MANY-BODY WAVEFUNCTIONS FOR QUANTUM IMPURITIES OUT OF EQUILIBRIUM

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ABSTRACT OF THE DISSERTATION

Many-body Wavefunctions for Quantum Impurities out of Equilibrium

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We present a new method for calculating the time-dependent many-body wavefunction that follows a local quench. We use the method to find the exact wavefunction of several quantum impurity models, focusing mainly on the nonequilibrium Kondo model driven by a bias voltage. The Bethe ansatz is not used, and integrability does not appear to play any role. We show that the long time limit (with the system size taken to infinity first) of the time-evolving wavefunction is a current-carrying nonequilibrium steady state, which we can also find directly with our method. We evaluate the steady state current in the regimes of strong and weak coupling, finding a new universal regime of strong ferromagnetic coupling with Kondo temperature \( T_K = De^{-\frac{3\pi^2}{8}\rho|J|} \) \( (J < 0, \rho|J| \to \infty) \). In this regime, the differential conductance \( dI/dV \) reaches the unitarity limit \( 2e^2/h \) asymptotically at large voltage or temperature.
Acknowledgments

My aim in writing this thesis was to make each successive idea or step forward seem logical, or better yet, obvious. My actual experience of doing this research, though, was much more complicated, and I had many moments of feeling discouraged by the uncertain path ahead. I have many people to thank for helping me through this long process. Most especially, I thank my advisor, Natan Andrei, for years of support, encouragement, and discussions of physics.

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Dedication

To my parents, for life and education.
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Chapter 1

Introduction

Textbooks on many-body physics often begin by explaining why it is typically impossible to understand the behavior of a macroscopic system by solving the $N$-body Schrödinger equation. The reason is the exponential growth of the Hilbert space. Even if each of the $N$ particles has just two degrees of freedom, the dimension of the Hilbert space is $2^N$: a formidably large number if we take $N \sim N_{\text{Avagadro}} \sim 10^{24}$ as a rough estimate. To account for spatial degrees of freedom, one needs a function of all coordinates $x_1, \ldots, x_N$. Unless the system is non-interacting, with the function factorizing into a product of single-variable functions, one can expect the full wavefunction to be both difficult to find and difficult to use in calculating observable quantities.

Nonetheless, there are some cases in which the full wavefunction can be found and used to calculate observable quantities. These special cases are important for a number of reasons. First, an exact solution can probe regimes inaccessible to perturbation theory. Second, the exact solution in a special case serves as a benchmark for other methods; after checking that a more approximate method agrees reasonably well with the exact answer, one can use the more approximate method with greater confidence in problems for which no exact solution is available. Third, an exact solution can serve as a starting point for new types of approximations.

The principal method available for finding exact wavefunctions is known as the Bethe ansatz. This is a method well-suited to understanding a system in equilibrium in which case one can use the powerful basic tool of statistical thermodynamics: the partition function. Techniques that work out of equilibrium are far less developed.
In this thesis, I present a new method for finding the many-body wavefunction _out of equilibrium_ and calculating expectation values of observables. I apply the method to a few _quantum impurity_ models to find the exact wavefunction, and in some cases I find an exact formula for an observable in terms of the \( N \) quantum numbers of the wavefunction. The methods of Bethe ansatz make no appearance. This new method is the first of two main points of this thesis.

In the problems I consider, it is necessary for technical reasons to take the thermodynamic limit (\( N \to \infty \) with a fixed density of particles) to get physically-meaningful answers. Taking this limit is a formidable task. In this thesis, I take a more modest approach of calculating the thermodynamic limit order-by-order to a few powers in an expansion parameter, which (in the _Kondo model_) can be either the coupling constant or its inverse. In the latter case, the expansion probes a new strongly coupled regime of the model; the predictions in this regime are the second main point of this thesis. If a way can be found – whether analytical or numerical – of taking the thermodynamic limit without expansion, then the new method could attain for nonequilibrium problems the same importance that the Bethe ansatz has in equilibrium.

### 1.1 Quantum impurities and the physics of many scales

In the broad, modern use of the term, a “quantum impurity” is any quantum system which has a small number of degrees of freedom and which is coupled to another quantum system with a much larger number of degrees of freedom [1]. I defer discussion of the history of the subject, including the origin of the name “impurity,” to the next section, and present here a conceptual overview of the main focus of the thesis: nonequilibrium transport in the _Kondo model_, a particular flavor of quantum impurity system. The Kondo model and variations thereof have an interesting feature, known as the “physics of many scales” [2, 3], that occurs also in a range of other situations in disparate areas of physics. This thesis develops a method for calculations in the Kondo model (and variants), with a particular
focus on nonequilibrium aspects. Much less is understood about the physics of many scales out of equilibrium, compared to what is known in equilibrium.

“Many scales” refers to the idea of a system in which a wide range of energy scales (or distance scales) are of importance, where “wide” means orders of magnitude. To see what an uncommon situation this is, it is useful to consider what is the more typical case. Usually, there is a relatively narrow range of scales which are important, with fluctuations in the remaining scales either ignored or averaged over. For instance, in calculating the trajectory of a baseball, it is a good approximation to average over the fluctuations of the individual atoms (the center of mass of the projectile is just the average position of the atoms) and to take the Earth as stationary. The same idea underlies mean field theory, in which the effects of interactions are approximated by an average (e.g. each spin in a ferromagnetic material responding to an external magnetic field determined by averaging over all other spins).

In some systems, however, there are orders of magnitude of fluctuations which have an effect not captured by a simple average. The most visible examples are turbulent fluids: the churning water in the wake of a ship or in whitewater rapids, or the smoke rising from a chimney, or weather patterns in the atmosphere, have “whirls within whirls” which are all of importance even in calculating properties at distances much larger than the scale of the smallest of these fluctuations. The physics of many scales is completely ubiquitous in elementary particle physics, and occurs also in two broad classes of condensed matter systems. The first broad class consists of second-order phase transitions, also known as the theory of “critical phenomena.” Examples include the critical point of a liquid-gas phase transition (the point at which the distinction between liquid and gas breaks down) and the Curie temperature, at which a ferromagnetic material loses its magnetism due to thermal fluctuations. In either case, when the system is tuned to be close to the transition, the thermal fluctuations are important over many orders of magnitude of distance scales. The

\[1\text{The following discussion draws mainly on the Nobel lecture of K. Wilson [4], as well as on Refs. [5] and [6].}\]
second broad class of systems consists of quantum impurities, with the Kondo model as a central example.\(^2\)

As a prelude to introducing quantum impurities and the Kondo model, it is interesting to note that the mechanism for why many scales are important can be quite different in each case. In critical phenomena, for instance, the fluctuations are classical (statistical fluctuations described by the partition function), while in particle physics they are quantum. In particle physics, Lorentz invariance requires that interactions are local – we must have, e.g., \(\phi(x)^4\) in the Lagrangian, not \(\phi(x)^2\) times \(\phi(x')^2\) for some \(x'\) away from \(x\). Writing each \(\phi(x)\) as an expansion in energy modes then means that modes of vastly different energies are coupled equally. Roughly speaking, having fields at different points coupled by a delta function couples widely separated modes, since a delta function is “spread out” in momentum space.

In the Kondo model, the impurity is a single spin connected to one or more reservoirs of electrons – the larger system – by spin exchange. (Hewson’s textbook [9] is a standard reference for the Kondo model.) While the main focus in this thesis will be the case of two reservoirs, the case of one reservoir will be an important starting point. The Kondo Hamiltonian with one reservoir is:

\[
H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{k,k',|\epsilon_k|,|\epsilon_{k'}|<D} J c_k^\dagger \sigma_{aa'} c_{k'}^\dagger \cdot \mathbf{S}, \tag{1.1}
\]

where the reservoir degrees of freedom have the bandwidth \(D\) as an energy cutoff and have a density of states per spin (denoted \(\rho\)) assumed to be constant. Spin sums are implicit, and the impurity operator \(S^j = \frac{\hbar}{2} \sigma^j\) acts on fixed impurity states \(|\uparrow\rangle\) and \(|\downarrow\rangle\). Notice that the spin exchange term couples modes of very different energies. Equivalently, for large bandwidth the spin exchange term is approximately a delta function in position space. The physics of many scales arises in this case because the impurity spin’s interaction with the

\(^2\)The physics of many scales also leads to the “effective field theory” concept that provides a conceptual underpinning of many important ideas in condensed matter physics, including Landau-Fermi theory. While the physics of the Kondo model is essentially one-dimensional, the geometry of the Fermi surface plays a more prominent role in higher dimensions. See, e.g., Refs. [7] and [8].
reservoir electrons is sharply peaked in position space.

For reasons to be clarified shortly, the case of two reservoirs is known as the nonequilibrium Kondo model:

\[
H = \sum_{k} \epsilon_k \left(c_{1ka}^\dagger c_{1ka} + c_{2ka}^\dagger c_{2ka}\right) + \frac{1}{2} \sum_{k,k'} J \left(c_{1ka}^\dagger + c_{2ka}^\dagger\right) \sigma_{aa'} \left(c_{1k'a'} + c_{2k'a'}\right) \cdot S,
\]

where 1 and 2 are the labels for the two reservoirs. A number of simplifying assumptions have been made here, including that the reservoirs have the same energy spectrum \(\epsilon_k\), and that the spin exchange within an individual lead has the same coefficient as the spin exchange between leads. Upon rotation to new fields defined by \((c_{1ka} \pm c_{2ka})/\sqrt{2}\), the model decouples into a free field (the \(-\) combination) and a copy of the single reservoir case (1.1) (involving the \(+\) combination). The scaling properties of the model (1.2), discussed below, are essentially identical to the scaling of the simpler model (1.1).

The experimental realization of this model occurs in “quantum dots,” which consist of a relatively small number of electrons – of order 100 – confined to a nanoscale region of semiconductor material. The dot has a sequence of discrete energy levels, and hence can be thought of as an “artificial atom.” The dot can be connected by quantum tunneling to two-dimensional electron gases, which serve as the reservoirs. The reservoirs are called “leads,” since they can form an electric circuit, with a voltage difference imposed between the “source” lead and the “drain” lead, and with the dot as a circuit element between them. The system can be tuned so that only the uppermost occupied level is of any significance, at least for a certain range of parameters (one must ensure that the energy gap to the level below is sufficiently large). With an odd number of electrons on the dot, the singly-occupied level at the top acts as the quantum impurity, or fixed Kondo spin \(S\). (Often, this uppermost level itself is referred to as “the dot.”) The interactions between electrons on the dot must not be too large. For a much more detailed account of obtaining the Kondo model as a description of a quantum dot in the low energy regime, and the approximations
involved, see Ref. [10].

How does the physics of many scales manifest itself in this problem? To see this, one can calculate an observable quantity such as the differential conductance \( G \equiv \partial I / \partial V_{sd} \), where \( I \) is the electric current and \( V_{sd} \) is the source-drain voltage. Let us consider the conductance at \( V_{sd} = 0 \) as a function of the temperature \( T \). (This is an equilibrium quantity, accessible by linear response theory.) The result is:

\[
G = \frac{2e^2}{h} \frac{3\pi^2}{16} \left( (2g)^2 + 2(2g)^3 \ln \frac{D}{k_BT} + 3(2g)^4 \ln^2 \frac{D}{k_BT} + \ldots \right),
\]

where \( g = \rho J \) is the dimensionless coupling constant. In writing this expression, we have made a few approximations. The temperature (or rather, \( k_B T \)) has been taken to be much smaller than the bandwidth. Equivalently, we can imagine sending the bandwidth to infinity, and keeping only the terms that are constant or divergent in this limit. General arguments based on renormalizability and dimensional analysis (see [5]) imply that the most general term that can remain takes the form \( g^{2+n} \ln^m \frac{D}{k_BT} \), with \( n \geq 0 \) and \( 0 \leq m \leq n \). We have made the “leading log” approximation of keeping only the terms with \( m = n \).

The presence of logarithmic divergences is a sign of the physics of many scales. The idea is that a log divergence arises from some integral over energy of the form \( \int d\epsilon \frac{1}{\epsilon} \), suitably cutoff at high energies by the bandwidth and at low energies by an external scale at which the system is probed (in this case, \( k_B T \)). Each order of magnitude of energies contributes the same amount to the conductance; for instance, the range from \( k_B T \) to \( 10k_B T \) and the range from \( 10k_B T \) to \( 100k_B T \) each contribute \( \ln 10 \). In the pre-Wilson view of field theory, one would say that the \( g^3 \) and higher terms in the perturbation series “diverge as the cutoff is sent to infinity.” While this notion is sometimes useful as a shorthand (and even as a practical tool in calculations), it must be kept in mind that the cutoff \( D \) represents a real, fixed quantity, and not an artificial parameter put in by hand.

Summing the leading log series yields:

\[
G = \frac{2e^2}{h} \frac{3\pi^2}{16} \left( \frac{2g}{1 + 2g \ln \frac{D}{T}} \right)^2 = \frac{2e^2}{h} \frac{3\pi^2}{16 \ln^2 \frac{T}{k_BT}},
\]

(1.4)
where the *Kondo temperature* $T_K$ is given (in leading log approximation) by:

$$k_B T_K = D e^{-\frac{\Gamma}{g}}. \quad (1.5)$$

The appearance of the Kondo temperature is an example of *dimensional transmutation* [11], meaning that interactions generate a dimensionful scale even though the problem itself has no intrinsic scale (aside from the cutoff). Here, the only quantity besides the cutoff that is intrinsic to the problem is the coupling constant $g$, which is dimensionless.

The main message is that the observable we calculated, which seemed to depend on $D$, $g$, and $T$, turns out to depend only on the ratio $T/T_K$. The “microscopic” details of the model have vanished, and a *universal* answer has emerged. Indeed, the same answer would be obtained starting from a more general model, with an energy-dependent density of states $\rho(\epsilon)$ and a Kondo coupling of the form $J_{kk'}$ (instead of the isotropic $J$). The point is that for sufficiently low energies (i.e. close to the Fermi level), both $\rho(\epsilon)$ and $J_{kk'}$ can be approximated as constant. The bandwidth $D$ in the simplified model used above is replaced by the energy scale at which $\rho(\epsilon)$ and $J_{kk'}$ start to deviate significantly from their value at the Fermi energy, and all modes beyond this value make no significant contribution. It turns out that there remains a considerable range of energies over which this approximation is valid. It is important that the Kondo coupling is antiferromagnetic ($J > 0$, and recall that we are in the weakly coupled regime $g \ll 1$), so $k_B T_K \ll D$ and the generated scale is well within the appropriate regime. In the opposite case of ferromagnetic coupling ($J < 0$, still with $|g| \ll 1$), we have $k_B T_K \gg D$, the generated scale is well outside the regime of our approximations, and the result for the conductance is *non-universal* – that is, it reflects only what would happen if the simplified model itself (with constant $\rho$ and $J$) were realized.

The summation of leading logs (1.4), presented above as a simple extrapolation that higher terms of the series would continue to fit the pattern $\sum_{n=0}^{\infty} n x^n$, can be understood at a deeper level as an example of *renormalization group (RG) improvement* of a perturbation series (see Ref. [5] and references therein). The starting point is to note that the perturbation series for the conductance satisfies the Callan-Symanzik (or RG scaling)
equation:
\[
(D \frac{\partial}{\partial D} + \beta(g)) G(D, g, T) = 0, \text{ where: } \beta(g) = -2g^2 + O(g^3).
\] (1.6)

While this is only seen above to a few orders in \( g \), the existence of such an equation is guaranteed by the fact that the theory is renormalizable. (To be more precise, the renormalizability is known to all orders in equilibrium; out of equilibrium it is a reasonable conjecture.) It is important to note that this scaling equation holds for \( G \) only after we make the approximation \( k_B T \ll D \) (which results in simple powers of logarithms); within this large bandwidth part of answer, we then consider \( D \) as a variable (with no restriction anymore on the relative sizes of \( k_B T \) and \( D \)). This scaling equation is a reformulation of the statement that the conductance depends on \( D \), \( g \), and \( T \) only through the ratio \( T/T_K \). The beta function \( \beta(g) \) describes the change of the “running” coupling \( g_R \) with the negative sign indicating that \( g_R \) is larger at lower energy scales. Indeed, the running coupling is given in the leading log approximation by \( g_R = \frac{1}{2 \ln \frac{T}{T_K}} \), and the RG improved answer is obtained from the perturbation series (1.3) by replacing \( g \to g_R \) and deleting the logarithmic terms (see Sec. A.4 in the Appendix for more detail).

As often happens in the RG improvement of a perturbation series, there is some restriction remaining even after resummation of the large logarithms. In this case, the answer (1.4) is only valid for high temperatures – that is, high compared to \( T_K \) while still much smaller than the bandwidth \( (k_B T_K \ll k_B T \ll D) \).

What happens as \( T \) is reduced to be of order \( T_K \), or all the way to 0? Answering this requires techniques more powerful than perturbation theory. The results (see next section for references to the literature) can be summarized as follows: (1) the running coupling \( g_R \) continues to grow as \( T \) is reduced; (2) the conductance \( G \) also grows as \( T \) is reduced, reaching a peak value at \( T = 0 \) that is the maximal allowed value of \( 2e^2/h \) (the “unitarity limit”); and (3) the low temperature regime of the model, i.e. \( T \ll T_K \), can be described by a different perturbation theory (or effective field theory) that essentially takes the \( g_R \to \infty \) strong coupling fixed point as the starting point.
Much of the above discussion carries through in case of $\partial I/\partial V_{sd}$ at $T = 0$ with $V_{sd}$ as the independent variable – that is, a nonequilibrium setup. A leading log series identical to Eq. (1.3) is obtained with $eV$ replacing $k_B T$. More generally, including both voltage and temperature, we expect the conductance to be given by a universal form:

$$G = f_{\text{universal}} \left( \frac{eV_{sd}}{k_B T_K}, \frac{T}{T_K} \right),$$

provided that we stay in the universal regime – that is, $eV$ and $k_B T$ much smaller than the bandwidth. The universal function reaches the unitarity limit at $eV_{sd} = k_B T = 0$, and its behavior near this point (that is, all scales much smaller than $T_K$) is described by the effective field theory approach mentioned above. The leading log series in $g$ yields the leading behavior in the opposite limit, in which at least one of the external scales is much larger than $T_K$. (The extrapolation to all orders relies on renormalizability theorems whose applicability is not completely clear in the nonequilibrium case; however, the low orders of the series fit the expected pattern and the extension to all orders is a reasonable conjecture.)

One of the main conclusions, or rather predictions, of this thesis is the existence of another universal regime of the Kondo model: strong ferromagnetic coupling ($g < 0, |g| \to \infty$). The new method I present for calculating the many-body wavefunction permits the calculation of the conductance $G$ to several orders either in powers of $g$ or in powers of $1/g$. The first case serves as a check, recapitulating the leading log calculation presented above. The second case results, by similar scaling arguments, in a universal conductance curve that reaches the unitarity limit asymptotically at high energies:

$$G = f_{\text{universal}}(V, T) = \frac{2e^2}{\hbar} \left( 1 - \frac{3\pi^2}{16 \ln^2 \sqrt{\left( eV \right)^2 + (k_B T)^2}} \right) + \ldots,$$

where $\left( \sqrt{(eV)^2 + (k_B T)^2} \right) \gg T_K$, $T_K \equiv D e^{-\frac{3\pi^2 |g|}{\pi}}$ ($g < 0, |g| \to \infty$).

In this way, the expansion in $1/g$ yields the high energy (relative to $T_K$) part of the universal conductance curve. What about the full curve? The most natural guess is that it falls to zero at $eV_{sd} = k_B T = 0$, with the running coupling flowing from a large negative value
initially down to zero from below. The calculation of the full curve is a formidable task towards which this thesis makes only a partial step. The remaining obstacle is to find either a way of resumming the series in $1/g$ to all orders in a controlled way, or a way of taking the thermodynamic limit (large system size with fixed density) without making an expansion in $1/g$. The same comments apply to the case of finding the full conductance curve in the standard antiferromagnetic model (which has, however, been calculated by other means; see next section).

1.2 Survey of prior work

Quantum impurities have a long and distinguished history in physics, with the interplay of experiment and theory generating many new ideas. My brief summary below draws on Refs. [9], [12], and [13].

Starting in the 1930s, experiments detected an unexpected minimum in the low temperature resistivity of nonmagnetic metals such as copper or gold. In 1964, Kondo showed [14] that this minimum could be explained by the presence of trace amounts of magnetic atoms, such as iron – naturally-occurring “impurities” in a nearly “pure” sample. The impurities were sufficiently dilute so that the calculation could first be done with a single magnetic impurity in a non-magnetic host, then generalized to account for a random distribution of impurities too far way to interact with each other. Kondo’s calculation of the impurity contribution to the resistivity resulted in:

$$R_{\text{imp}} \sim (2g)^2 + 2(2g)^3 \ln \frac{D}{k_B T} + \ldots$$

The logarithmic dependence with temperature produced the required minimum when balanced against the phonon contribution to the overall resistivity.

Up to the overall prefactor, the Kondo result (1.9) exactly coincides with the first two orders of the conductance series presented above (1.3). In 1965, Abrikosov [15] resummed the most strongly divergent terms of the series (the leading logs), and obtained for the
resistivity the analog of Eq. (1.4). Similar calculations were carried out for other quantities, such as the impurity contribution to the magnetic susceptibility, again resulting in logarithmic divergences and the emergence of the Kondo temperature.

There followed the puzzle of understanding the behavior of the theory as the temperature is reduced to $T_K$ (at which point the perturbative results break down), and beyond to $T = 0$. First to get the right answer were Anderson, Yuval, and Hamannn [16], who argued that the susceptibility at zero temperature approaches a constant. Part of the argument featured “scaling laws” for a bandwidth-dependent coupling constant – equivalent to the leading order beta function $\beta(g) = -2g^2$ discussed above.\(^3\) Shortly thereafter, Anderson [17] introduced the idea of progressively reducing the bandwidth of the model, providing a simpler way of obtaining the same scaling laws with a clearer connection to renormalization group ideas.

In 1973, Wilson [18, 2] carried out a more detailed analysis, confirming the constant susceptibility and calculating the full crossover from high to low temperature, using a novel numerical implementation of the renormalization group. This calculation helped clarify the connection between the Kondo model and other problems in which “divergences” occur; indeed, Wilson played a large role recognizing these problems as all being instances of the physics of many scales. In 1974, Nozières [19] developed a simple description of the theory at low temperatures, with results in agreement with Wilson’s in that regime. (See also the later work of Nozières and Blandin [20] extending the idea to other variations of the Kondo model.) In 1980, an analytical solution of the Kondo model was obtained independently by Andrei [21] and Wiegmann [22] by means of the Bethe ansatz, in good agreement with Wilson’s calculation.

Many other directions of work proceeded beyond the (single impurity) Kondo model, including multichannel generalizations, the renormalization group study of the more general Anderson model, and the idea of a lattice of Kondo impurities. My story follows a different

---

\(^3\)To be more precise, Anderson et al. allowed anisotropy in the Kondo interaction – i.e. $\mathcal{J} \mathbf{\sigma} \cdot \mathbf{S} \rightarrow 2\mathcal{J}_\perp (\sigma^+ S^- + \sigma^- S^+) + \mathcal{J}_z \sigma^z S^z$ – and found (in modern terms) the beta functions for both $g_\perp$ and $g_z$. 
thread, beginning with experimental advances that allowed the Kondo model to be realized in quantum dots and explored out of equilibrium.

Even before the advent of quantum dots, nonequilibrium Kondo physics was studied in the context of tunnel junctions. (See the introduction of Ref. [23] and references therein.) Of particular note was the prediction of Glazman and Raikh [24] in 1988 that the Kondo effect would manifest itself in this case as a peak – the unitarity limit – of the conductance at zero temperature and bias. In 1998, Goldhaber-Gordon [25] experimentally observed the beginning of this unitarity peak developing in a quantum dot (with the peak being suppressed when there were an even number of electrons on the dot). Further improvement by van der Wiel et al. in 2000 resulted in the first observation of the conductance essentially reaching the full unitarity limit. In 2011, Kretinin et al. [26] showed the universality of the conductance curve (as a function of the source-drain voltage, at a fixed low temperature) by collapsing various experimental curves onto a single-parameter curve, at least at sufficiently low energies.

This line of experimental work stimulated a great amount of theoretical effort at understanding the Kondo model out of equilibrium. An extensive list of theoretical works on this subject can be found in the references in [27]. The universal antiferromagnetic regime of the nonequilibrium Kondo model has been studied theoretically by a variety of approaches, including Keldysh perturbation theory [28, 29, 30], flow equations [31], the real-time renormalization group [32], and the variational principle [27]; the Kondo regime has also been studied in the Anderson model using perturbation theory [33], Fermi liquid theory [34], integrability [35], the Scattering Bethe ansatz [36], Dynamical Mean Field Theory [37], and quantum Monte Carlo [38]. Of particular note is a recent calculation that, through a combination of NRG and other powerful tools such as matrix product states, calculates the full conductance curve with voltage [39].

In contrast, the regime of strong ferromagnetic coupling has apparently received little attention in the literature.
1.3 Nonequilibrium Kondo as a quench problem

In a broad sense, there is only one way for a system to be in equilibrium, while there are many ways for it to be out of equilibrium. A quantum dot subject to source-drain voltage, discussed above, is an example of steady state (or time-independent) nonequilibrium. The applied voltage represents some external battery continually supplying energy, and so the system is described by some non-equilibrium steady state instead of by a Boltzmann distribution. Another type of nonequilibrium is quench dynamics: the sudden change of a system’s Hamiltonian. Equivalently, a quench consists of an eigenstate of one Hamiltonian evolving in time by a different Hamiltonian.

This thesis finds, in the Kondo model, both the nonequilibrium steady of the quantum dot, and the time-evolving state following a certain quench (to be described below) that leads to this steady state in the long time limit. The method introduced is therefore a way of studying both quench dynamics and steady state nonequilibrium. The quench dynamics part, aside from being interesting in its own right, also serves as a way to “legalize” the direct calculation of the steady state. (This is similar to a familiar story from single particle scattering theory: the time-independent formalism is convenient for calculations, but has certain apparent irregularities that are resolved by deriving it as the limit of a time-dependent approach.)

It must be mentioned that there a vast number of other possibilities in the realm of nonequilibrium. An AC voltage instead of DC corresponds to periodic or “Floquet” driving, quenches can be gradual instead of sudden, and so on. It also worth noting that quench dynamics (or its equivalent, before the introduction of the term) was long considered a purely theoretical exercise, due to the short coherence times in real quantum systems. Experimental improvements starting in the early 2000s, however, opened up new possibilities for observing coherent time evolution in optical lattices of ultracold atoms.

The quench setup for the quantum dot attached to leads has the initial state with Fermi
seas in each lead; the difference in chemical potentials represents the source-drain voltage.

The quench at $t = 0$ consists of switching on the coupling to the dot, after which an electric current develops – see Fig. 1.1. More experimentally relevant than this “interaction” quench would be a “voltage” quench, in which the tunneling to the dot is always present and the source-drain voltage is turned on suddenly. However, it has been shown in the Kondo model that the steady state limit is the same either way [30].

Since time evolution of a state by a Hamiltonian is unitary, quench calculations are usually applied to closed systems (i.e. isolated from the environment). However, it is sometimes possible to use a quench setup to make predictions for an open, driven system.

In the quantum dot driven by voltage, we can take the limit of infinite system size – that is, infinitely large leads – and find that the leads serve as thermal reservoirs. The idea is that for a sudden and spatially localized quench, the long time limit (with the system size always large enough so that the effect of the quench does not reach the boundaries) yields a nonequilibrium steady state (NESS) that carries current and generates entropy.

Figure 1.1: Schematic of the quench process. Prior to $t = 0$, the leads are filled with free electrons, with no tunneling to the dot allowed. From $t = 0$ onward, the system evolves with the many-body Hamiltonian $H$, with tunneling to and from the leads resulting in an electric current.

A simple physical quantity to characterize a quench is the expectation value of an observable: $\mathcal{O}(t) = \langle \Psi | e^{iHt} \hat{O} e^{-iHt} | \Psi \rangle$, where $| \Psi \rangle$ is the initial state and $H$ is a Hamiltonian that is switched on suddenly at $t = 0$. Some basic questions arise: does $\mathcal{O}(t)$ reach a limit as $t \to \infty$? If so, does this limit coincide with the expectation value in the NESS state – that is, do we have $\lim_{t \to \infty} \mathcal{O}(t) = \langle \Psi_{NESS} | \hat{O} | \Psi_{NESS} \rangle$? In the case of the electric current in
the Kondo model, we answer both questions with “yes.” The methods of calculation that we introduce to arrive at these answers could be of wider use.

In this thesis, the end goal of our calculations is the universal form of a given observable (primarily the current or conductance), which arises when all external energy scales are much smaller than the bandwidth. In particular, we wish to express final answers not in terms of “microscopic” quantities \((g, D)\), but in terms of the Kondo temperature \(T_K\) (or more generally, in terms of renormalization group invariants). This is a situation that often occurs in the physics of many scales. A time-honored strategy in these cases is to modify the high energy fluctuations of the theory in such a way as to make the calculation easier.

Taking the density of states in the Kondo model to be constant, as we did above, is one example of this strategy. A more complicated density of states would lead to the same answer (in terms of \(T_K\)) in the low energy regime, provided that the density of states is reasonably smooth at the Fermi level. In particle physics, this strategy goes by the more respectable sounding description of “freedom to choose the cutoff scheme,” and it is well-known that a great variety of different schemes (sharp cutoff, dimensional regularization, Pauli-Villars, etc.) for “regulating the divergences” yield the same final answers (expressed in terms of, e.g., the renormalized electron charge) in perturbative quantum field theory. These different schemes represent different ways of modifying the theory at high energies. Though it is not completely clear what constitutes a valid modification, the strategy has been successful in practice.

With universality in mind, we consider the one-dimensional version of the two lead Kondo Hamiltonian introduced earlier [Eq. (1.2)] with no bounds on the energy spectrum:

\[
H_{\text{Kondo}} = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^{2} \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) + \sum_{\gamma, \gamma' = 1, 2} \frac{1}{2} J_{\gamma a \gamma' a'}(0) \sigma_{aa'} \psi_{\gamma a}(0) \cdot \sigma_{\gamma' a'} \cdot S - BS^2. \quad (1.10)
\]

The reduction to one dimension is obtained by standard steps of linearizing the energy spectrum about the Fermi level and unfolding to obtain right-moving electrons. With the bandwidth sent to infinity, the Hamiltonian takes a convenient form in position space: the
linear spectrum \( \sum_k kc^+_{\gamma ka} c_{\gamma ka} \) becomes a linear derivative and the Kondo interaction term becomes a delta function. A magnetic field \( B \hat{z} \) on the dot is included, as well. The Kondo coupling \( J \) is dimensionless in our convention; we can make contact with the previous convention (which is more common) by expressing our final results in terms of the dimensionless quantity \( g \equiv \rho_{\text{per length}} J \) (where \( \rho_{\text{per length}} = \frac{1}{2\pi} \) is the density of states per spin unit length, so that \( \rho_{\text{per length}} J = \rho J \) is the same dimensionless coupling constant \( g \) discussed earlier.)

The bandwidth \( D \), having been removed from the Hamiltonian, must still make an appearance somewhere in the problem in order for us to get a finite answer (which we then re-express in terms of \( T_K \) in the limit of large bandwidth). It is helpful to recall how this works in the equilibrium case [40] (see also [41]). The exact solution of the one lead model also starts with an unbounded Hamiltonian. The approach taken there is to diagonalize the Hamiltonian by means of the Bethe ansatz, then calculate the partition function with a lower cutoff on energy.\(^4\) Physical quantities such as the impurity susceptibility are then expressed in terms of \( T_K \), and the same answer is obtained as in the NRG calculations.\(^5\) The conclusion here is that the procedure of (1) diagonalizing the unbound Hamiltonian, and then (2) imposing a cutoff on the energy spectrum (in the basis of exact eigenstates), constitutes a valid modification of the high energy details. The use of the unbound Hamiltonian is a convenience, as it preserves the integrability of the model, permitting the solution by Bethe ansatz.

For the nonequilibrium situations considered in this thesis, the partition function is not sufficient; instead, we calculate time evolution. The use of the unbound Hamiltonian is a convenience for allowing the time-evolving wavefunction (and its steady state limit) to be calculated exactly. The bandwidth appears in this case as a cutoff on the initial state (more generally, density matrix) that is the initial condition for the quench.

To see this, we now discuss the quench setup in more detail. Prior to the quench, the

\(^4\)An upper cutoff is not necessary, due to the exponential decay of the Boltzmann factor.
\(^5\)This agreement holds despite the fact that \( T_K \) takes a different form, in terms of \( D \) and \( g \), than it does in the conventional cutoff scheme, once one goes beyond the leading log approximation. Since the goal is to get the universal answer as a function of \( T_K \), the form of \( T_K \) in terms of \( g \) is not of any significance by itself.
source-drain voltage is applied but the tunneling to the dot is blocked. That is, the initial density matrix $\rho$ is a product of filled Fermi seas in each lead (cutoff by the bandwidth $D$), with the bias voltage appearing as $V = \mu_1 - \mu_2$. In particular:

$$
\rho = \exp \left[ -\frac{1}{T_1} \sum_{|k|<D} (k - \mu_1) c_{1ka}^\dagger c_{1ka} \right] \otimes \exp \left[ -\frac{1}{T_2} \sum_{|k|<D} (k - \mu_2) c_{2ka}^\dagger c_{2ka} \right]. \quad (1.11)
$$

For clarity, we present the calculation at zero temperature; once we have an expression for the current, we make an obvious generalization to the case of arbitrary $T_1$ and $T_2$. (We have verified that starting with the density matrix $\rho$ leads to the same answer.) The zero temperature initial state is:

$$
|\Psi\rangle = \left( \prod_{\gamma=1,2} \prod_{j=1}^{N_\gamma} c_{\gamma j\uparrow}^\dagger c_{\gamma j\downarrow} \right) |a_0\rangle, \quad (1.12)
$$

where $|a_0\rangle$ is the fixed impurity spin, and where the momenta in the leads are:

$$
k_j = -D + \frac{2\pi}{L} j, \quad (1.13a)$$

$$
D = \frac{2\pi}{L} N_1 \quad \text{(i.e., } \mu_1 = 0), \quad (1.13b)$$

$$
V = \frac{2\pi}{L} (N_1 - N_2) \quad \text{(i.e., } \mu_2 = -V). \quad (1.13c)
$$

At $t = 0$, we turn on the Kondo coupling $J$, and the system evolves via the many-body Hamiltonian $H$. Since the total number of electrons in the system is conserved, the (average) electric current at time $t$ is the time derivative of the number of electrons in one of the leads:

$$
I(t) = -\frac{d}{dt} \langle \psi | e^{iHt} \hat{N}_1 e^{-iHt} | \psi \rangle, \quad (1.14)
$$

where $\hat{N}_1 = \int_{-L/2}^{L/2} dx \psi_{1a}^\dagger(x) \psi_{1a}(x)$. (We note here that although we focus on the current, our formalism can also be used to calculate other quantities.) Since we have linearized the spectrum, the answers we obtain for small numbers of electrons have no physical meaning. Rather than evaluate our results for a large but finite number of electrons, we find it more convenient to take the thermodynamic limit – the limit of infinitely many electrons with fixed density:

$$
\lim_{\text{thermodynamic}} = \lim_{N_1 \to \infty, N_2 \to \infty, L \to \infty} \frac{N_1}{2\pi} \frac{L}{N_1} = D, \frac{N_2}{2\pi} (N_1 - N_2) = V. \quad (1.15)
$$
In this limit, the time $t$ is held fixed. This guarantees that the effects of the quench, which travel at the Fermi velocity, never reach the (artificial) boundaries of the system.

One of the main results of this thesis is the exact and nonperturbative solution of the many-body wavefunction $e^{-iH_{\text{Kondo}}t}|\Psi\rangle$. The new method we introduce allows us to find the exact time evolution starting from any number of electrons with arbitrary lead indices, momenta, and spins. We show that in the long time limit, with the system size always larger, the time-evolving wavefunction becomes a Lippmann-Schwinger “in” state – that is, an eigenstate of the Hamiltonian that satisfies the incoming boundary condition of $N$ plane waves with the specified quantum numbers. This provides an exact and explicit example of a nonequilibrium steady state (NESS) in a many-body problem. We can also solve for this NESS directly using a time-independent version of our formalism.

With the many-body wavefunction in hand, we turn to the calculation of the current at time $t$ following the quench. A lengthy calculation based on Wick’s Theorem brings the current to a form in which is suitable for taking the thermodynamic limit; this limit yields a series expression for the current. This series has the interesting property that it really yields two series: one in powers of $J$ for small $J$, and one in powers of $1/J$ for large $|J|$.

We show that our series expression for the current reaches a long time limit to all orders (in either $J$ or $1/J$), and that this limit agrees with the expectation value of the current operator in the NESS. We then evaluate the first several terms of the series, focusing on both the usual universal regime of weak antiferromagnetic coupling and a new universal regime of strong ferromagnetic coupling. In each regime, we allow the external parameters $T_1, T_2,$ and $V$ to be arbitrary in order to investigate the scaling properties of the steady state current using the Callan-Symanzik equation. We find the standard scaling at leading order for weak antiferromagnetic coupling, and a new $T_K$ for strong ferromagnetic coupling.

The method can also be applied to other impurity models, though results for observables are more preliminary. We also consider two impurity models with charge fluctuations,
namely, the interacting resonant level model:

\[ H_{\text{IRL}} = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma}^\dagger(x) \frac{d}{dx} \psi_{\gamma}(x) + \epsilon d^\dagger d \]

\[ + \sum_{\gamma=1}^{N_{\text{leads}}} \left[ \frac{v}{\sqrt{N_{\text{leads}}}} \psi_{\gamma}^\dagger(0) d_a + \text{h.c.} \right] + U \psi^\dagger(0) \psi(0) d^\dagger d, \quad (1.16) \]

and the Anderson model:

\[ H_{\text{And.}} = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) + \epsilon d^\dagger_a d_a \]

\[ + \sum_{\gamma=1}^{N_{\text{leads}}} \left[ \frac{v}{\sqrt{N_{\text{leads}}}} \psi_{\gamma a}^\dagger(0) d_a + \text{h.c.} \right] + U n_a^\dagger n_a, \quad (1.17) \]

where we have let the number of leads be arbitrary. We find the exact time-evolving wavefunction of the IRL; in the AIM, we find the NESS for small \( U \) or infinite \( U \). We calculate observables at the leading order, verifying the answer by comparing to a conventional calculation.

In these charge fluctuation models, there is some overlap between our work and that of Nishino and collaborators. Refs. [42], [43], and [44] present the NESS of the two lead IRL. The results seem to agree with ours for \( N = 2, 3 \) electrons; while the authors obtained the general \( N \) case as well, it is not written explicitly. Ref. [44] allows the tunnelings and Coulomb interactions to be lead-dependent, which is a more general case than we consider. NESS wavefunctions for \( N = 2, 3 \) electrons were obtained in Refs. [45], [46] in a double-dot version of the IRL. In Ref. [47], Imamura et. al. find the two electron NESS for the one lead AIM – a result that we reproduce by our method, and extend to arbitrary \( N \) electrons in the cases of small and large Coulomb interaction \( U \).

1.4 Outline of thesis

Chapter 2 describes the new method for calculating the many-body wavefunction and expectation values. The calculations there are set up in a fairly abstract way, without specifying a particular model. Chapter 3 discusses two non-interacting models from the same point of
view that is applied to interacting models in subsequent chapters; the non-interacting case serves as a warm-up and illustrates some points that arise, in a more complicated way, in the interacting case. The main results of the thesis are in Chapter 4, which applies the new method to the nonequilibrium Kondo model. Chapters 5 and 6 show that the method has wider scope by applying it to the interacting resonant level model and Anderson model. Finally, Chapter 7 gives a summary and discusses a number of possible future directions.

I have presented some of this work already – in particular, the work on the Kondo model, and the associated general formalism – in three arXiv preprints co-authored with Natan Andrei. The first two, Refs. [48] and [49], cover the Kondo model in detail, and the third, Ref. [50], is a short summary. Some passages in this thesis are taken verbatim, or with small alterations, from these preprints. All three have been submitted for publication and returned with comments from reviewers. It is my intention to resubmit the work in the following way: Refs. [48] and [49] will be combined into one paper, the new version of Ref. [50] will summarize both the Kondo results and the results on charge fluctuations, and a new paper (still with Natan Andrei as co-author) will be added that covers charge fluctuations in detail.

1.5 Notes on conventions

I use natural units: $\hbar = e = k_B = 1$. Conductance is dimensionless in these units, and I sometimes restore its dimensions by noting that the conductance quantum is $G_0 \equiv 2e^2/h = 1/\pi$. In the linearized models that are my main focus, I also set the Fermi velocity to unity ($v_F = 1$), which implies that momentum and $1/\text{length}$ have dimensions of energy.
My Fourier transform conventions in one dimension are given by:

\[ c_k = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{-ikx} \psi(x) \rightarrow \int \frac{dk}{2\pi} \ e^{-ikx} \psi(x) \]  
(1.18a)

\[ \psi(x) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} c_k \rightarrow \int \frac{dk}{2\pi} e^{ikx} c_k \]  
(1.18b)

\[ \{ c_{k'}, c_k^\dagger \} = \delta_{kk'} \rightarrow \{ c_{k'}, c_k^\dagger \} = 2\pi \delta(k - k') \]  
(1.18c)

where the momenta are quantized according to \( k_j = \frac{2\pi}{L} j \) (\( j \in \mathbb{Z} \)) for finite \( L \) and where the arrow indicates the \( L \rightarrow \infty \) limit, in which the Kronecker-normalized operators are replaced by Dirac-normalized operators (each indicated by the same notation \( c_k \)) via \( \sqrt{L}c_k \rightarrow c_k \),  
\[ \frac{1}{L} \sum_k \rightarrow \int \frac{dk}{2\pi}. \]

Some authors write the Kondo interaction term as \( \pm \sigma \cdot \sigma_0 \) or \( \pm s \cdot S \) (where \( s = \sigma/2 \) and \( S = \sigma_0/2 \)), with a corresponding change in \( g \); the convention I use agrees with, e.g., Refs. [9] and [51].
Chapter 2
General formalism

2.1 Overview

This chapter presents a new method for calculating the time-evolving many-body wavefunction and expectation values of operators. Concrete calculations in particular models are deferred to later chapters; here the goal is to use model-independent properties to take care of much bookkeeping that is common to all applications of the new method. After the time-dependent case is treated in detail, it is shown that minor adjustments produce a time-independent version of the formalism.

2.2 Many-body wavefunction

We present a direct method for finding the time-dependent many-body wavefunction given a simple initial state. More precisely, given some fairly mild assumptions, we write the time-evolving wavefunction in terms of a family of time-dependent “crossing states,” and show that the Schrodinger equation holds provided that these crossing states satisfy certain differential equations. We cannot claim that this alone solves the problem, since the differential equations for the crossing states could be (and for a generic Hamiltonian, are) no less difficult to solve than the original Schrodinger equation. The real interest in this method, then, is that we are able to write exact, explicit expressions for the crossing states (and hence, for the full wavefunction) in several interacting models.

The explicit construction of the crossing states in particular models is deferred to later chapters. In each case, it is found that the single particle \( T \)-matrix for an electron scattering
off (i.e. crossing) the impurity is a basic ingredient in the construction, and this is the reason for the name “crossing.”

In this section, we describe the general setup and construction of the wavefunction, and state the main results (the differential equations that the crossing states must satisfy). The next two sections provide proofs of the main results. The final section shows that, in a two lead model which some linear combination of leads is non-interacting, the wavefunction can be written simply in terms of the crossing states of the corresponding one lead model.

We suppose the system is described by a Hamiltonian $H$ whose degrees of freedom are given by some operators $c_{\alpha}^\dagger$ and a set of “fixed impurity states” $|\beta\rangle$. That is, an arbitrary state in the Hilbert space can be written as a superposition of states of the form:

$$c_{\alpha_n}^\dagger \ldots c_{\alpha_1}^\dagger |\beta\rangle,$$

where any $c_{\alpha}$ annihilates any fixed impurity state:

$$c_{\alpha}|\beta\rangle = 0.$$  \hspace{1cm} (2.2)

We write the Hamiltonian as the sum of a non-interacting term plus an interacting term:

$$H = H^{(0)} + H^{(1)},$$  \hspace{1cm} (2.3)

and we make the following assumptions on the fixed impurity states:

$$e^{-iH^{(0)}t}|\beta\rangle = \sum_{\beta'} f_{\beta'\beta}(t)|\beta'\rangle \quad \text{[some coefficients } f_{\beta'\beta}(t)]\hspace{1cm} (2.4a)$$

$$H^{(1)}|\beta\rangle = 0.$$  \hspace{1cm} (2.4b)

That is, we assume that time evolution by the non-interacting term sends any fixed impurity state into a superposition of fixed impurity states, and that the interacting term annihilates any fixed impurity state. The results of this section are valid even if $H^{(0)}$ is an interacting Hamiltonian [as long as (2.4a) and (2.4b) hold]; however, it seems that $H^{(0)}$ must be non-interacting for these results to be useful.
Let us consider some examples. In the Kondo model, the index $\alpha$ stands for momenta and spin (and also a lead index, in the case of a multi-lead model). The states $|\beta\rangle$ are the fixed Kondo spin ($\beta \in \{\uparrow, \downarrow\}$), and the assumption (2.4a) holds even if $H^{(0)}$ contains a magnetic field term. In the Anderson model, there is only one fixed impurity state $|0\rangle$ (the empty dot), and the index $\alpha$ takes on additional values including only spin (with no momentum or lead index) to represent the dot operators $d^\dagger_\uparrow$ and $d^\dagger_\downarrow$. In both models, the assumptions (2.4a) and (2.4b) are easily verified.

We can now state the problem of interest. We are given an initial state with quantum numbers $\alpha_1, \ldots, \alpha_N$ and $\beta$:

$$|\Psi_{\alpha_1\ldots\alpha_N,\beta}\rangle \equiv c^\dagger_{\alpha_N} \ldots c^\dagger_{\alpha_1} |\beta\rangle,$$

and we wish to find the time evolution:

$$|\Psi_{\alpha_1\ldots\alpha_N,\beta}(t)\rangle \equiv e^{-iHt}|\Psi_{\alpha_1\ldots\alpha_N,\beta}\rangle.$$

We must therefore solve the Schrodinger equation with the given initial condition:

$$\left( H - i \frac{d}{dt} \right) |\Psi_{\alpha_1\ldots\alpha_N,\beta}(t)\rangle = 0,$$  \hspace{1cm} (2.7a)

$$|\Psi_{\alpha_1\ldots\alpha_N,\beta}(0)\rangle = |\Psi_{\alpha_1\ldots\alpha_N,\beta}\rangle.$$

To begin our construction of the solution, we define time-evolving fixed impurity states that evolve by $H^{(0)}$ only:

$$|\beta(t)\rangle = e^{-iH^{(0)}t}|\beta\rangle,$$

and we also define a set of time-dependent operators $c^\dagger_{\alpha}(t)$ that describe the free evolution of the $\alpha$ quantum numbers:

$$c^\dagger_{\alpha}(t) = e^{-iH^{(0)}t}c^\dagger_{\alpha}e^{iH^{(0)}t}.$$

Note that the sign in the exponent is the opposite from the interaction picture. The motivation for these definitions is that in the simplest case $H^{(1)} = 0$ (no interaction), the full
solution for the time evolution is:

\[ |\Psi^0(t)\rangle \equiv \left( \prod_{j=1}^{N} c^\dagger_{\alpha_j}(t) \right) |\beta(t)\rangle, \quad (2.10) \]

as can be seen by cancelling each factor of 1 = \( e^{iH^{(0)}t} e^{-iH^{(0)}t} \). So far, this is essentially the approach used by Gurvitz to study transport in non-interacting Floquet models [52]. To allow interactions, we will systematically add a finite number of correction terms to \( |\Psi^0(t)\rangle \) to arrive at the full, exact solution \( |\Psi(t)\rangle \).

Let us emphasize that we are using the Schrodinger picture: the state vector evolves in time, while observables are represented by time-independent operators. The time-evolving state vector is conveniently written in terms of the time-dependent operators \( c^\dagger_{\alpha}(t) \).

Before presenting the case of general \( N \), let us work with \( N = 1, 2 \) and 3 in some detail. We ask, by how much does the freely-evolving state \( |\Psi^0_{\alpha_1...\alpha_N,\beta}(t)\rangle \) fail in solving the full Schrodinger equation? For \( N = 1 \), we have:

\[
\left( H - i \frac{d}{dt} \right) |\Psi^0_{\alpha_1,\beta}(t)\rangle = \left( H - i \frac{d}{dt} \right) c^\dagger_{\alpha_1}(t) |\beta(t)\rangle = \left( [H, c^\dagger_{\alpha_1}(t)] - i \frac{\partial}{\partial t} c^\dagger_{\alpha_1}(t) \right) |\beta(t)\rangle, \quad (2.11a) \\
\]

where we have used \( (H - i \frac{d}{dt}) |\beta(t)\rangle = 0 \), which follows from the definition (2.8) and the two assumptions (2.4a) and (2.4b) we made regarding the fixed impurity states. The operator in parentheses turns out to be very useful, so we give it a name:

\[ A_{\alpha}(t) \equiv [H, c^\dagger_{\alpha}(t)] - i \frac{\partial}{\partial t} c^\dagger_{\alpha}(t). \quad (2.12) \]

Thus, the freely-evolving state \( |\Psi^0_{\alpha_1,\beta}(t)\rangle \) satisfies the initial condition \( |\Psi^0_{\alpha_1,\beta}(0)\rangle = |\Psi_{\alpha_1,\beta}\rangle \), but can fail to satisfy the Schrodinger equation due to a non-zero \( A(t) \) operator:

\[
\left( H - i \frac{d}{dt} \right) |\Psi^0_{\alpha_1,\beta}(t)\rangle = A_{\alpha}(t) |\beta(t)\rangle. \quad (2.13) \\
\]

The \( N = 1 \) problem is solved, then, provided that we can find a time-dependent state vector...
that cancels the leftover term without disturbing the initial condition:

\[
(H - i \frac{d}{dt}) |\Phi_{\alpha_1,\beta}(t)\rangle = -A_{\alpha_1}(t) |\beta(t)\rangle,
\]

(2.14a)

\[
|\Phi_{\alpha_1,\beta}(0)\rangle = 0.
\]

(2.14b)

As long as we continue on this abstract level, there is little content in the previous two equations. Indeed, one can say that the Schrodinger equation has a unique solution \(|\Psi_{\alpha_1,\beta}(t)\rangle\), and define \(|\Phi_{\alpha_1,\beta}(t)\rangle\) to be \(|\Psi_{\alpha_1,\beta}(t)\rangle - |\Psi^0_{\alpha_1,\beta}(t)\rangle\); then the properties of \(|\Phi_{\alpha_1,\beta}(t)\rangle\) follow immediately. But this is not what we have in mind. We have set up the equations for \(|\Phi_{\alpha_1,\beta}(t)\rangle\) because in particular models (including the Kondo model), the solution can be constructed explicitly. We postpone the construction to a later chapter. Given \(|\Phi_{\alpha_1,\beta}(t)\rangle\), the full solution is then:

\[
|\Psi_{\alpha_1,\beta}(t)\rangle = |\Psi^0_{\alpha_1,\beta}(t)\rangle + |\Psi^1_{\alpha_1,\beta}(t)\rangle, \text{ where } |\Psi^1_{\alpha_1,\beta}(t)\rangle = |\Phi_{\alpha_1,\beta}(t)\rangle.
\]

(2.15)

We proceed to \(N = 2\). We have:

\[
(H - i \frac{d}{dt}) |\Psi^0_{\alpha_1,\alpha_2,\beta}(t)\rangle = \left( H - i \frac{d}{dt} \right) c^\dagger_{\alpha_2}(t)c^\dagger_{\alpha_1}(t) |\beta(t)\rangle = A_{\alpha_2}(t)c^\dagger_{\alpha_1}(t) |\beta(t)\rangle + c^\dagger_{\alpha_2}(t)A_{\alpha_1}(t) |\beta(t)\rangle,
\]

(2.16a)

(2.16b)

where we have again used \((H - i \frac{d}{dt}) |\beta(t)\rangle = 0\). Anticommuting the \(A(t)\) operator to the right, we obtain:

\[
(H - i \frac{d}{dt}) |\Psi^0_{\alpha_1,\alpha_2,\beta}(t)\rangle = -c^\dagger_{\alpha_1}(t)A_{\alpha_2}(t) |\beta(t)\rangle + c^\dagger_{\alpha_2}(t)A_{\alpha_1}(t) |\beta(t)\rangle + B_{\alpha_1\alpha_2}(t) |\beta(t)\rangle,
\]

(2.17)

where we have defined another operator that will be very useful hereafter:

\[
B_{\alpha_1\alpha_2}(t) = \{ A_{\alpha_2}(t), c^\dagger_{\alpha_1}(t) \}.
\]

(2.18)

Why the anticommutator and not the commutator? The Hamiltonian is bosonic (i.e. the total number of fermionic operators in any term is even); hence the commutator \([H, c^\dagger_{\alpha}(t)]\) is fermionic. Therefore the anticommutator written above will be simpler than the corresponding commutator.
A useful property of the $B(t)$ operator is that it is antisymmetric:

$$B_{\alpha_1 \alpha_2}(t) = -B_{\alpha_2 \alpha_1}(t),$$

which follows from $B_{\alpha_1 \alpha_2}(t) + B_{\alpha_2 \alpha_1}(t) = [H, \{c_{\alpha_1}^\dagger(t), c_{\alpha_2}^\dagger(t)\}] - i \frac{d}{dt} \{c_{\alpha_1}^\dagger(t), c_{\alpha_2}(t)\}$ and the observation that the anticommutation relation $\{c_{\alpha_1}^\dagger, c_{\alpha_2}\} = 0$ is preserved under unitary time evolution of the field operators. The $B(t)$ operator can therefore be written as an antisymmetrization of what we will call a “reduced” operator:

$$B_{\alpha_1 \alpha_2}(t) = B_{\alpha_1 \alpha_2}^{(\text{red})}(t) - B_{\alpha_2 \alpha_1}^{(\text{red})}(t).$$

While there is a considerable freedom in the choice of $B_{\alpha_1 \alpha_2}^{(\text{red})}(t)$ (for instance, $B_{\alpha_1 \alpha_2}^{(\text{red})}(t) = \frac{1}{2} B_{\alpha_1 \alpha_2}(t)$ is always an option), the most convenient choice is usually clear in practice.

A model will be called “type A” if $B_{\alpha_1 \alpha_2}(t) = 0$ for all times and for any quantum numbers. These are the simplest interacting models from the point of view of the methods of this chapter. The Kondo model is of this type: since the interaction term is of the form $c^\dagger \hat{O}_{\text{imp}} c$ (where $\hat{O}_{\text{imp}}$ is an operator that commutes with all field operators), the $A(t)$ operator is of the form $c^\dagger \hat{O}_{\text{imp}}$. (This is done in more detail in Chapter 4.) We focus on type A models for some time before considering the next level of difficulty.

We again have found that the freely-evolving state does not satisfy the Schrödinger equation. The trick is to use the same states $|\Phi_{\alpha_1,\beta}(t)\rangle$ that we used in the $N = 1$ solution to cancel the leftover terms. We define:

$$|\Psi_{\alpha_1 \alpha_2, \beta}(t)\rangle = c_{\alpha_2}^\dagger(t)|\Phi_{\alpha_1, \beta}(t)\rangle - c_{\alpha_1}^\dagger(t)|\Phi_{\alpha_2, \beta}(t)\rangle.$$  

Then we obtain:

$$\left(H - i \frac{d}{dt}\right) |\Psi_{\alpha_1 \alpha_2, \beta}(t)\rangle = -c_{\alpha_2}^\dagger(t) A_{\alpha_1}(t) |\beta(t)\rangle + c_{\alpha_1}^\dagger(t) A_{\alpha_2}(t) |\beta(t)\rangle$$

$$+ A_{\alpha_2}(t) |\Phi_{\alpha_1, \beta}(t)\rangle - A_{\alpha_1}(t) |\Phi_{\alpha_2, \beta}(t)\rangle.$$  

(2.22a)

Combining with what we found for the action of $H - i \frac{d}{dt}$ on the freely-evolving state, and remembering that we are considering the case of $B_{\alpha_1 \alpha_2}(t) = 0$ for now, we obtain:

$$\left(H - i \frac{d}{dt}\right) \left(|\Psi_{\alpha_1 \alpha_2, \beta}(t)\rangle + |\Psi_{\alpha_1 \alpha_2, \beta}(t)\rangle\right) = A_{\alpha_2}(t) |\Phi_{\alpha_1, \beta}(t)\rangle - A_{\alpha_1}(t) |\Phi_{\alpha_2, \beta}(t)\rangle.$$  

(2.23)
We therefore have new leftover terms to cancel. Let us suppose that we can construct a
time-evolving state $|\Phi_{\alpha_1\alpha_2,\beta}(t)\rangle$ that cancels these leftover terms without affecting the initial condition at $t = 0$:

$$\left(H - i\frac{d}{dt}\right)|\Phi_{\alpha_1\alpha_2,\beta}(t)\rangle = A_{\alpha_2}(t)|\Phi_{\alpha_1,\beta}(t)\rangle - A_{\alpha_1}(t)|\Phi_{\alpha_2,\beta}(t)\rangle,$$

(2.24a)

$$|\Phi_{\alpha_1\alpha_2,\beta}(t = 0)\rangle = 0.$$  

(2.24b)

Given such a state, the full solution for two particles is:

$$|\Psi_{\alpha_1\alpha_2,\beta}(t)\rangle = |\Psi^0_{\alpha_1\alpha_2,\beta}(t)\rangle + |\Psi^1_{\alpha_1\alpha_2,\beta}(t)\rangle + |\Psi^2_{\alpha_1\alpha_2,\beta}(t)\rangle,$$

where

$$|\Psi^0_{\alpha_1\alpha_2,\beta}(t)\rangle = c^\dagger_{\alpha_3}(t)c^\dagger_{\alpha_2}(t)c^\dagger_{\alpha_1}(t)|\beta(t)\rangle,$$

(2.27a)

$$|\Psi^1_{\alpha_1\alpha_2,\beta}(t)\rangle = c^\dagger_{\alpha_3}(t)c^\dagger_{\alpha_2}(t)|\Phi_{\alpha_1,\beta}(t)\rangle - c^\dagger_{\alpha_3}(t)c^\dagger_{\alpha_1}(t)|\Phi_{\alpha_2,\beta}(t)\rangle + c^\dagger_{\alpha_2}(t)c^\dagger_{\alpha_1}(t)|\Phi_{\alpha_3,\beta}(t)\rangle,$$

(2.27b)

$$|\Psi^2_{\alpha_1\alpha_2,\beta}(t)\rangle = c^\dagger_{\alpha_3}(t)|\Phi_{\alpha_1\alpha_2,\beta}(t)\rangle - c^\dagger_{\alpha_2}(t)|\Phi_{\alpha_1\alpha_3,\beta}(t)\rangle + c^\dagger_{\alpha_1}(t)|\Phi_{\alpha_2\alpha_3,\beta}(t)\rangle,$$

(2.27c)

$$|\Psi^3_{\alpha_1\alpha_2,\beta}(t)\rangle = |\Phi_{\alpha_1\alpha_2\alpha_3,\beta}(t)\rangle,$$

(2.27d)

and $|\Phi_{\alpha_1\alpha_2\alpha_3,\beta}(t)\rangle$ is a new state we must construct, satisfying:

$$\left(H - i\frac{d}{dt}\right)|\Phi_{\alpha_1\alpha_2\alpha_3,\beta}(t)\rangle =$$

$$- (A_{\alpha_3}(t)|\Phi_{\alpha_1\alpha_2,\beta}(t)\rangle - A_{\alpha_2}(t)|\Phi_{\alpha_1\alpha_3,\beta}(t)\rangle + A_{\alpha_1}(t)|\Phi_{\alpha_2\alpha_3,\beta}(t)\rangle),$$

(2.28a)

$$|\Phi_{\alpha_1\alpha_2\alpha_3,\beta}(t = 0)\rangle = 0.$$  

(2.28b)

We now outline what happens in the case of general $N$, with the formal proof in the
following section. The action of $H - i\frac{d}{dt}$ on the freely-evolving state $|\Psi^0_{\alpha_N,\beta}(t)\rangle$ produces
Figure 2.1: The wavefunction for $N = 1, 2, \text{and } 3$. Each line represents a quantum number of the initial state ($\alpha_1, \alpha_2, \alpha_3$). Ordinary lines represent $c^\dagger(t)$ operators, while each line that ends on a circle represents a quantum number assigned to the crossing state $|\chi(t)\rangle$. Sign factors, antisymmetrizations, and dependence on $t$ are all implicit.

A sum of states that each have $N - 1$ free creation operators and a single $A(t)$. To cancel this, we add a state $|\Psi_{N,\beta}(t)\rangle$, which is a sum of states that each have $N - 1$ free creation operators acting on a $|\Phi_{\alpha,\beta}(t)\rangle$ state. Acting with $H - i \frac{d}{dt}$ on $|\Psi_{N,\beta}(t)\rangle$ cancels the leftover terms from $|\Psi_{0,\beta}(t)\rangle$ but leaves new leftovers: $N - 2$ creation operators acting on $A_{j_2}(t)|\Psi_{\alpha_{j_1},\beta}(t)\rangle$. We cancel these by adding $|\Psi_{N,\beta}(t)\rangle$, which is a sum of terms consisting of $N - 2$ free creation operators acting on $|\Phi_{\alpha_{j_1},\alpha_{j_2},\beta}(t)\rangle$ states. Proceeding in this way, the number of free creation operators in the leftover terms gets reduced from $N$ down to one, when we are left with a sum of terms of the form $A_{\alpha_{j_N}}(t)|\Phi_{\alpha_{j_1},\ldots,\alpha_{j_{N-1}},\beta}(t)\rangle$ to cancel. We cancel these by adding $|\Psi_{N,\beta}(t)\rangle = |\Phi_{\alpha_{N},\beta}(t)\rangle$, and then we are done.

We still need to find the $|\Phi(t)\rangle$ states. This may be, for a generic Hamiltonian, no easier than finding solutions to the Schrodinger equation in its original form. However, there is some reason to expect the construction we are using to be useful in a quantum dot model with a linearized spectrum. In such a model, the Fermi velocity sets an upper speed limit (which we always set to unity). If the quantum dot is located at $x = 0$, then the effect of the quench spreads out in a “light cone.” Of course, the real interest in the construction
we are using is that the $|\Phi(t)\rangle$ states can be found explicitly in several interacting quantum dot models.

Before proceeding with the formal proof for general $N$, let us consider the case of non-vanishing $B_{\alpha_1 \alpha_2}(t)$. When we act $H - i\frac{d}{dt}$ on a list of free creation operators, we obtain an $A(t)$ operator in each possible position, as shown in the following two examples:

\[
\left( H - i\frac{d}{dt} \right) c_{\alpha_3}^\dagger(t) c_{\alpha_2}^\dagger(t) c_{\alpha_1}(t) |\beta(t)\rangle = \\
A_{\alpha_3}(t) c_{\alpha_2}^\dagger(t) c_{\alpha_1}(t) |\beta(t)\rangle + c_{\alpha_3}^\dagger(t) A_{\alpha_2}(t) c_{\alpha_1}(t) |\beta(t)\rangle + c_{\alpha_3}(t) c_{\alpha_2}(t) A_{\alpha_1}(t) |\beta(t)\rangle, 
\]

\[
(2.29a)
\]

\[
\left( H - i\frac{d}{dt} \right) c_{\alpha_3}(t) c_{\alpha_2}(t) c_{\alpha_1}^\dagger(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle = A_{\alpha_3}(t) c_{\alpha_1}^\dagger(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle + c_{\alpha_3}^\dagger(t) A_{\alpha_1}(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle. 
\]

\[
(2.29b)
\]

If the $B(t)$ operator vanishes, this means that each $A(t)$ operator can be brought to the right of all the remaining $c^\dagger(t)$ operators, with a minus sign for every $c^\dagger(t)$ operator it passes on the way. If $B(t)$ does not vanish, we obtain (continuing the two examples given above):

\[
\left( H - i\frac{d}{dt} \right) c_{\alpha_3}^\dagger(t) c_{\alpha_2}^\dagger(t) c_{\alpha_1}(t) |\beta(t)\rangle = \\
c_{\alpha_2}(t) c_{\alpha_1}^\dagger(t) A_{\alpha_3}(t) |\beta(t)\rangle - c_{\alpha_3}(t) c_{\alpha_1}^\dagger(t) A_{\alpha_2}(t) |\beta(t)\rangle + c_{\alpha_3}(t) c_{\alpha_2}(t) A_{\alpha_1}(t) |\beta(t)\rangle \\
+ B_{\alpha_2\alpha_3}(t) c_{\alpha_1}^\dagger(t) |\beta(t)\rangle - c_{\alpha_2}(t) B_{\alpha_1\alpha_3}(t) |\beta(t)\rangle + c_{\alpha_3}(t) B_{\alpha_1\alpha_2}(t) |\beta(t)\rangle, 
\]

\[
(2.30a)
\]

\[
\left( H - i\frac{d}{dt} \right) c_{\alpha_3}(t) c_{\alpha_1}^\dagger(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle = -c_{\alpha_3}^\dagger(t) A_{\alpha_3}(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle + c_{\alpha_3}^\dagger(t) A_{\alpha_1}(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle \\
+ B_{\alpha_1\alpha_3}(t) |\Phi_{\alpha_2\alpha_4,\beta}(t)\rangle. 
\]

\[
(2.30b)
\]

What if we bring each $B(t)$ past all of the $c^\dagger(t)$ operators to its right? (There is only one such term in the examples above, but it is easy to see by consider larger products that we can have a $B(t)$ to the left of any number of $c^\dagger(t)$ operators.) The next simplest type of model to consider would be one in which the $B(t)$ and $c^\dagger(t)$ operators commute, so that the $B(t)$ operators could be brought to the right without generating any additional terms. This turns out to be slightly too general. We call a model “type B” if the $B(t)$ and $c^\dagger(t)$
operators commute and the $A(t)$ operators annihilate the fixed impurity states; that is,

\begin{align}
[B_{\alpha_2\alpha_3}(t), c_{\alpha_1}(t)] &= 0 & \text{for any } \alpha_1, \alpha_2, \alpha_3, t \tag{2.31a} \\
A_\alpha(t)|\beta\rangle &= 0 & \text{for any } \alpha, \beta, t \tag{2.31b}
\end{align}

We look at the commutator rather than the anticommutator because $B(t)$ is bosonic, being the anticommutator of the fermionic operators $A(t)$ and $c^\dagger(t)$. As further motivation for this definition of type B models, consider that the interaction term in the Hamiltonian often takes the form $c^\dagger c^\dagger c c$ (with summations over various quantum numbers). In this case, the $A(t)$ operator has the form $c^\dagger c^\dagger c$ (which annihilates the only fixed impurity state), and the $B(t)$ operator has the form $c^\dagger c^\dagger$ (which commutes with any $c^\dagger(t)$). The Anderson model is of this type. More generally, it seems that the condition of $A(t)$ annihilating fixed impurity states does not in fact reduce the space of suitable Hamiltonians at all, seeing as the $A(t)$ operator must have an annihilation operator in order for the $B(t)$ operator to be non-vanishing.

Although we restrict our attention to type A and type B models, we note that the process of generalization can be continued indefinitely. We could define $C_{\alpha_1\alpha_2\alpha_3}(t) = [B_{\alpha_2\alpha_3}(t), c_{\alpha_1}(t)]$ and consider the case of non-vanishing $C(t)$; a “type C” model would then be one in which any $C(t)$ anticommutes with any $c^\dagger(t)$, and so on with higher nested commutators and anticommutators. The methods we describe in this chapter can probably be generalized to cover all of these cases, with greater difficulty as the models get more and more general.

2.2.1 Interlude – notation for manipulating lists

Before presenting our main results on type A and type B models, we introduce a compact notation for manipulating lists of indices and products of operators. This notation allows us to do calculations that would be excessively lengthy if all indices were written out in full. It is used throughout the remainder of this thesis.
We use boldface letters to stand for lists of indices: \( m = (1, 3, 6, 7) \), for example. We use \( m_j \) and \( m(j) \) interchangeably to refer to individual list elements, such as \( m_2 = m(2) = 3 \).

Boldface letters in subscripts indicate products in the manner of the following examples (in which \( m \) has length \( n \), a small circle stands for composition, and \( \sigma \in \text{Sym}(n) \)):

\[
c_{\alpha m} = c_{\alpha_{m(1)} \cdots \alpha_{m(n)}}, \quad c_{\alpha m^{\sigma}} = c_{\alpha_{m(\sigma_1)} \cdots \alpha_{m(\sigma_n)}},
\]

\[
c_{\alpha m}^\dagger = c_{\alpha_{m(n)}^\dagger \cdots \alpha_{m(1)}^\dagger}, \quad c_{\alpha m^{\sigma}}^\dagger = c_{\alpha_{m(\sigma_n)}^\dagger \cdots \alpha_{m(\sigma_1)}^\dagger}.
\]

(2.32a)

(2.32b)

(Note that taking the adjoint reverses the order of the indices.) We also use boldface letters in subscripts to stand for lists of quantum numbers; for instance, the initial state of the quench problem is written as:

\[
|\Psi_{\alpha N, \beta}\rangle = |\Psi_{\alpha_1 \cdots \alpha_N, \beta}\rangle, \quad \langle \Psi_{\alpha N, \beta}| = \langle \Psi_{\alpha_1 \cdots \alpha_N, \beta}|,
\]

(2.33)

with \( N = (1, \ldots, N) \). (Note the convention that taking the adjoint of a state does not reverse the order of the quantum numbers).

Given any list \( m \) of increasing indices \((m_1 < \cdots < m_n)\), we define \( \mathcal{I}_j(m) \) to be the set of increasing lists of length \( j \) chosen from \( m \):

\[
\mathcal{I}_j(m) = \{ \ell = (\ell_1, \ldots, \ell_j) \subset m \mid \ell_1 < \cdots < \ell_j \}. \quad (2.34)
\]

For instance, if \( m = (1, 3, 6, 7) \), then \( \mathcal{I}_3(m) = \{(1, 3, 6), (1, 3, 7), (3, 6, 7)\} \).

It is often convenient to write a sum over a single index \( \ell_1 \) as a sum over lists \( \ell \) of length 1 (i.e., \( \ell \in \mathcal{I}_1(m) \)) in order to use the notation we define in the next paragraph.

Given \( \ell \in \mathcal{I}_j(m) \), we define \( \overline{\text{perm}}[\ell] \) to be the permutation of \( m \) that brings all the entries of \( \ell \) to the left of all the remaining entries of \( m \); we define \( \overline{\text{perm}}[\ell] \) similarly. For example, if \( m = (1, 3, 6, 7) \) and \( \ell = (1, 6) \), then \( \overline{\text{perm}}[\ell] \) maps \( (1, 3, 6, 7) \to (1, 6, 3, 7) \) and \( \overline{\text{perm}}[\ell] \) maps \( (1, 3, 6, 7) \to (3, 7, 1, 6) \). Note that \( \overline{\text{perm}}[\ell] \) and \( \overline{\text{perm}}[\ell] \) depend implicitly on the list \( m \) from which the entries in \( \ell \) are chosen. We write the sign factors for these
permutations in the following way:

\[ \hat{\text{sgn}} \ell \equiv \text{sgn} \hat{\text{perm}}[\ell], \quad (2.35a) \]
\[ \text{sgn} \ell \equiv \text{sgn} \text{perm}[\ell]. \quad (2.35b) \]

The slash notation \( m/\ell \) indicates the list \( m \) with the indices belonging to \( \ell \) all removed; in the example given above, \( m/\ell = (3, 7) \). The same slash notation also applies for removing a single entry of list: for instance, \( m/3 = (1, 6, 7) \).

When a boldface letter is used without any defining statement, it can be assumed to refer to a simple increasing list:

\[ n = (1, \ldots, n). \quad (2.36) \]

The above notation suffices for the analysis of type A models. For type B models, we also need to consider lists divided into smaller parts in various ways. Given a list \( m \), we define a **partition** of \( m \) to be a separation of the list elements into **cells of length 2 or greater**. Partitions are denoted by underlined, boldface letters (typically the letter \( p \), as in \( p \)). Take \( m = (1, 3, 6, 7) \) as an example; the two partitions of \( m \) are \( p = (1, 3, 6, 7) \) (one cell) and \( p = (1, 3|6, 7) \) (two cells).

A partition with \( s \) cells can be written as \( p = (p_1|\ldots|p_s) \), where each \( p_j \) is a list. Elements of these lists are written as \( p_j(\ell) = p_{j\ell} = p(j\ell) \). The set of all partitions of a list \( m \) is written as \( \mathbb{P}(m) \):

\[ \mathbb{P}(m) = \left\{ p \equiv (p_1|\ldots|p_s) \mid 1 \leq s \leq |m|/2, \ (p_1, \ldots, p_s) = m, \ |p_j| \geq 2 \text{ for all } j \right\}. \quad (2.37) \]

The set of partitions whose last cell has length \( q \) is denoted with a subscript \( q \):

\[ \mathbb{P}_q(m) = \left\{ p \equiv (p_1|\ldots|p_s) \in \mathbb{P}(m) \mid |p_s| = q \right\} \quad (2.38) \]

2.2.2 Statement of results

In either type of model (type A or type B), the wavefunction takes the following form:

\[ |\Psi_{\alpha N,\beta}(t)\rangle = \sum_{n=0}^{N} |\Psi_{\alpha N,\beta,n}(t)\rangle, \quad (2.39) \]
where:

\[ |\Psi^n_{\alpha N, \beta}(t)\rangle = \sum_{m \in L_n(N)} (\text{sgn } m) c_{\alpha N/m}^\dagger(t) |\Phi_{\alpha m, \beta}(t)\rangle. \]  

(2.40)

We set \(|\Phi, \beta(t)\rangle = |\beta(t)\rangle\); then the \(n = 0\) term above is \(|\Psi^0_{\alpha N, \beta}(t)\rangle = c_{\alpha N}^\dagger(t) |\beta(t)\rangle\), which is exactly the freely-evolving state defined earlier. The interpretation of this wavefunction is the following: any number \(n\) of the given \(N\) quantum numbers can be chosen to be put into a “crossing state” \(|\Phi(t)\rangle\) (the reason for this name will be given in a later chapter), while the remaining quantum numbers are assigned to \(c^\dagger(t)\) operators.

We have not defined the \(|\Phi(t)\rangle\) states yet; we will see shortly that they must satisfy certain differential equations. The essential point of this chapter is to reduce the time evolution problem to the solution of these differential equations. In some sense, we are getting the combinatorics out of the way in order to focus on the core difficulty of the problem. We can do this for any Hamiltonian, but it is certainly not always possible to solve the differential equations we end up with. Thus, while we will continue to keep the discussion fairly general, it must be kept in mind that the main interest of the method is that for particular interacting models, the differential equations are solvable and the \(|\Phi(t)\rangle\) states can be found explicitly.

We now state the main results of this chapter. Proofs are given in the next two sections.

In a type A model, we have:\footnote{The small circle on the right-hand side stands for composition; written in full, this equation reads: \(|\Phi_{\alpha m_1 \ldots m_n, \beta}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) |\chi_{\alpha m_1 \ldots m_n, \beta}(t)\rangle. \) If \( m \) is the empty sequence, we understand it to mean \(|\Phi, \beta(t)\rangle = |\chi, \beta(t)\rangle. \)
}

\[ |\Phi_{\alpha m, \beta}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) |\chi_{\alpha m, \sigma, \beta}(t)\rangle, \]  

(2.41)

where the “unsymmetrized crossing states” \(|\chi(t)\rangle\) satisfy:

\[ \left( \hat{H} - i \frac{d}{dt} \right) |\chi_{\alpha_1 \ldots \alpha_n, \beta}(t)\rangle = -A_{\alpha_n}(t) |\chi_{\alpha_1 \ldots \alpha_{n-1}, \beta}(t)\rangle, \]  

(2.42a)

\[ |\chi_{\alpha_1 \ldots \alpha_n, \beta}(t = 0)\rangle = 0, \]  

(2.42b)

\[ |\chi_{\beta}(t)\rangle = |\beta(t)\rangle. \]  

(2.42c)
(The third equation ensures that for \( n = 1 \), the first equation becomes the same as equation (2.14a) from the \( N = 1 \) warm-up case.)

In a type B model, we have:

\[
|\Phi_{\alpha,\beta}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn} \, \sigma) \sum_{p \in \mathcal{P}(m)} |\chi_{\alpha_{p\sigma},\beta}(t)\rangle,
\]

where the crossing states \( |\chi(t)\rangle \) satisfy a more complicated condition than in the type A case, which we now state. Given a partition \( p \) of \((1,\ldots,n)\), the crossing state condition is:

\[
\left( H - i \frac{d}{dt} \right) |\chi_{p\sigma,\beta}(t)\rangle = \begin{cases} 
-\mathcal{D}^{\text{red}}_{\alpha_1-\alpha_n}(t)|\chi_{p_{/\alpha_1},\beta}(t)\rangle & q = 2 \\
-A_{\alpha_n}(t)|\chi_{p_{/\alpha_n},\beta}(t)\rangle & 3 \leq q \leq n 
\end{cases},
\]

\( |\chi_{p\sigma,\beta}(t = 0)\rangle = 0 \), \( \langle \chi_{\alpha,\beta}(t) | \beta(t) \rangle \).

In type B models, the crossing state with just one quantum number always vanishes \( (|\Phi_{\alpha_1,\beta}(t)\rangle = |\chi_{\alpha_1,\beta}(t)\rangle = 0) \)

### 2.2.3 Proof for type A models

We show that, given crossing states \( |\chi(t)\rangle \) satisfying the conditions listed, the construction satisfies the Schrodinger equation. That is, we show \( \langle H - i \frac{d}{dt} | \Psi_{\alpha_{N},\beta}(t) \rangle = 0 \).

Our first task is to show that the crossing state condition implies that the states \( |\Phi(t)\rangle \) satisfy a very similar condition:

\[
\left( H - i \frac{d}{dt} \right) |\Phi_{\alpha_{m},\beta}(t)\rangle = -\sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \, \ell) A_{\alpha_\ell}(t)|\Phi_{\alpha_{m/\ell},\beta}(t)\rangle.
\]

Recall that \( m \) is an increasing sequence of length \( n \) chosen from the larger index set \( N = (1,\ldots,N) \). We are therefore trying to prove a statement about the \( |\Phi(t)\rangle \) state corresponding to the quantum numbers \( \alpha_{m_1},\ldots,\alpha_{m_n} \) (and \( \beta \)). Since these quantum numbers are arbitrary, we can just as well do the proof for \( \alpha_1,\ldots,\alpha_n \) to simplify the notation.
Equivalently, we can say that we are doing the proof for the case \( m = (1, \ldots, n) \) \( \equiv n \), which suffices to prove the claim for general \( m \).

We have:

\[
\left( H - i \frac{d}{dt} \right) |\Phi_{\alpha_n,\beta}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \left( H - i \frac{d}{dt} \right) |\chi_{\alpha_{\sigma_1} \ldots \alpha_{\sigma_n},\beta}(t)\rangle \tag{2.46a}
\]

\[
= - \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) A_{\alpha_{\sigma_n}}(t) |\chi_{\alpha_{\sigma_1} \ldots \alpha_{\sigma_{n-1}},\beta}(t)\rangle \tag{2.46b}
\]

\[
= - \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) A_{\alpha_{\sigma_n}}(t) |\chi_{\alpha_{\sigma[n/n]},\beta}(t)\rangle. \tag{2.46c}
\]

The trick is to separate the \( n \)th term of the permutation \( \sigma \). A permutation of \( n \) elements is equivalent to a choice of one element (\( \sigma_n \)) to be brought to the right of the list, then a permutation of the remaining \( n - 1 \) elements. We therefore have:

\[
\left( H - i \frac{d}{dt} \right) |\Phi_{\alpha_n,\beta}(t)\rangle = - \sum_{\ell \in \mathcal{I}_1(n)} (\text{sgn } \ell) \sum_{\sigma \in \text{Sym}(n-1)} (\text{sgn } \sigma) A_{\alpha_{\ell_1}}(t) |\chi_{\alpha_{(n/\ell)n/\ell},\beta}(t)\rangle \tag{2.47a}
\]

\[
= - \sum_{\ell \in \mathcal{I}_1(n)} (\text{sgn } \ell) A_{\alpha_{\ell_1}}(t) |\Phi_{\alpha_{n/\ell},\beta}(t)\rangle. \tag{2.47b}
\]

This completes the proof of equation (2.45).

The next step is to write down a formula for the action of \( H - i \frac{d}{dt} \) on a product of \( c^\dagger(t) \) operators. If \( |X(t)\rangle \) is any time-dependent state and \( m \) any non-empty list of indices, then we have:

\[
\left( H - i \frac{d}{dt} \right) \left( c_{\alpha_m}^\dagger(t)|X(t)\rangle \right) = \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn } \ell) c_{\alpha_{m/\ell}}^\dagger(t) A_{\alpha_{\ell_1}}(t) |X(t)\rangle
\]

\[
+ c_{\alpha_m}^\dagger(t) \left( H - i \frac{d}{dt} \right) |X(t)\rangle. \tag{2.48}
\]

The first term on the right-hand side comes from commuting \( H \) past each \( c^\dagger(t) \) operator; the sign factor \( \text{sgn } \ell \) appears because the \( A(t) \) generated by the commutator then anticommutes (using the assumption that the model is type A) past each remaining \( c^\dagger(t) \) to the right.
Applying the formula (2.48), we obtain:

\[
(H - i \frac{d}{dt}) |\Psi_{\alpha N, \beta}(t)\rangle = \left( H - i \frac{d}{dt} \right) \sum_{n=0}^{N} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) c_{\alpha N/m}^{\dagger}(t) |\Phi_{\alpha m, \beta}(t)\rangle \tag{2.49a}
\]

\[
= \sum_{n=0}^{N-1} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) \sum_{\ell \in I_1(N/m)} (\hat{\text{sgn}} \ell) c_{\alpha N/m/\ell}^{\dagger}(t) A_{\alpha \ell}^{(1)}(t) |\Phi_{\alpha m, \beta}(t)\rangle + \sum_{n=1}^{N} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) c_{\alpha N/m}^{\dagger}(t) (H - i \frac{d}{dt}) |\Phi_{\alpha m, \beta}(t)\rangle. \tag{2.49b}
\]

Note that in the first term, we dropped the \( n = N \) part of the sum, since it is zero – if all quantum numbers are chosen to be put into \( |\Phi(t)\rangle \), then there are no \( c^{\dagger}(t) \) operators to commute with and so no \( A(t) \) is generated. Similarly, in the second term we dropped the \( n = 0 \) part, since \( (H - i \frac{d}{dt}) |\Phi_{\alpha \beta}(t)\rangle = (H - i \frac{d}{dt}) |\beta(t)\rangle = 0 \). (The purpose of the assumptions (2.4a) and (2.4b) we made regarding the fixed impurity states was to make this term vanish.)

We now make a judicious relabelling of summation indices in the first term of (2.49b). As it stands, we are choosing a list \( m \) of \( n \) indices from \( N \) to bring to the left (of \( N \)), then choosing one index (i.e. a list \( \ell \) of length 1) from the remainder and bringing it to the left (of \( N/m \)). Schematically, this amounts to:

\[
\begin{align*}
N & \xrightarrow{\text{choose}} m \quad m/N \xrightarrow{\text{choose}} \ell \quad m \quad \ell/m. \tag{2.50}
\end{align*}
\]

We can just as well choose \( n + 1 \) indices from \( N \) and bring them to the left (of \( N \)), then choose one of the \( n + 1 \) to bring to the right (of the \( n + 1 \)).\(^2\) We therefore have:

\[
\text{first term of (2.49b)} = \sum_{n=0}^{N-1} \sum_{m \in I_{n+1}(N)} (\hat{\text{sgn}} m) \sum_{\ell \in I_1(m)} (\hat{\text{sgn}} \ell) c_{\alpha N/m}^{\dagger}(t) A_{\alpha \ell}^{(1)}(t) |\Phi_{\alpha m/\ell, \beta}(t)\rangle \tag{2.51a}
\]

\[
= \sum_{n=1}^{N} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) c_{\alpha N/m}^{\dagger}(t) \sum_{\ell \in I_1(m)} (\hat{\text{sgn}} \ell) A_{\alpha \ell}^{(1)}(t) |\Phi_{\alpha m/\ell, \beta}(t)\rangle. \tag{2.51b}
\]

\(^2\) To be precise, we are noting that \( \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) \sum_{\ell \in I_1(m)} (\hat{\text{sgn}} \ell) X(m, \ell) = \sum_{m \in I_{n+1}(N)} (\hat{\text{sgn}} m) \sum_{\ell \in I_1(m)} (\hat{\text{sgn}} \ell) X(m, \ell, \ell) \) for any function \( X \) as long as \( n + q \leq N \) and \( q \leq n \). We are here using this formula for \( q = 1 \), while in the type B proof, we will need \( q = 1 \) and \( q = 2 \).
It is then clear from (2.45) that the two terms of (2.49b) cancel each other. This completes the proof.

2.2.4 Proof for type B models

We show that, given crossing states $|\chi(t)\rangle$ satisfying the conditions listed, the construction satisfies the Schrodinger equation. That is, we show \( (H - i\frac{d}{dt}) |\Psi_{\alpha_N,\beta}(t)\rangle = 0 \). The reader may find it helpful to warm up by going through the type A proof first, since the manipulations are similar.

Our first task is to show that the crossing state condition implies that the symmetrized crossing states $|\Phi(t)\rangle$ satisfy a very similar condition:

\[
(H - i\frac{d}{dt}) |\Phi_{\alpha_m,\beta}(t)\rangle = -\sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \ell) A_{\alpha_1}(t) |\Phi_{\alpha_{m/\ell},\beta}(t)\rangle \\
- \sum_{\ell \in \mathcal{I}_2(m)} (\text{sgn} \ell) B_{\alpha_1,\alpha_{\ell_2}}(t) |\Phi_{\alpha_{m/\ell},\beta}(t)\rangle.
\]  

(2.52a)

Unlike the corresponding proof of Eq. (2.45) for type A models, the proof we now consider does not look any simpler when one sets $m = (1, \ldots, n)$; we therefore keep $m$ arbitrary (with length $n$).

We can split up any sum over all partitions into sums over those with specified lengths of the last cell:

\[
\sum_{p \in \mathcal{F}(m)} X(p) = \sum_{q=2}^{n} \sum_{p \in \mathcal{F}_q(m)} X(p),
\]  

(2.53)

where $X$ is any function. In particular, we separate the $q = 2$ partitions from the others in
order to apply the crossing state condition:

\[
(H - i \frac{d}{dt}) |\Phi_{\alpha_m,\beta}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{p \in \mathbb{P}(m)} \left( H - i \frac{d}{dt} \right) |\chi_{\alpha_{p^\sigma},\beta}(t)\rangle
\]

(2.54a)

\[
= \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{p \in \mathbb{P}_2(m)} \left( H - i \frac{d}{dt} \right) |\chi_{\alpha_{p^\sigma},\beta}(t)\rangle
\]

\[
+ \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{q=3}^{n} \sum_{\substack{\mathbb{P}_q(m) \ni p \neq \ell \rangle}} \left( H - i \frac{d}{dt} \right) |\chi_{\alpha_{p^\sigma},\beta}(t)\rangle
\]

(2.54b)

\[
= - \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{p \in \mathbb{P}_2(m)} B^{(\text{red})}_{\alpha_{p(\sigma_{n-1})\alpha_{p(\sigma_n)}}}(t) |\chi_{\alpha_{p(\sigma_{n-1})\alpha_{p(\sigma_n)}},\beta}(t)\rangle
\]

\[
- \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{q=3}^{n} \sum_{\substack{\mathbb{P}_q(m) \ni p \neq \ell \rangle}} A_{\alpha_{p(\sigma_{n-1})},\beta}(t) |\chi_{\alpha_{p(\sigma_{n-1})}\alpha_{p(\sigma_n)}},\beta(t)\rangle.
\]

(2.54c)

The two terms on the right-hand side will now be massaged separately. By steps similar to
the type A proof, we relabel summation indices to obtain:

**First term of (2.54c)**

\[
- \sum_{\ell \in \mathbb{I}_2(m)} (\text{sgn } \ell) \left( B^{(\text{red})}_{\alpha_{\ell_1,\ell_2}}(t) - B^{(\text{red})}_{\alpha_{\ell_2,\ell_1}}(t) \right) \sum_{\sigma \in \text{Sym}(n-2)} (\text{sgn } \sigma)
\]

\[
\times \sum_{p \in \mathbb{P}(m/\ell)} |\chi_{\alpha_{p^\sigma},\beta}(t)\rangle
\]

(2.55a)

\[
- \sum_{\ell \in \mathbb{I}_2(m)} (\text{sgn } \ell) B_{\alpha_{\ell_1,\ell_2}}(t) |\Phi_{\alpha_m/\ell,\beta}(t)\rangle
\]

(2.55b)

and:

**2nd term of (2.54c)**

\[
- \sum_{\ell \in \mathbb{I}_1(m)} (\text{sgn } \ell) A_{\alpha_{\ell_1}}(t) \sum_{\sigma \in \text{Sym}(n-1)} (\text{sgn } \sigma) \sum_{q=3}^{n} \sum_{\substack{\mathbb{P}_{q-1}(m/\ell) \ni p \neq \ell \rangle}} |\chi_{\alpha_{p^\sigma},\beta}(t)\rangle
\]

(2.56a)

\[
= - \sum_{\ell \in \mathbb{I}_1(m)} (\text{sgn } \ell) A_{\alpha_{\ell_1}}(t) \sum_{\sigma \in \text{Sym}(n-1)} (\text{sgn } \sigma) \sum_{q=2}^{n-1} \sum_{\substack{\mathbb{P}_{q}(m/\ell) \ni p \neq \ell \rangle}} |\chi_{\alpha_{p^\sigma},\beta}(t)\rangle
\]

(2.56b)

\[
= - \sum_{\ell \in \mathbb{I}_1(m)} (\text{sgn } \ell) A_{\alpha_{\ell_1}}(t) |\Phi_{\alpha_m/\ell,\beta}(t)\rangle.
\]

(2.56c)

This completes the proof of Eq. (2.52a).

The next step is to write down a formula for the action of \( H - i \frac{d}{dt} \) on a product of \( c_\alpha^\dagger(t) \) operators. If \( |X(t)\rangle \) is any time-dependent state and \( m \) is any non-empty list of indices, then
we have:

\[
(H - i \frac{d}{dt}) c_{\alpha m}^\dagger(t)|X(t)\rangle = \sum_{\ell \in I_1(m)} (\hat{\text{sgn}} \ell) c_{\alpha m/\ell}^\dagger(t) A_{\alpha_{\ell_1}}(t)|X(t)\rangle + \sum_{\ell \in I_2(m)} (\hat{\text{sgn}} \ell) c_{\alpha m/\ell}(t) B_{\alpha_{\ell_1} \alpha_{\ell_2}}(t)|X(t)\rangle + c_{\alpha m}^\dagger(t) \left( H - i \frac{d}{dt} \right) |X(t)\rangle. \tag{2.57}
\]

This reduces to the type A formula (2.48) if we set \(B(t) = 0\). We now complete the proof by applying formula (2.57):

\[
(H - i \frac{d}{dt}) |\Psi_{\alpha N, \beta}(t)\rangle = \left( H - i \frac{d}{dt} \right) \sum_{n=0}^{N} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) c_{\beta N/m}^\dagger(t) \Phi_{\alpha m, \beta}(t) \tag{2.58a}
\]

\[
= \sum_{n=1}^{N-1} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) \sum_{\ell \in I_1(N/m)} (\hat{\text{sgn}} \ell) c_{\alpha N/m/\ell}^\dagger(t) A_{\alpha_{\ell_1}}(t) \Phi_{\alpha m, \beta}(t) \\
+ \sum_{n=0}^{N-2} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) \sum_{\ell \in I_2(N/m)} (\hat{\text{sgn}} \ell) c_{\alpha N/m/\ell}^\dagger(t) B_{\alpha_{\ell_1} \alpha_{\ell_2}}(t) \Phi_{\alpha m, \beta}(t) \\
+ \sum_{n=2}^{N} \sum_{m \in I_n(N)} (\hat{\text{sgn}} m) c_{\alpha N/m}^\dagger(t) \left( H - i \frac{d}{dt} \right) \Phi_{\alpha m, \beta}(t). \tag{2.58b}
\]

Note that in the first term, we dropped the \(n = N\) part of the sum, since it is zero – if all quantum numbers are chosen to be put into \(|\Phi(t)\rangle\), then there are no \(c^\dagger(t)\) operators to commute with and so no \(A(t)\) is generated. We also dropped the \(n = 0\) part because \(A_{\alpha_j}(t)|\Phi_{\beta}(t)\rangle = A_{\alpha_j}(t)|\beta(t)\rangle = 0\) (using the type B condition and the assumption (2.4a) we made regarding the fixed impurity states.) In the second term, we dropped the \(n = N-1\) and \(n = N\) parts of the sum, since there must be at least two \(c^\dagger(t)\) operators in order to produce a \(B(t)\) operator. In the third term we dropped the \(n = 0\) part, since \((H - i \frac{d}{dt}) |\Phi_{\beta}(t)\rangle = (H - i \frac{d}{dt}) |\beta(t)\rangle = 0\) (using the fixed impurity state assumptions (2.4a)\(\)and\(\) (2.4b)), and the \(n = 1\) part, since \(|\Phi_{\alpha_j, \beta}(t)\rangle = 0\). (We could have dropped the \(|\Phi_{\alpha_j, \beta}(t)\rangle\) contributions to the first two terms of (2.58b), but have left them in to simplify the notation.)

We now relabel the summation variables in the first two terms of (2.58b), in exactly the
same way as in the second paragraph below (2.49b) and in the footnote there, obtaining:

\[
\text{first term of (2.58b)} = \sum_{n=1}^{N-1} \sum_{m \in \mathcal{I}_{n+1}(N)} (\text{sgn } m) \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn } \ell) c_{\alpha N/m/\ell}^\dagger(t) A_{\alpha_{\ell_1}}(t) |\Phi_{\alpha_{m/\ell},\beta}(t)\rangle
\]

\[
= \sum_{n=2}^{N} \sum_{m \in \mathcal{I}_n(N)} (\text{sgn } m) c_{\alpha N/m}^\dagger(t) \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn } \ell) A_{\alpha_{\ell_1}}(t) |\Phi_{\alpha_{m/\ell},\beta}(t)\rangle \quad (2.59)
\]

and:

\[
\text{second term of (2.58b)} = \sum_{n=0}^{N-2} \sum_{m \in \mathcal{I}_{n+2}(N)} (\text{sgn } m) \sum_{\ell \in \mathcal{I}_2(m)} (\text{sgn } \ell) c_{\alpha N/m}^\dagger(t) B_{\alpha_{\ell_1} \alpha_{\ell_2}}(t) |\Phi_{\alpha_{m/\ell},\beta}(t)\rangle \quad (2.60a)
\]

\[
= \sum_{n=2}^{N} \sum_{m \in \mathcal{I}_n(N)} (\text{sgn } m) c_{\alpha N/m}^\dagger(t) \sum_{\ell \in \mathcal{I}_2(m)} (\text{sgn } \ell) B_{\alpha_{\ell_1} \alpha_{\ell_2}}(t) |\Phi_{\alpha_{m/\ell},\beta}(t)\rangle. \quad (2.60b)
\]

It is then clear from the $|\Phi(t)\rangle$ condition (2.52a) that the first two terms of (2.58b) exactly cancel the third. This completes the proof.

### 2.3 N-particle expectation values

#### 2.3.1 Overview

In order to make use of the many-body wavefunction, we must find a way to calculate something physical. In this section, we develop the necessary formalism for calculating overlaps and expectation values.

Since the many-body wavefunction $|\Psi(t)\rangle$ is a sum over all subsets of the initial quantum numbers, an expectation value $\langle\Psi(t)|\mathcal{O}|\Psi(t)\rangle$ is a double sum over subsets. The main message of this section is that this double sum actually diagonalizes to a single sum (over subsets). The main tool in the calculation is Wick’s Theorem. While the proof is somewhat technical, the overall picture is simple: bringing all the $c^\dagger(t)$ operators to the left of all the $c(t)$ operators generates contractions which are in this case Kronecker deltas, and these diagonalize the double sum over subsets.

We begin the section by presenting a general formula that equates an expectation value in a single state $|\Psi(t)\rangle$ to some derivatives of the overlap $\langle\Psi(t)|\bar{\Psi}(t)\rangle$, where the barred
state evolves via a Hamiltonian with a varying parameter (the notation is explained below). Wick’s Theorem is again useful in diagonalizing the double sum over subsets that appears in such overlaps, as we will show explicitly.

### 2.3.2 Derivative formula

A standard trick for calculating correlation functions is to calculate some overlap (typically the vacuum-to-vacuum transition amplitude) in the presence of a source term (e.g., $e^{i \int dx \, J(x)\phi(x)}$) and then differentiate with respect to the source $\left( \frac{\delta}{\delta J(x)} \right)$. Usually this is done in the Lagrangian formalism. In this section, we state and prove a version of this trick in the Hamiltonian formalism. We will see that the calculation of an expectation value (as a function of time, following a quench) reduces to differentiating the overlap of two states that evolve in time by Hamiltonians with different values of one or more parameters. This motivates the considerations of the following section, in which we develop a formula for such overlaps.

We now state the simplest form of the result. Consider a family of Hamiltonians depending on a real parameter $\lambda$ in the following way:

$$H_\lambda = H_{\text{ref}} + \lambda O,$$

(2.61)

where $H_{\text{ref}}$ is some “reference” Hamiltonian and $O$ is an operator representing an observable we are interested in. Suppose that the physical Hamiltonian of interest is $H_{\lambda_0} = H_{\text{ref}} + \lambda_0 O$, and that we want to calculate the expectation value of $O$ as a function of time given an initial state $|\psi\rangle$. We will show the following result:

$$\langle \psi | e^{i H_{\lambda_0} t} O e^{-i H_{\lambda_0} t} | \psi \rangle = i \frac{\partial}{\partial \lambda} \bigg|_{\lambda=\lambda_0} \frac{\partial}{\partial t} \langle \psi | e^{i H_{\lambda_0} t} e^{-i H_{\lambda} t} | \psi_{\lambda} \rangle. \quad (2.62a)$$

Here, $|\psi_{\lambda}\rangle$ can be any family of states that satisfies $|\psi_{\lambda_0}\rangle = |\psi\rangle$ and depends “reasonably smoothly” on $\lambda$ near $\lambda = \lambda_0$. (We make the smoothness requirement more precise in the next paragraph.) To derive this result, we first do the time derivative on the right-hand
right-hand side of (2.62a), yielding:
\[
\text{right-hand side of (2.62a)} = \frac{\partial}{\partial \lambda} \bigg|_{\lambda=\lambda_0} \langle \Psi | e^{iH_{\lambda_0}t} (H_\lambda - H_{\lambda_0}) e^{-iH_{\lambda_0}t} | \Psi \rangle = \frac{\partial}{\partial \lambda} \bigg|_{\lambda=\lambda_0} (\lambda - \lambda_0) \langle \Psi | e^{iH_{\lambda_0}t} O e^{-iH_{\lambda_0}t} | \Psi \rangle. \tag{2.63b}
\]

The result (2.62a) then follows immediately if we grant that \( \frac{\partial}{\partial \lambda} \langle \Psi | e^{iH_{\lambda_0}t} O e^{-iH_{\lambda_0}t} | \Psi \rangle \) does not diverge as \( \lambda \to \lambda_0 \); we take this as the definition of the requirement that \( | \Psi_\lambda \rangle \) is “reasonably smooth” near \( \lambda = \lambda_0 \).\(^3\)

While this simple formula suffices for some observables, for others (including the electric current in the Kondo model), we need a more general version. Consider again a family of Hamiltonians:
\[
H_\lambda = H_{\text{ref}} + \sum_{j=1}^n f_j(\lambda) O_j. \tag{2.64}
\]

With a very similar calculation, we obtain a generalization of Eq. (2.62a):
\[
\langle \Psi | e^{iH_{\lambda_0}t} \left( \sum_{j=1}^n f_j(\lambda_0) O_j \right) e^{-iH_{\lambda_0}t} | \Psi \rangle = i \frac{\partial}{\partial \lambda} \bigg|_{\lambda=\lambda_0} \frac{\partial}{\partial t} \langle \Psi | e^{iH_{\lambda_0}t} e^{-iH_{\lambda_0}t} | \Psi \rangle. \tag{2.65a}
\]

In order for this formula to be useful, we have to be able to bring the observable we are interested in to the form \( \sum_{j=1}^n f_j(\lambda_0) O_j \). We will see that this is true for the current with \( n = 2 \).

We also note that in order to apply the derivative formula beyond perturbation theory, we have to be able to solve the quench problem for the Hamiltonian \( H_\lambda \). One might expect that even if \( H_{\text{ref}} \) is solvable, the addition of the \( \lambda \)-dependent terms will spoil this; however, we will see that at least in the case of the current operator, there is essentially no increase in difficulty. In the case of the magnetization, the difficulty increases but the model is still solvable.

Let us introduce a convenient shorthand notation that we will use whenever we do a calculation via the derivative formula. The varying real parameter \( \lambda \) will instead be called \( \bar{\lambda} \) (where the bar is just a label and does not signify complex conjugation), and the physical

\(^3\)In fact, the result holds even if \( \langle \Psi | e^{iH_{\lambda_0}t} O e^{-iH_{\lambda_0}t} | \Psi \rangle \) diverges like \( \left( \frac{1}{\lambda - \lambda_0} \right)^a \) with \( a < 1 \).
value of interest $\lambda_0$ will be called $\lambda$. A bar over any quantity indicates that it is evaluated using the variable $\lambda$, and “removing the bar” corresponds to setting $\lambda = \lambda_0$. Thus, the simple form (2.62a) becomes:

$$\langle \Psi(t) | \mathcal{O} | \Psi(t) \rangle = i \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda_0} \frac{\partial}{\partial t} \langle \Psi(t) | \overline{\Psi}(t) \rangle,$$

where:

$$| \overline{\Psi}(t) \rangle = e^{-i\mathcal{H}t} | \overline{\Psi} \rangle, \quad | \Psi(t) \rangle = e^{-iHt} | \Psi \rangle.$$  (2.67)

This second equation in the line above is actually redundant, since it is a special case of the first – one just removes the bar. Also, the condition that the family of states $| \overline{\Psi} \rangle$ reduces to the original state $| \Psi \rangle$ when we set $\lambda = \lambda_0$ is built into the notation – again, it follows by removing the bar. The more general formula (2.65a) becomes:

$$\langle \Psi(t) | \left( \sum_{j=1}^{n} f_j^{(\lambda)} \mathcal{O}_j \right) | \Psi(t) \rangle = i \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda_0} \frac{\partial}{\partial t} \langle \Psi(t) | \overline{\Psi}(t) \rangle.$$  (2.68)

For the quench problems we are interested in, the initial state with quantum numbers $\alpha_1, \ldots, \alpha_N$ and $\beta$ takes the form:

$$| \Psi_{\alpha N, \beta} \rangle \equiv c_{\alpha N}^\dagger | \beta \rangle \quad (N \equiv (1, \ldots, N)).$$  (2.69)

We assume that $\overline{H}$ and $H$ have the same Hilbert space. We also assume that $\overline{H}$ satisfies the same requirements as $H$ – namely, the degrees of freedom of $\overline{H}$ are described by operators $\overline{c}_\alpha^\dagger$ and fixed impurity states $| \beta \rangle$, and $\overline{H} = \overline{H}^{(0)} + \overline{H}^{(1)}$, where time evolution by $\overline{H}^{(0)}$ sends fixed impurity states to fixed impurity states and $\overline{H}^{(1)}$ annihilates any fixed impurity state. Then we can write a one-parameter family of initial states generalizing $| \Psi_{\alpha N, \beta} \rangle$, namely:

$$| \overline{\Psi}_{\alpha N, \beta} \rangle = \overline{c}_{\alpha N}^\dagger | \beta \rangle.$$  (2.70)

The time-evolving state has the same form as the time evolution of $| \Psi_{\alpha N, \beta} \rangle$ under $H$, but with a bar over everything:

$$| \overline{\Psi}_{\alpha N, \beta}(t) \rangle \equiv e^{-i\overline{H}t} | \overline{\Psi}_{\alpha N, \beta} \rangle$$  (2.71a)

$$= \sum_{n=0}^{N} \sum_{m \in I_n(N)} (\text{sgn } m) \overline{c}_{\alpha N/m}^\dagger(t) | \overline{\Psi}_{\alpha m, \beta}(t) \rangle.$$  (2.71b)
In applications of the derivative formula, we find that there is some freedom in the definition of the $c^\dagger$ operators (even after $\overline{H}$ has been chosen so that a particular observable can be obtained by differentiation). A judicious definition of the operators can make the calculation easier. We find that the derivative approach is usually more efficient than the direct approach, but not always. Even when the direct approach is less efficient, it is still useful as a check.

### 2.3.3 Main results for overlaps and matrix elements

Let $O_{\text{imp}}$ be a “fixed impurity operator,” by which we mean that it commutes with any field operator (and hence can act non-trivially only on fixed impurity states):

\[
[O_{\text{imp}}, c^\dagger_\alpha] = [c^\dagger_\alpha', O_{\text{imp}}] = 0 \quad \text{for any } \alpha, \alpha'
\]  

(2.72)

(In the Kondo model, the fixed impurity operators are the impurity spin operators $S^j$ and the identity; in the Anderson model, the only fixed impurity operator is the identity.) Let $O^\dagger_1$ and $O^\dagger_2$ be linear combinations of field operators $c^\dagger_\alpha$. The precise form is unimportant for now; we only make use of the anticommutation properties and the fact that each $O_j$ annihilates any fixed impurity state:\footnote{Strictly speaking, these properties only follow from $O^\dagger_j$ being a linear combination of field operators once we specify that $\{c^\dagger_{\alpha_1}, c^\dagger_{\alpha_2}\} = 0$ and that $\{c^\dagger_\alpha', c^\dagger_\alpha\}$ is always a complex number – properties that are true for every model considered in this thesis, but which were not needed when setting up the general method of finding the wavefunction.}

\[
\{O^\dagger_j, c^\dagger_\alpha\} = 0 \quad \text{for any } \alpha,
\]

(2.73a)

\[
\{c^\dagger_\alpha', O^\dagger_j\} \text{ is a complex number for any } \alpha', \quad O_j|\beta\rangle = 0.
\]

(2.73b)

The expectation value of a fixed impurity operator (at some time $t$ following the quench) is one quantity we study. We also consider the overlap between states evolving with different Hamiltonians – the right-hand side of equation (2.66) – since this allows to access various observables. Finally, we consider the expectation value of $O^\dagger_1 O^\dagger_2 O_{\text{imp}}$, which is a sufficiently general form to encompass the current operator in the Kondo model and in the Anderson model.
Ultimately, we are interested in these quantities for a particular choice of the initial quantum numbers $\alpha_N$ — namely, the quantum numbers that describe filled Fermi seas. One might think that the most efficient approach would be to fix $\alpha_N$ to be the desired values from the beginning. However, it turns out that we need to understand the case of arbitrary quantum numbers because the calculation involving $|\Psi_{\alpha_N,\beta}(t)\rangle$ becomes a sum over (normal ordered) expectation values in the state $|\Psi_{\alpha_m,\beta}(t)i\rangle \equiv e^{-i\mathcal{H}t}c_{\alpha_m}^{\dagger}|\beta\rangle$, with the quantum numbers $\alpha_m$ summed over all possible subsets of the original quantum numbers.

We will make this statement precise after we define the notion of normal ordering and specify the normalizations of the field operators and fixed impurity states.

We declare that the normal ordering symbol $: (\text{anything}) :$ moves all field creation operators $c_i^{\dagger}$ (with or without the bar) to the left of all field annihilation operators $c_{\alpha'}$, with the usual fermion sign factor. (This corresponds to normal ordering relative to the bare fixed impurity states, rather than the more commonly used notion of normal ordering relative to the filled Fermi sea state.) The operators $\mathcal{O}_1^{\dagger}$ and $\mathcal{O}_2$ are treated the same way as $c_i^{\dagger}$ and $c_i$. Our convention is that the normal ordering symbol has no effect at all on the crossing states ($|\mathcal{F}(t)\rangle$, with or without the bar and in either bra or ket position), even though such states are themselves linear combinations of field operators. Here are some examples:

- $: (\Phi_{\alpha_1',\alpha_2',\alpha_3',\beta'}(t)|\mathcal{O}_2c_3^{\dagger}(t)|\Phi_{\alpha_2\alpha_4\alpha_5}(t)) : = -(\Phi_{\alpha_1',\alpha_2',\alpha_3',\beta'}(t)|c_3^{\dagger}(t)\mathcal{O}_2|\Phi_{\alpha_2\alpha_4\alpha_5}(t))$

- $: (\Phi_{\alpha_1',\alpha_2',\beta'}(t)|c_{\alpha_1'}(t)c_3^{\dagger}(t)|\Phi_{\alpha_6,\beta}(t)) : = (\Phi_{\alpha_1',\alpha_2',\beta'}(t)|c_3^{\dagger}(t)\mathcal{F}_{\alpha_6,\beta}(t))$

The fixed impurity states and field operators are assumed to be unit normalized:

$$\langle \beta | \beta \rangle = \delta_{\beta \beta'}, \quad \text{(2.74a)}$$

$$\{ c_{\alpha'}, c_{\alpha}^{\dagger} \} = \delta_{\alpha \alpha'}. \quad \text{(2.74b)}$$

The main results we will use in subsequent chapters for calculating observables are the following:
Normal ordered formula 1 (The normal ordered overlap of any two states vanishes unless they are both fixed impurity states).

\[
: \langle \Psi_{\alpha_N^\prime,\beta^\prime}(t) | \Psi_{\alpha_N,\beta}(t) \rangle : = \begin{cases} 
0 & \text{N is non-empty} \\
\delta_{\beta^\prime} & \text{N is the empty list}
\end{cases} \quad (2.75)
\]

Note that the quantum numbers on either side are arbitrary. This generality will be useful even for calculations of expectation values, as we will see later.

The next three results are concerned with the case of having the same quantum numbers on each side. We use the notation \( \mathbf{m} = (m_1, \ldots, m_n) \) when \( \mathbf{m} \) appears inside a sum over \( m_1, \ldots, m_n \).

Normal ordered formula 2 (Expectation value of a fixed impurity operator).

\[
\langle \Psi_{\alpha_N,\beta}(t) | \mathcal{O}_{\text{imp}} | \Psi_{\alpha_N,\beta}(t) \rangle = \langle \beta(t) | \mathcal{O}_{\text{imp}} | \beta(t) \rangle + \sum_{n=1}^{N} \frac{1}{n!} \sum_{m_1, \ldots, m_n = 1}^{N} \langle \Psi_{\alpha_{m_1},\beta}(t) | \mathcal{O}_{\text{imp}} | \Psi_{\alpha_{m_1},\beta}(t) \rangle : \quad (2.76)
\]

Normal ordered formula 3 (Expectation value of a generic operator in derivative form).

\[
i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda} \langle \Psi_{\alpha_N,\beta}(t) | \overline{\Psi}_{\alpha_N,\beta}(t) \rangle = i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda} \left( \langle \beta(t) | \overline{\beta}(t) \rangle \right) + \sum_{m=1}^{N} \langle \beta(t) | \overline{\beta}(t) \rangle : + \sum_{n=1}^{N} \frac{1}{n!} \sum_{m_1, \ldots, m_n = 1}^{N} \langle \Psi_{\alpha_{m_1},\beta}(t) | \overline{\Psi}_{\alpha_{m_1},\beta}(t) \rangle : \quad (2.77)
\]

Normal ordered formula 4 (Expectation value of a fixed impurity operator with bilinear).

\[
\langle \Psi_{\alpha_N,\beta}(t) | \mathcal{O}_{\mathbf{1}}^\dagger \mathcal{O}_{\mathbf{2}} \mathcal{O}_{\text{imp}} | \Psi_{\alpha_N,\beta}(t) \rangle = \sum_{n=1}^{N} \sum_{m_1, \ldots, m_n = 1}^{N} \left( \frac{1}{n!} : \langle \Psi_{\alpha_{m_1},\beta}(t) | \mathcal{O}_{\mathbf{1}}^\dagger \mathcal{O}_{\mathbf{2}} \mathcal{O}_{\text{imp}} | \Psi_{\alpha_{m_1},\beta}(t) \rangle : \right.
\]
\[
+ \frac{1}{(n-1)!} \{ \mathcal{O}_{\mathbf{2}}, c_{\alpha_{m_1}}^\dagger (t) \} : \langle \Psi_{\alpha_{m_1},\beta}(t) | \mathcal{O}_{\mathbf{1}}^\dagger \mathcal{O}_{\text{imp}} | \Psi_{\alpha_{m_1},\beta}(t) \rangle : 
\]
\[
+ \frac{1}{(n-1)!} \{ c_{\alpha_{m_1}} (t), \mathcal{O}_{\mathbf{1}}^\dagger \} : \langle \Psi_{\alpha_{m_1},\beta}(t) | \mathcal{O}_{\mathbf{2}} \mathcal{O}_{\text{imp}} | \Psi_{\alpha_{m_1},\beta}(t) \rangle : 
\]
\[
+ \frac{1}{(n-1)!} \sum_{\mathbf{\ell} \in \mathcal{L}(\mathbf{m})} (\text{sgn} \mathbf{\ell}) \{ c_{\alpha_{m_1}} (t), \mathcal{O}_{\mathbf{1}}^\dagger \} \{ \mathcal{O}_{\mathbf{2}}, c_{\alpha_{\mathbf{1}(\mathbf{1})}}^\dagger (t) \} : \langle \Psi_{\alpha_{m_1},\beta}(t) | \mathcal{O}_{\text{imp}} | \Psi_{\alpha_{m_1},\beta}(t) \rangle : \quad (2.78)
\]
In each case, we assume that the initial quantum numbers $\alpha_N$ are all distinct (no repeats); note that any repeat would imply that the initial state vanishes.

Another identity we use in later chapters is that the normal ordered inner product between two states of arbitrary quantum numbers is zero:

$$\langle \Psi_{\alpha'_{\beta'}, \beta'}(t) | \Psi_{\alpha_N, \beta}(t) \rangle : = 0 \quad (\text{non-empty } N).$$  \hfill (2.79)$$

The restriction to non-empty sequences $N$ is necessary because for empty $N$, the normal ordered overlap is:

$$\langle \beta(t) | \beta(t) \rangle = \delta_{\beta \beta'}.$$

The derivation of these results takes several steps. First, we demonstrate some symmetry properties of normal ordered overlaps and matrix elements. We review Wick’s Theorem and write it in our notation. Then we prove a useful lemma for rearranging sums. With Wick’s Theorem and the lemma, we derive two “off-diagonal” identities – that is, identities for matrix elements in which the quantum numbers on either side could be different. We use these identities and the symmetry properties to find the three final results given above, as well as the identity (2.79).

### 2.3.4 Symmetry properties of normal ordered overlaps and matrix elements

The field operators appearing in the initial state $\hat{c}_{\alpha_N}^\dagger |\beta\rangle$ can be written in any order, as long as one accounts for the fermionic sign factor associated with each interchange of two operators. By linearity, the time-evolving states have the same fermionic symmetry:

$$|\Psi_{\alpha \sigma \beta}(t)\rangle = (\text{sgn } \sigma) |\Psi_{\alpha \beta}(t)\rangle \quad [\sigma \in \text{Sym}(n)].$$  \hfill (2.80)$$

This symmetry property is inherited by matrix elements in an obvious way – for instance, the matrix elements of a fixed impurity operator between two time-evolving states satisfies:

$$\langle \Psi_{\alpha'_{\sigma'} \alpha \beta}(t) | O_{\text{imp}} | \Psi_{\alpha \sigma \beta}(t) \rangle = (\text{sgn } \sigma) (\text{sgn } \sigma') \langle \Psi_{\alpha'_{\sigma'} \alpha \beta}(t) | O_{\text{imp}} | \Psi_{\alpha \beta}(t) \rangle \quad [\sigma, \sigma' \in \text{Sym}(n)].$$  \hfill (2.81)$$
A useful fact, which we will demonstrate below, is that the same symmetry properties hold also for overlaps and matrix elements that are normal ordered. For instance, the above equation also holds if both sides are normal ordered:

\[
\langle \Psi_{\sigma' \sigma n, \beta'(t)} | O_{\text{imp}} | \Psi_{\sigma \sigma n, \beta(t)} \rangle : = (\text{sgn } \sigma)(\text{sgn } \sigma') \langle \Psi_{\sigma' \sigma n, \beta'(t)} | O_{\text{imp}} | \Psi_{\alpha n, \beta(t)} \rangle :
\]

\[
[\sigma, \sigma' \in \text{Sym}(n)]. \quad (2.82)
\]

This is not as trivial as it may seem; normal ordering is a notation, not an operation that one can safely apply to both sides of an equation. For example, normal ordering both sides of the equation \( cc^\dagger + c^\dagger c = 1 \) yields \( 0 = 1 \); evidently, replacing operators by numbers using anticommutation relations does not commute with normal ordering. What we must show, then, is that converting the state \( | \Psi_{\sigma \sigma n, \beta(t)} \rangle \) to the state \( (\text{sgn } \sigma)| \Psi_{\alpha n, \beta(t)} \rangle \) commutes with normal ordering. This is true because of two facts: first, normal ordering has no effect on crossing states; and second, rearranging creation operators into different order (with the appropriate fermionic sign factor) commutes with normal ordering.

At the risk of belaboring what may be an obvious point, let us consider the case of \( N = 2 \), with \( \sigma \) being the permutation that exchanges \( 1 \leftrightarrow 2 \). We compare:

\[
| \Psi_{\alpha 2 \alpha 1, \beta(t)} \rangle = c_{\alpha 1}^\dagger (t)c_{\alpha 2}^\dagger (t)| \Phi_{\alpha, \beta}(t) \rangle + c_{\alpha 1}^\dagger (t)| \Phi_{\alpha 2, \beta}(t) \rangle - c_{\alpha 2}^\dagger (t)| \Phi_{\alpha 1, \beta}(t) \rangle + | \Phi_{\alpha 2 \alpha 1, \beta}(t) \rangle \quad (2.83)
\]

with:

\[
- | \Psi_{\alpha 1 \alpha 2, \beta}(t) \rangle = - \left[ c_{\alpha 2}^\dagger (t)c_{\alpha 1}^\dagger (t)| \Phi_{\alpha, \beta}(t) \rangle + c_{\alpha 1}^\dagger (t)| \Phi_{\alpha 2, \beta}(t) \rangle - c_{\alpha 2}^\dagger (t)| \Phi_{\alpha 1, \beta}(t) \rangle \right]
\]

\[
+ | \Phi_{\alpha 1 \alpha 2, \beta}(t) \rangle. \quad (2.84)
\]

Crossing states are totally antisymmetric by construction, so \( -| \Phi_{\alpha 1 \alpha 2, \beta}(t) \rangle = | \Phi_{\alpha 2 \alpha 1, \beta}(t) \rangle \).

Making this replacement commutes with normal ordering, since normal ordering ignores the crossing states completely. Rearranging \( -c_{\alpha 2}^\dagger (t)c_{\alpha 1}^\dagger (t) \) to \( c_{\alpha 2}^\dagger (t)c_{\alpha 1}^\dagger (t) \) to also commutes with normal ordering, due to the fact that normal ordering keeps account of all the sign factors from exchanging fermionic operators.
It is not difficult to present the same argument for general $N$. The $N$-particle wavefunction starting from rearranged quantum numbers is:

$$|\Psi_{\alpha N, \beta}(t)\rangle = \sum_{n=0}^{N} \sum_{m \in \mathbb{N}} (\text{sgn } m) c_{\alpha N/N \gamma}^{\dagger}(t) |\Phi_{\alpha N, \gamma}(t)\rangle. \quad (2.85)$$

For any fixed $m \in \mathcal{I}_n(N)$, we rearrange the creation operators to $c_{\alpha N/m}^{\dagger}(t)$ and the crossing state to $|\Phi_{\alpha m, \beta}(t)\rangle$, with a fermionic sign factor in each case. As discussed above, these rearrangements commute with normal ordering. The product of the two sign factors is equal to $\text{sgn } \sigma$, and so we obtain exactly $(\text{sgn } \sigma)|\Psi_{\alpha N, \beta}(t)\rangle$ – with the quantum numbers in the original order – using only manipulations that commute with normal ordering.

The above arguments all carry through if instead of considering a wavefunction, we consider a normal ordered matrix element, as in Eq. (2.82); the fixed impurity operator is unaffected by normal ordering. The same arguments carry through even if there are field operator insertions (such as $\hat{O}_1^\dagger \hat{O}_2$); in particular, we have:

$$: \langle \Psi_{\alpha' \alpha \gamma}^{\sigma'} \beta'(t) | \hat{O}_1^\dagger \hat{O}_2 \hat{O}_{\text{imp}} | \Psi_{\alpha \gamma}^{\sigma \beta}(t) \rangle : = (\text{sgn } \sigma)(\text{sgn } \sigma') : \langle \Psi_{\alpha' \alpha \gamma}^{\sigma'} \beta'(t) | \hat{O}_1^\dagger \hat{O}_2 \hat{O}_{\text{imp}} | \Psi_{\alpha \gamma}^{\sigma \beta}(t) \rangle : \quad [\sigma, \sigma' \in \text{Sym}(n)]. \quad (2.86)$$

and:

$$: \langle \Psi_{\alpha' \alpha(n/n) \gamma}^{\sigma'} \beta'(t) | c_{\alpha' \alpha}^{\dagger}(t) | \Psi_{\alpha \gamma}^{\sigma \beta}(t) \rangle : = (\text{sgn } \sigma)(\text{sgn } \sigma') : \langle \Psi_{\alpha' \alpha(n/n) \gamma}^{\sigma'} \beta'(t) | c_{\alpha \alpha}^{\dagger}(t) | \Psi_{\alpha \gamma}^{\sigma \beta}(t) \rangle : \quad [\sigma \in \text{Sym}(n), \sigma' \in \text{Sym}(n-1)]. \quad (2.87)$$

The latter equation will be used in calculating the current.

### 2.3.5 Wick’s Theorem

Recall that in the usual presentation of Wick’s Theorem, the contraction of two time-dependent operators is defined as the difference between the time-ordered product and the normal-ordered product:

$$\phi_1(t_1)\phi_2(t_2) = \mathcal{T} \phi_1(t_1)\phi_2(t_2) - : \phi_1(t_1)\phi_2(t_2) :. \quad (2.88)$$

Wick’s Theorem asserts:
\[
\mathcal{T} \phi_{m_1}(t_{m_1}) \ldots \phi_{m_n}(t_{m_n}) = \sum_{\text{contractions}} :\phi_{m_1}(t_{m_1}) \ldots \phi_{m_n}(t_{m_n}) :. 
\] (2.89)

Most of the operators in the quantities we are interested in are evaluated at the same time \(t\). We therefore redefine contraction, replacing time-ordering by “original-ordering” – that is, the order in which the operators in the original product appear. Then the left-hand side of Wick’s Theorem becomes simply the original product of operators. In a product of the form \(\prod c(t) \prod \bar{c}^\dagger(t)\), all contractions are zero except for:
\[
\bar{c}_{\alpha'}(t) \bar{c}^\dagger_{\alpha}(t) = \{c_{\alpha'}(t), \bar{c}^\dagger_{\alpha}(t)\}. 
\] (2.90)

In deriving the third normal ordered formula (2.78), we encounter products of the same form with the bilinear \(O_1 O_2^\dagger\) inserted. In addition to the contraction (2.90) with the bar removed, there are two more non-zero contractions:
\[
\bar{c}_{\alpha'}(t) O_1^\dagger = \{c_{\alpha'}(t), O_1^\dagger\}, \quad (2.91a) 
\]
\[
O_2 \bar{c}^\dagger_{\alpha}(t) = \{O_2, c^\dagger_{\alpha}(t)\}. \quad (2.91b) 
\]

Note that \(O_1^\dagger O_2 = 0\), since the original order of these operators is the same as the normal order. This reflects the fact that in bringing all annihilation operators to the right, we never need to bring \(O_2\) past \(O_1^\dagger\). Given two index lists \(m\) and \(m'\), Wick’s Theorem yields:
\[
c_{\alpha_{m'}}(t) O_1^\dagger \bar{c}^\dagger_{\alpha_m}(t) = \sum_{\text{contractions}} :c_{\alpha_{m'}}(t) O_1^\dagger \bar{c}^\dagger_{\alpha_m}(t) :. 
\] (2.92a)

\[
c_{\alpha_{m'}}(t) O_1^\dagger O_2 O_1^\dagger \bar{c}^\dagger_{\alpha_m}(t) = \sum_{\text{contractions}} :c_{\alpha_{m'}}(t) O_1^\dagger O_2 O_1^\dagger \bar{c}^\dagger_{\alpha_m}(t) :. 
\] (2.92b)

The fixed impurity operator is purely a spectator. (Formally, since it commutes with any field operator, its contractions are all zero.) For further progress, we need to write these contractions explicitly. The first case is simpler:
\[
c_{\alpha_{m'}}(t) O_1^\dagger \bar{c}^\dagger_{\alpha_m}(t) = \sum_{p=0}^{\min(|m|,|m'|)} \sum_{\ell \in I_p(m)} (\text{sgn } \ell) \sum_{\ell' \in I_q(m')} (\text{sgn } \ell') \times \sum_{\sigma \in \text{Sym}(p)} (\text{sgn } \sigma) \left( \prod_{j=1}^{p} \{c_{\alpha'_{\ell'(\sigma_j)}}(t), \bar{c}^\dagger_{\sigma_j}(t)\} \right) :c_{\alpha_{m'/\ell'}}(t) O_1^\dagger \bar{c}^\dagger_{m'/\ell'}(t) :. 
\] (2.93)
This formula is perhaps best understood by looking at an example. We will temporarily drop the spectator $O_{\text{imp}}$ and use an obvious shorthand notation for the dependence on the $\alpha$ quantum numbers (we will also suppress the time dependence and the bar); then, an example term in the Wick’s Theorem expression for $c_1^* c_2^* c_3^* c_4^* c_1 c_2 c_3 c_4$ is:

$$
: \text{c}_1^* \text{c}_2^* \text{c}_3^* \text{c}_4^* \text{c}_1 \text{c}_2 \text{c}_3 \text{c}_4 : = - \text{c}_2^* \text{c}_1^* \text{c}_3^* \text{c}_2 \text{c}_3 \text{c}_4 \text{c}_1 : = \text{c}_2^* \text{c}_1^* \text{c}_3 \text{c}_2 \text{c}_4 \text{c}_1 : = \\
\{ \text{c}_3^*, \text{c}_2^* \} \{ \text{c}_1^*, \text{c}_3 \} : \text{c}_2^* \text{c}_4^* \text{c}_1^* : . (2.94)
$$

There are two contractions ($p = 2$). In the first step, we bring the indices that will be contracted [$\ell = (2, 3)$ and $\ell' = (1, 3)$] to the middle, introducing a factor of $\text{sgn} ^{\text{c}_3^*} \text{c}_2^* = 1$ and a factor of $\text{sgn} ^{\text{c}_1^*} \text{c}_2 = -1$. We then move the operators around so that contractions only occur between adjacent operators; this can be thought of as rearranging the indices in $\ell'$ by a permutation $\sigma$, which yields a factor of $\text{sgn} \sigma$ (which is $-1$ in this case, since $\sigma$ interchanges $1'$ and $3'$). The final step simply replaces the contractions by anticommutators.

It is convenient for now to leave the uncontracted operators as they are (i.e., we do not explicitly carry out the normal ordering). More generally, we have to sum over the total number $p$ of contractions (which cannot exceed the number of operators of either type, since contractions occur in pairs), and this yields Eq. (2.93).

The second case, with the operators $O_1^\dagger O_2$ inserted, is messier. There are four types of contraction, seeing as each of the inserted operators can either be contracted or not. By
similar reasoning, we find:

\[
c_{\alpha'_{m'/\ell'}}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_m}(t) = \sum_{p=0}^{\min\{\left|\mathbf{m}\right|,\left|\mathbf{m}'\right|\}} \sum_{\ell_1 \in \mathcal{I}_p(\mathbf{m})} \sum_{\ell'_1 \in \mathcal{I}_p(\mathbf{m}')}(\text{sgn} \ell) \sum_{\ell \in \mathcal{I}_p(\mathbf{m})} \sum_{\ell' \in \mathcal{I}_p(\mathbf{m}')} \sum_{\sigma \in \text{Sym}(p)} (\text{sgn} \sigma) \left( \prod_{j=1}^{p} \{c_{\alpha'_{\ell_1}(j)}(t), c_{\alpha_{\ell_1}(j)}(t)\} \right) : c_{\alpha'_{m'/\ell'}}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_m}(t) : \\
+ \sum_{s \in \mathcal{I}_1(\mathbf{m}/\ell)} (\text{sgn} s) \{O_2, c_{\alpha_s(1)}(t)\} : c_{\alpha'_{m'/\ell'}}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_m}(t) :
\]

\[
+ \sum_{s' \in \mathcal{I}_1(\mathbf{m}'/\ell')} (\text{sgn} s') \{c_{\alpha'_{s'(1)}}(t), O_1^{\dagger}\} : c_{\alpha'_{m'/\ell'}}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_m}(t) :
\]

\[
+ \sum_{s \in \mathcal{I}_1(\mathbf{m}/\ell)} (\text{sgn} s) \{O_2, c_{\alpha_s(1)}(t)\} \sum_{s' \in \mathcal{I}_1(\mathbf{m}'/\ell')} (\text{sgn} s') \{c_{\alpha'_{s'(1)}}(t), O_1^{\dagger}\} \times : c_{\alpha'_{m'/\ell'/s'}}(t)O_{\text{imp}} c_{\alpha_m}(t) : .
\]

(2.95)

Note that the sums over \( s \) and \( s' \) may sometimes yield zero. For instance, if \( \ell = \mathbf{m} \), then each sum over \( s \in \mathcal{I}_1(\mathbf{m}/\ell) \) yields zero (there are no lists of length one chosen from the empty list); in this case, every \( c_{\alpha}^{\dagger}(t) \) operator is contracted with a \( c(t) \) operator, which implies that there is no \( c_{\alpha}^{\dagger}(t) \) operator available to contract with \( O_2 \).

### 2.3.6 A lemma for rearranging sums

For any function \( X \), we have:

**Lemma.**

\[
\sum_{n,n'=0}^{N} \sum_{\mathbf{m} \in \mathcal{I}_n(N)} \sum_{\mathbf{m}' \in \mathcal{I}_{n'}(N)} (\text{sgn} \mathbf{m}) \sum_{\min\{N-n,N-n'\}} \sum_{p=0}^{\min\{N-n,N-n'\}} \sum_{\ell \in \mathcal{I}_p(N/\mathbf{m})} \sum_{\ell' \in \mathcal{I}_p(N/\mathbf{m}')}(\text{sgn} \ell) \\
\times \sum_{\ell \in \mathcal{I}_p(N/\mathbf{m})} \sum_{\ell' \in \mathcal{I}_p(N/\mathbf{m}')} (\text{sgn} \ell) X (\mathbf{m}, \mathbf{m}', \ell, \ell') = \\
\sum_{p=0}^{N} \sum_{\ell, \ell' \in \mathcal{I}_p(N)} (\text{sgn} \ell) (\text{sgn} \ell') \sum_{n,n'=0}^{N} \sum_{\mathbf{m} \in \mathcal{I}_n(\ell)} \sum_{\mathbf{m}' \in \mathcal{I}_{n'}(\ell')}(\text{sgn} \mathbf{m}) \sum_{\min\{N-n,N-n'\}} \sum_{p=0}^{\min\{N-n,N-n'\}} \sum_{\ell \in \mathcal{I}_p(\mathbf{m})} \sum_{\ell' \in \mathcal{I}_p(\mathbf{m}')} \sum_{\sigma \in \text{Sym}(p)} (\text{sgn} \sigma) \left( \prod_{j=1}^{p} \{c_{\alpha'_{\ell_1}(j)}(t), c_{\alpha_{\ell_1}(j)}(t)\} \right) : c_{\alpha'_{\ell_1}(j)}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_{\ell_1}(j)}(t) : \\
\times : c_{\alpha'_{\ell_1}(j)}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_m}(t) : \\
\times : c_{\alpha'_{\ell_1}(j)}(t)O_2^\dagger O_{\text{imp}} c_{\alpha_m}(t) : .
\]

(2.96)

The proof is an exercise in rearranging sums and relabelling indices. We start by interchanging the order of summations on the left-hand side. In particular, we want to do the
sums over \( n, n', m, \) and \( m' \) before \( p, \ell, \) and \( \ell' \). The range of the integers \( n, n' \), and \( p \) on the left-hand side is described by the following inequalities:

\[
0 \leq n \leq N, \ 0 \leq n' \leq N, \ 0 \leq p \leq N - \max\{n, n'\},
\]

which are equivalent to:

\[
0 \leq p \leq N, \ 0 \leq n \leq N - p, \ 0 \leq n' \leq N - p.
\]

Hence, we can replace:

\[
\sum_{n,n'=0}^{N} \sum_{p=0}^{N-p} \min \{ N-n, N-n' \} \sum_{p=0}^{N-p} \sum_{n,n'=0}^{N} \equiv \sum_{p=0}^{N} \sum_{n,n'=0}^{N} \sum_{m=0}^{\min \{ N-n, N-n' \}} \sum_{m'=0}^{\min \{ N-n, N-n' \}} \sum_{m,m'=0}^{\min \{ N-n, N-n' \}}.
\]

Rather than first choosing a sequence \( m \) from \( N \) and then choosing a sequence \( \ell \) from the remainder \( N/m \), we can just as well choose \( \ell \) first and then \( m \) from the remainder. Schematically, the two different orders are:

\[
N \rightarrow m \ N/m \rightarrow m \ N/m/\ell \ell \quad \text{original order,} \quad (2.100a)
\]

\[
N \rightarrow N/\ell \ell \rightarrow m \ N/\ell/m \ell \quad \text{new order.} \quad (2.100b)
\]

The sign factors \( \bar{\text{sgn}} m \) and \( \bar{\text{sgn}} \ell \) can differ between the original order and the new order, but the product is the same because it is equal to the sign of the permutation that maps \( N \rightarrow m \ N/m/\ell \ell \). Thus, the sign factors can be left as they are. We can therefore make the replacement:

\[
\sum_{m \in \mathbb{Z}_n(N)} (\bar{\text{sgn}} m) \sum_{\ell \in \mathbb{Z}_{p}(N/m)} (\bar{\text{sgn}} \ell) \rightarrow \sum_{\ell \in \mathbb{Z}_{p}(N)} (\bar{\text{sgn}} \ell) \sum_{m \in \mathbb{Z}_n(N/\ell)} (\bar{\text{sgn}} m).
\]

Doing the same exchange of sums with \( m' \) and \( \ell' \) as well, we obtain:

\[
\text{left-hand side of (2.96) = } \sum_{p=0}^{N} \sum_{n,n'=0}^{N} \sum_{\ell,\ell'=\mathbb{Z}_{p}(N)} (\bar{\text{sgn}} \ell) (\bar{\text{sgn}} \ell') \times \sum_{m \in \mathbb{Z}_n(N/\ell)} (\bar{\text{sgn}} m) \sum_{m' \in \mathbb{Z}_{n'}(N/\ell')} (\bar{\text{sgn}} m') X (m, m', \ell, \ell').
\]
We relabel \( p \to N - p, \ell \to N/\ell, \) and \( \ell' \to N/\ell' \), which flips the sign factors from \( \text{sgn} \ell \) and \( \text{sgn} \ell' \) to \( \text{-sgn} \ell \) and \( \text{-sgn} \ell' \). We thus obtain:

left-hand side of (2.96) = \[ \sum_{p=0}^{N} \sum_{n,n'=0}^{p} \sum_{\ell, \ell' \in I_p(N)} \left( \text{sgn} \ell \right) \left( \text{sgn} \ell' \right) \times \sum_{m \in I_n(\ell)} \left( \text{-sgn} m \right) \sum_{m' \in I_{n'}(\ell')} \left( \text{-sgn} m' \right) X \left( m, m', N/\ell, N/\ell' \right). \] (2.103)

We are then free to do the sums over \( \ell \) and \( \ell' \) before \( n \) and \( n' \), which completes the proof of the lemma.

2.3.7 Off-diagonal identities

We prove two identities involving inner products or matrix elements in which the two states involves each have arbitrary quantum numbers. We refer to these identities as “off-diagonal,” bearing mind that they also hold even in the “diagonal” case (i.e. the same quantum numbers on both sides). We later use the first identity to derive normal ordered formula 1, 2, and 3 [Eq. (2.75), (2.76), (2.77)], and the more complicated second identity to derive normal ordered formula 4 [(2.78)].

**Off-diagonal identity 1** (Fixed impurity operator/derivative form).

\[ \langle \Psi_{\sigma'_{\alpha_{N}}, \beta'}(t) | O_{\text{imp}} | \bar{\Psi}_{\alpha_{N}, \beta}(t) \rangle = \sum_{n=0}^{N} \sum_{m, m' \in I_n(N)} \left( \text{sgn} m \right) \left( \text{sgn} m' \right) \sum_{\sigma \in \text{Sym}(N-n)} \text{sgn} \sigma \times \left( \prod_{j=1}^{N-n} \left\{ c_{\sigma'_{\alpha_{j}/m'}}(t), c_{\sigma_{\alpha_{j}/m}}(t) \right\} \right) : \langle \Psi_{\sigma'_{\alpha_{N}}, \beta'}(t) | O_{\text{imp}} | \bar{\Psi}_{\alpha_{m}, \beta}(t) \rangle : \] (2.104)

Note that in this first identity, we can remove the bar to obtain matrix elements of a fixed impurity operator, or we can set the fixed impurity operator to be the identity to obtain the overlap that is needed for the derivative formula. In case it is not clear, we note here that the \( n = 0 \) term in the sum is \( \left( \prod_{j=1}^{N} \left\{ c_{\sigma'_{\alpha_{j}}}(t), c_{\sigma_{\alpha_{j}}}(t) \right\} \right) : \langle \Psi_{\beta'}(t) | O_{\text{imp}} | \bar{\Psi}_{\beta}(t) \rangle : \)
Off-diagonal identity 2 (Fixed impurity operator with bilinear).

\[
\langle \Psi_{\alpha_{N}, \beta'}(t) | O_1^\dagger O_2 O_{\text{imp}} | \Psi_{\alpha_{N}, \beta}(t) \rangle = \sum_{n=1}^{N} \sum_{m,m' \in \mathcal{I}_n(N)} (\delta_{\text{sign}} m) (\delta_{\text{sign}} m') \sum_{\sigma \in \text{Sym}(N-n)} (\text{sgn} \sigma) 
\times \left( \prod_{j=1}^{N-n} \{c_{\alpha_{(N/m)}}(t), c_{\alpha_{(N/m')}\sigma_j}(t)\} \right) \langle \Psi_{\alpha_{m'}', \beta'}(t) | O_1^\dagger O_2 O_{\text{imp}} | \Psi_{\alpha_{m}, \beta}(t) \rangle 
+ \sum_{\ell \in \mathcal{I}_1(m)} (\delta_{\text{sign}} \ell) \{O_2, c_{\alpha_{(1)} \ell}(t)\} : \langle \Psi_{\alpha_{m'}, \beta'}(t) | O_1^\dagger O_{\text{imp}} | \Psi_{\alpha_{m}, \beta}(t) \rangle 
+ \sum_{\ell' \in \mathcal{I}_1(m')} (\delta_{\text{sign}} \ell') \{c_{\alpha_{(1)} \ell'}(t), O_1^\dagger\} \langle \Psi_{\alpha_{m'}, \beta'}(t) | O_2 O_{\text{imp}} | \Psi_{\alpha_{m}, \beta}(t) \rangle 
\times \langle \Psi_{\alpha_{m'}, \beta'}(t) | O_{\text{imp}} | \Psi_{\alpha_{m}, \beta}(t) \rangle. \tag{2.105}
\]

Proof of Off-diagonal identity 1.

We begin by writing the wavefunctions on the left-hand side of Eq. (2.104) explicitly in terms of field operators and crossing states:

\[
\langle \Psi_{\alpha_{N}, \beta'}(t) | O_{\text{imp}} | \overline{\Psi}_{\alpha_{N}, \beta}(t) \rangle = \sum_{n,m' \in \mathcal{I}_n(N)} (\delta_{\text{sign}} m) (\delta_{\text{sign}} m') \sum_{\sigma \in \text{Sym}(N-n)} (\text{sgn} \sigma) 
\times \langle \Phi_{\alpha_{m'}, \beta'}(t) | c_{\alpha_{(N/m')}\sigma}(t), \overline{\Psi}_{\alpha_{N}, \beta}(t) \rangle. \tag{2.106}
\]

Inserting Wick’s Theorem in the form (2.93) (with \( m \) and \( m' \) replaced by \( N/m \) and \( N/m' \)), we obtain:

\[
\langle \Psi_{\alpha_{N}, \beta'}(t) | O_{\text{imp}} | \overline{\Psi}_{\alpha_{N}, \beta}(t) \rangle = \sum_{n,m' \in \mathcal{I}_n(N)} (\delta_{\text{sign}} m) (\delta_{\text{sign}} m') \sum_{\sigma \in \text{Sym}(N-n)} (\text{sgn} \sigma) 
\times \left( \prod_{j=1}^{N-n} (\delta_{\text{sign}} \ell_j) \{c_{\alpha_{(N/m')}\sigma_j}(t), \overline{\Psi}_{\alpha_{N}, \beta}(t) \} \right) 
\times \langle \Phi_{\alpha_{m'}, \beta'}(t) | c_{\alpha_{(N/m')\ell}(t)}^{\dagger} O_{\text{imp}} \overline{\Psi}_{\alpha_{N}, \beta}(t) \rangle. \tag{2.107}
\]

Normal-ordering, by our convention, does nothing to the crossing states; hence we are free to write the normal ordering symbols outside the inner product. Since \(|N/m| = N - n\) and
\[ |N/m'| = N - n', \] the expression above is of the form of the lemma (2.96), with \( X \) given by:

\[
X(m, m', \ell, \ell') = \sum_{\sigma \in \text{Sym}(p)} (\text{sgn } \sigma) \left( \prod_{j=1}^{p} \{ c_{\alpha'_{(\ell')}(\sigma_j)}(t), \bar{c}^{\dagger}_{\alpha_{(\ell)}(\sigma_j)}(t) \} \right)
\]

\[
\times \langle \Phi_{\alpha'_{m'\ell'},\beta'}(t) | c_{\alpha'_{N/\ell'/m'}}(t) \Omega_{\text{imp}} \bar{c}^{\dagger}_{\alpha_{N/\ell'/m}}(t) | \bar{\Phi}_{\alpha_{m},\beta}(t) \rangle, \quad (2.108)
\]

where \( p = |\ell| \). Using the lemma, we obtain:

\[
\langle \Psi_{\alpha'_{N},\beta'}(t) | \Omega_{\text{imp}} | \bar{\Psi}_{\alpha_{N},\beta}(t) \rangle = \sum_{p=0}^{N} \sum_{\ell, \ell' \in I_p(N)} (\text{sgn } \ell) (\text{sgn } \ell') \left( \prod_{n,n' = 0}^{p} (\text{sgn } m) \right)
\]

\[
\times \sum_{m' \in I_{n'}(\ell')} (\text{sgn } m') \sum_{\sigma \in \text{Sym}(N-p)} (\text{sgn } \sigma) \left( \prod_{j=1}^{N-p} \{ c_{\alpha'_{(\ell')}(\sigma_j)}(t), \bar{c}^{\dagger}_{\alpha_{(\ell)}(\sigma_j)}(t) \} \right)
\]

\[
\times \langle \Phi_{\alpha'_{m'\ell'},\beta'}(t) | c_{\alpha'_{\ell'/m'}}(t) \Omega_{\text{imp}} \bar{c}^{\dagger}_{\alpha_{\ell'/m}}(t) | \bar{\Phi}_{\alpha_{m},\beta}(t) \rangle. \quad (2.109)
\]

The sums over \( n, n', m, \) and \( m' \) then yield:

\[
\langle \Psi_{\alpha'_{N},\beta'}(t) | \Omega_{\text{imp}} | \bar{\Psi}_{\alpha_{N},\beta}(t) \rangle = \sum_{p=0}^{N} \sum_{\ell, \ell' \in I_p(N)} (\text{sgn } \ell) (\text{sgn } \ell') \left( \prod_{\sigma \in \text{Sym}(N-p)} (\text{sgn } \sigma) \right)
\]

\[
\times \left( \prod_{j=1}^{N-p} \{ c_{\alpha'_{(\ell')}(\sigma_j)}(t), \bar{c}^{\dagger}_{\alpha_{(\ell)}(\sigma_j)}(t) \} \right) : \langle \Psi_{\alpha'_{\ell'},\beta'}(t) | \Omega_{\text{imp}} | \bar{\Psi}_{\alpha_{\ell},\beta}(t) \rangle :, \quad (2.110)
\]

which is exactly the identity (2.104) that we set out to prove, just with different labels for some of the summation indices \( (p \leftrightarrow n, \ell \leftrightarrow m, \ell' \leftrightarrow m') \).

**Proof of Off-diagonal identity 2.**

This is similar to the calculation above, though more messy. We again begin by writing the wavefunctions explicitly in terms of field operators and crossing states:

\[
\langle \Psi_{\alpha'_{N},\beta'}(t) | \Omega_{1}^{\dagger} \Omega_{2} \Omega_{\text{imp}} | \Psi_{\alpha_{N},\beta}(t) \rangle = \sum_{n,n'=0}^{N} \sum_{m \in I_{n}(N)} (\text{sgn } m) \sum_{m' \in I_{n'}(N)} (\text{sgn } m')
\]

\[
\times \langle \Phi_{\alpha'_{m'\ell'},\beta'}(t) | c_{\alpha'_{N/m'}}(t) \Omega_{1}^{\dagger} \Omega_{2} \Omega_{\text{imp}} \bar{c}^{\dagger}_{\alpha_{N/m}}(t) | \Phi_{\alpha_{m},\beta}(t) \rangle. \quad (2.111)
\]
Inserting Wick’s Theorem in the form (2.95) (with \( \mathbf{m} \) and \( \mathbf{m}' \) replaced by \( \mathbf{N}/\mathbf{m} \) and \( \mathbf{N}/\mathbf{m}' \)), we obtain:

\[
\langle \Psi_{\alpha_{\mathbf{n}},\beta}(t) | \mathcal{O}_1 | \mathcal{O}_2 \mathcal{O}_{\text{imp}} | \Psi_{\alpha_{\mathbf{N}},\beta}(t) \rangle = \sum_{n,n'=0}^{N} \sum_{\mathbf{m} \in \mathcal{I}_n(\mathbf{N})} \sum_{\mathbf{m}' \in \mathcal{I}_{n'}(\mathbf{N})} \langle \mathbf{m} | \mathbf{m}' \rangle \sum_{p=0}^{\min\{|\mathbf{N}/\mathbf{m}|,|\mathbf{N}/\mathbf{m}'|\}}
\]

\[
\times \sum_{\ell \in \mathcal{I}_p(\mathbf{N}/\mathbf{m})} \langle \mathbf{m} | \mathbf{m}' \rangle \sum_{\ell' \in \mathcal{I}_p(\mathbf{N}/\mathbf{m}')} \langle \mathbf{m}' | \mathbf{m} \rangle \sum_{\sigma \in \text{Sym}(p)} \langle \mathbf{m} | \mathbf{m}' \rangle \langle \mathbf{m}' | \mathbf{m} \rangle (\mathbf{m} | \mathbf{m}' \rangle \langle \mathbf{m}' | \mathbf{m} \rangle)
\]

\[
\times (\Phi_{\alpha_{\mathbf{m}},\beta}(t))(c_{\alpha_{\mathbf{m}},\beta}(t)) \mathcal{O}_1 | \mathcal{O}_2 \mathcal{O}_{\text{imp}} c_{\alpha_{\mathbf{N}},\beta}(t) \rangle.
\]

Since \( |\mathbf{N}/\mathbf{m}| = N - n \) and \( |\mathbf{N}/\mathbf{m}'| = N - n' \), the expression above is of the form of the lemma (2.96), with \( X \) given by:

\[
X(\mathbf{m}, \mathbf{m}', \ell, \ell') = \sum_{\sigma \in \text{Sym}(p)} \langle \mathbf{m} | \mathbf{m}' \rangle \langle \mathbf{m}' | \mathbf{m} \rangle \langle \mathbf{m} | \mathbf{m}' \rangle \langle \mathbf{m}' | \mathbf{m} \rangle (\mathbf{m} | \mathbf{m}' \rangle \langle \mathbf{m}' | \mathbf{m} \rangle)
\]

\[
\times (\Phi_{\alpha_{\mathbf{m}},\beta}(t))(c_{\alpha_{\mathbf{m}},\beta}(t)) \mathcal{O}_1 | \mathcal{O}_2 \mathcal{O}_{\text{imp}} c_{\alpha_{\mathbf{N}},\beta}(t) \rangle.
\]

(2.112)

(2.113)
where \( p = |\ell| \). Using the lemma, we obtain:

\[
\langle \Psi_{\alpha(N, \beta)} | O_1^\dagger O_2 O_{\text{imp}} | \Psi_{\alpha(N, \beta)} (t) \rangle = \sum_{p=0}^{N} \sum_{\ell, \ell' \in \mathcal{I}_p(N)} \langle \hat{\text{sgn}} \ell \rangle \langle \hat{\text{sgn}} \ell' \rangle \sum_{n,n'=0}^{p} \langle \hat{\text{sgn}} m \rangle \sum_{m' \in \mathcal{I}_p(\ell')} \langle \hat{\text{sgn}} m' \rangle \sum_{\sigma \in \text{Sym}(N-p)} \langle \text{sgn} \rangle \left( \prod_{j=1}^{N-p} \{ c_{\alpha\beta'_{(\ell')}} (t), c_{\alpha\beta'_{(\ell')}}^\dagger (t) \} \right) \\
\times \langle \Phi_{\beta'_{/m' \beta'}} (t) \rangle \left( c_{\alpha'_{/m' \beta'}} (t) O_1^\dagger O_2 O_{\text{imp}} c_{\alpha'_{/m' \beta'}}^\dagger (t) \right) \\
+ \sum_{s \in \mathcal{I}_1(\ell/m)} \langle \text{sgn} s \rangle \{ O_2, c_{\alpha_{s(1)}^{\dagger}} (t) \} c_{\alpha'_{/m' \beta'}} (t) O_1^\dagger O_{\text{imp}} c_{\alpha'_{/m' \beta'}}^\dagger (t) \\
+ \sum_{s' \in \mathcal{I}_1(\ell'/m')} \langle \text{sgn} s' \rangle \{ c_{\alpha'_{s'(1)}^{\dagger}} (t), O_1^\dagger \} c_{\alpha'_{/m' \beta'}} (t) O_1^\dagger c_{\alpha'_{/m' \beta'}}^\dagger (t) \\
+ \sum_{s \in \mathcal{I}_1(\ell/m)} \langle \text{sgn} s \rangle \{ O_2, c_{\alpha_{s(1)}^{\dagger}} (t) \} \sum_{s' \in \mathcal{I}_1(\ell'/m')} \langle \text{sgn} s' \rangle \{ c_{\alpha'_{s'(1)}^{\dagger}} (t), O_1^\dagger \}
\times c_{\alpha'_{/m' \beta'}} (t) O_{\text{imp}} c_{\alpha'_{/m' \beta'}}^\dagger (t) \langle \Phi_{\alpha_{m, \beta}} (t) \rangle : . \tag{2.114}
\]

As in the proof of the first off-diagonal identity, our goal is to carry out the sums over \( n, n', m, \) and \( m' \). This is straightforward for the first of the four terms in parentheses; for the others, it will take a couple of steps. First, we will bring the \( n, n', m, \) and \( m' \) sums inside the parentheses. Note that the sums over \( s \) and \( s' \) sometimes yield zero. For instance, if \( m = \ell \), then the sum over \( s \in \mathcal{I}_1(\ell/m) \) yields zero (there are no lists of length one chosen from the empty list); such terms correspond to contributions to Wick’s Theorem with the \( O_2 \) operator left uncontracted [see the comment below Eq. (2.95)]. Therefore, we can replace \( \sum_{n=0}^{p} \rightarrow \sum_{n=0}^{p-1} \) whenever there is a sum over \( s \) (seeing as \( n = p \) forces \( m = \ell \)).
Proceeding similarly with the $n'$ sum whenever there is a sum over $s'$, we obtain:

\[
= \sum_{p=0}^{N} \sum_{\ell, \ell' \in \mathcal{I}_p(N)} (\text{sgn } \ell) (\text{sgn } \ell') \sum_{\sigma \in \text{Sym}(N-p)} (\text{sgn } \sigma) \left( \prod_{j=1}^{N-p} \{c_{\alpha'_{(n'/j)}(\sigma_j)}(t), c_{\alpha_{(N-j)/j}}(t)\} \right) \\
\times \left( \sum_{n,n'=0}^{p} \sum_{m \in \mathcal{I}_n(\ell)} (\text{sgn } m) \sum_{m' \in \mathcal{I}_{n'}(\ell')} (\text{sgn } m') : (\Phi_{\alpha_{n'}, \beta'}(t)|c_{\alpha'_{n'/m'}}(t)\mathcal{O}_1^\dagger \mathcal{O}_2 \mathcal{O}_{\text{imp}} c_{c_{\alpha'_{n'/m'}}}(t)|\Phi_{\alpha_{n'}, \beta}(t)) : \right. \\
\left. + \sum_{n=0}^{p-1} \sum_{m \in \mathcal{I}_n(\ell)} (\text{sgn } m) \sum_{m' \in \mathcal{I}_{n'}(\ell')} (\text{sgn } m') \sum_{s \in \mathcal{I}_1(\ell/m)} (\text{sgn } s) \{\mathcal{O}_2, c_{c_{\alpha_{n'/s}}}(t)\} \right) \\
\times : (\Phi_{\alpha_{n'}, \beta'}(t)|c_{\alpha'_{n'/m'}}(t)\mathcal{O}_1^\dagger \mathcal{O}_2 \mathcal{O}_{\text{imp}} c_{c_{\alpha'_{n'/m'}}}(t)|\Phi_{\alpha_{n'}, \beta}(t)) : \\
+ \sum_{n=0}^{p-1} \sum_{m \in \mathcal{I}_n(\ell)} (\text{sgn } m) \sum_{m' \in \mathcal{I}_{n'}(\ell')} (\text{sgn } m') \sum_{s' \in \mathcal{I}_1(\ell')/m'} (\text{sgn } s') \{c_{\alpha_{n'/s'}}(t), \mathcal{O}_1^\dagger\} \\
\times : (\Phi_{\alpha_{n'}, \beta'}(t)|c_{\alpha'_{n'/m'}}(t)\mathcal{O}_2 \mathcal{O}_{\text{imp}} c_{c_{\alpha'_{n'/m'}}}(t)|\Phi_{\alpha_{n'}, \beta}(t)) : \\
+ \sum_{n,n'=0}^{p-1} \sum_{m \in \mathcal{I}_n(\ell)} (\text{sgn } m) \sum_{m' \in \mathcal{I}_{n'}(\ell')} (\text{sgn } m') \sum_{s \in \mathcal{I}_1(\ell/m)} (\text{sgn } s) \{\mathcal{O}_2, c_{c_{\alpha_{n'/s}}}(t)\} \\
\times \sum_{s' \in \mathcal{I}_1(\ell'/m')} (\text{sgn } s') \{c_{\alpha_{n'/s'}}(t), \mathcal{O}_1^\dagger\} : (\Phi_{\alpha_{n'}, \beta'}(t)|c_{\alpha'_{n'/m'}}(t)\mathcal{O}_{\text{imp}} c_{c_{\alpha'_{n'/m'}}}(t)|\Phi_{\alpha_{n'}, \beta}(t)) : \right). \quad (2.115)
\]

As mentioned, the first of the four terms in parentheses is already in the right form for us to do the sums over $n, n', m, \text{ and } m'$. In the remaining terms, we bring the $s$ and $s'$ sums
to the left of the $m$ and $m'$ sums to find:

$$
= \sum_{p=0}^{N} \sum_{\ell, \ell' \in \mathbb{I}_p(N)} \langle \text{sgn } \ell \rangle \langle \text{sgn } \ell' \rangle \sum_{\sigma \in \text{Sym}(N-p)} (\text{sgn } \sigma) \left( \prod_{j=1}^{N-p} \left\{ a'_{(N/\ell') \langle } \sigma(j) \rangle c_{\alpha_{(N/\ell)(j)}} \right\} \right)
\times \left( \langle \Phi_{\alpha_{\ell'}, \beta}(t) \rangle \| O_{1}^{\dagger} O_{2} O_{\text{imp}} | \Psi_{\alpha_{\ell}, \beta}(t) \rangle : \right)
\times \sum_{m \in \mathbb{I}_n(t/s)} \langle \text{sgn } m \rangle \sum_{m' \in \mathbb{I}_{n'}(t')} \langle \text{sgn } m' \rangle
\times \langle \Phi_{\alpha_{m'}, \beta}(t) | c_{\alpha_{m'/m}} \rangle \| O_{1}^{\dagger} O_{\text{imp}} | \alpha_{m} \rangle (t) \rangle : \right).

At last, we can do the remaining sums over $n, n', m$, and $m'$:

$$
= \sum_{p=0}^{N} \sum_{\ell, \ell' \in \mathbb{I}_p(N)} \langle \text{sgn } \ell \rangle \langle \text{sgn } \ell' \rangle \sum_{\sigma \in \text{Sym}(N-p)} (\text{sgn } \sigma) \left( \prod_{j=1}^{N-p} \left\{ a'_{(N/\ell') \langle } \sigma(j) \rangle c_{\alpha_{(N/\ell)(j)}} \right\} \right)
\times \left( \langle \Phi_{\alpha_{\ell'}, \beta}(t) \rangle \| O_{1}^{\dagger} O_{2} O_{\text{imp}} | \Psi_{\alpha_{\ell}, \beta}(t) \rangle : \right)
\times \sum_{m \in \mathbb{I}_n(t/s)} \langle \text{sgn } m \rangle \sum_{m' \in \mathbb{I}_{n'}(t')} \langle \text{sgn } m' \rangle
\times \langle \Phi_{\alpha_{m'}, \beta}(t) | c_{\alpha_{m'/m}} \rangle \| O_{1}^{\dagger} O_{\text{imp}} | \alpha_{m} \rangle (t) \rangle : \right).
$$

Once we show (momentarily) that the $p = 0$ term in the sum vanishes, we will have reached exactly the right-hand side of (2.105), just with different labels for some of the summation indices ($p \leftrightarrow n, \ell \leftrightarrow m, \ell' \leftrightarrow m', s \leftrightarrow \ell, s' \leftrightarrow \ell'$). If we take $p = 0$ in the sum, then $\ell$ and $\ell'$
are both forced to be the empty list; all sums over $s$ or $s'$ then vanish, leaving only a product of anticommutators multiplied by $:\langle \Psi_{s',s}(t)|\mathcal{O}_1^\dagger \mathcal{O}_2 \mathcal{O}_{\text{imp}}|\Psi_{s,s}(t)\rangle: = \langle \beta'(t)|\mathcal{O}_1^\dagger \mathcal{O}_2 \mathcal{O}_{\text{imp}}|\beta(t)\rangle = 0$ (where we recall that $\mathcal{O}_1$ and $\mathcal{O}_2$ annihilate any fixed impurity state $|\beta'\rangle$). This completes the proof.

### 2.3.8 Proof of main results

We use the first off-diagonal identity (2.104) to derive the first three normal ordered formulas – Eqs. (2.75), (2.76), and (2.77) – and the second off-diagonal identity (2.105) to derive the third normal ordered formula (2.78). For the first, the proof is by induction. For the latter three, the derivation proceeds by first specializing to the “diagonal” case (that is, the same quantum numbers on each side) of one of the off-diagonal identities, and then by using the symmetry properties of normal ordered overlaps discussed earlier (see 2.3.4) to replace the sum over increasing indices by an unrestricted sum over indices (that is, requiring the indices to be distinct, but not necessarily in order). The motivation for unrestricted sums will emerge later when we see that these sums become multiple integrals in the thermodynamic limit.

**Proof of Eq. (2.75) (normal ordered formula 1).**

Starting from the first off-diagonal identity, Eq. (2.104), we set $\mathcal{O}_{\text{imp}} = 1$ and remove the bar to find:

$$\langle \Psi_{a',a}(t)|\Psi_{a,a}(t)\rangle = \sum_{n=0}^{N} \sum_{m,m'\in I_n(N)} \left(\text{sgn } m\right) \left(\text{sgn } m'\right) \sum_{\sigma \in \text{Sym}(N-n)} (\text{sgn } \sigma)$$

$$\times \left(\prod_{j=1}^{N-n} \{c_{a'(N/m')}(t), c_{a(N/m)}(t)\}\right) :\langle \Psi_{a',a'}(t)|\Psi_{a,a}(t)\rangle: . \quad (2.118)$$

The $n = 0$ term of the sum is independent of time, and is easily evaluated at $t = 0$; then, the left-hand side is equal to the $n = 0$ term on the right-hand side, since the $c_{a}(t)$ operators
have the same anticommutation relations as the $c_{\frac{1}{2}}$ operators. Taking $N = 1$, we obtain:

$$0 = : \langle \Psi_{\alpha N(1)}, \beta (t) | \Psi_{\alpha N(1)}, \beta (t) \rangle :,$$

(2.119)

which is the first non-trivial case of the claimed Eq. (2.75). Since the $\alpha, \alpha'$ labels are arbitrary, we see that the $n = 1$ contribution on the right-hand side of Eq. (2.118) vanishes for any $N$. Taking $N = 2$ yields:

$$0 = : \langle \Psi_{\alpha N(1)}', \beta (t) | \Psi_{\alpha N(1)}', \beta (t) \rangle :,$$

(2.120)

and so on up to arbitrary $N \geq 1$ by induction. If instead $N = 0$ (i.e. $N$ is the empty list), the result (2.75) is immediate due to the definition $|\Psi, \beta (t) \rangle = |\beta (t) \rangle$. This completes the proof.

**Proof of Eq. (2.76) (normal ordered formula 2).**

Removing the bar in the first off-diagonal identity (2.104) causes the anticommutators to become Kronecker deltas. We set the quantum numbers to be equal ($\alpha'_{\frac{1}{2}} = \alpha_{\frac{1}{2}}, \beta' = \beta$)
and, for clarity, separate the $n = 0$ term from the rest of the sum, yielding:

\[ \langle \Psi_{\alpha_N,\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_N,\beta}(t) \rangle = \sum_{\sigma \in \text{Sym}(N)} \left( \prod_{j=1}^{N} \{ c_{\alpha_{\sigma(j)}}(t), c_{\dagger \alpha_{\sigma(j)}}(t) \} \right) \langle \beta(t) | \mathcal{O}_{\text{Imp}} | \beta(t) \rangle \]

\[ + \sum_{n=1}^{N} \sum_{\mathbf{m}, \mathbf{m}' \in \mathbb{I}_n(N)} \left( \frac{\text{sgn} \mathbf{m}}{\text{sgn} \mathbf{m}'} \right) \sum_{\sigma \in \text{Sym}(N-n)} \left( \prod_{j=1}^{N} \{ c_{\alpha_{(N/m')}(\sigma_j)}(t), c_{\dagger \alpha_{(N/m)(\sigma_j)}(t)} \} \right) : \langle \Psi_{\alpha_{m'},\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_{m},\beta}(t) \rangle : \]

\[ = \sum_{\sigma \in \text{Sym}(N)} \left( \prod_{j=1}^{N} \delta_{\alpha_j \alpha_{\sigma(j)}} \right) \langle \beta(t) | \mathcal{O}_{\text{Imp}} | \beta(t) \rangle \]

\[ + \sum_{n=1}^{N} \sum_{\mathbf{m}, \mathbf{m}' \in \mathbb{I}_n(N)} \left( \frac{\text{sgn} \mathbf{m}}{\text{sgn} \mathbf{m}'} \right) \sum_{\sigma \in \text{Sym}(N-n)} \left( \prod_{j=1}^{N-n} \delta_{\alpha_{(N/m')(\sigma_j)} \alpha_{(N/m)(\sigma_j)}} \right) : \langle \Psi_{\alpha_{m'},\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_{m},\beta}(t) \rangle : \]

\[ (2.121a) \]

The Kronecker deltas force $\sigma = \text{identity}$ and $\mathbf{m}' = \mathbf{m}$ in the sums,\(^5\) so we obtain:

\[ \langle \Psi_{\alpha_N,\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_N,\beta}(t) \rangle = \langle \beta(t) | \mathcal{O}_{\text{Imp}} | \beta(t) \rangle + \sum_{n=1}^{N} \sum_{\mathbf{m} \in \mathbb{I}_n(N)} : \langle \Psi_{\alpha_{m},\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_{m},\beta}(t) \rangle : . \]

\[ (2.122a) \]

To obtain the second normal ordered formula (2.76), we just need to note that the symmetry of the normal ordered matrix element [see Sec. 2.3.4] allows us to replace the restricted sum by the unrestricted sum if we compensate by a factor of $\frac{1}{n!}$:

\[ \sum_{\mathbf{m} \in \mathbb{I}_n(N)} : \langle \Psi_{\alpha_{m},\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_{m},\beta}(t) \rangle : = \frac{1}{n!} \sum_{m_1, \ldots, m_n} : \langle \Psi_{\alpha_{m},\beta}(t) | \mathcal{O}_{\text{Imp}} | \Psi_{\alpha_{m},\beta}(t) \rangle : . \]

\[ (2.123) \]

This completes the proof.

---

\(^5\)Here we use the assumption that the list $\alpha_N$ of initial quantum numbers contains no repeats.
Proof of Eq. (2.77) (normal ordered formula 3).

We begin by specializing the first off-diagonal identity (2.104) to the case of equal quantum numbers, with $O_{\text{imp}} = 1$. We also separate the $n = 0$ term of the sum from the rest:

$$
\langle \Psi_{\alpha N, \beta}(t) | \overline{\Psi}_{\alpha N, \beta}(t) \rangle = \sum_{\sigma \in \text{Sym}(N)} \langle \beta(t) | \overline{\beta}(t) \rangle (\text{sgn} \, \sigma) \left( \prod_{j=1}^{N} \{ c_{\alpha_{\sigma(j)}}(t), \overline{c}_{\alpha_{\sigma(j)}}(t) \} \right)
$$

$$
+ \sum_{n=1}^{N} \sum_{m \in \mathcal{I}_n(N)} (\text{sgn} \, m) \sum_{m' \in \mathcal{I}_n(N)} (\text{sgn} \, m') \sum_{\sigma \in \text{Sym}(N-n)} (\text{sgn} \, \sigma)
$$

$$
\left( \prod_{j=1}^{N-n} \{ c_{\alpha_{(N/m')(\sigma(j))}}(t), \overline{c}_{\alpha_{(N/m)(\sigma(j))}}(t) \} \right) : \langle \Psi_{\alpha_{m'}, \beta}(t) | \overline{\Psi}_{\alpha_{m'}, \beta}(t) \rangle :. \quad (2.124)
$$

Let us now act with $\frac{\partial}{\partial \lambda} |_{\lambda = \lambda}$ on both sides. In the first term, the derivative can act on any one of the anticommutators or on the overlap between the fixed impurity states. All anticommutators that are not differentiated have the bar removed and become Kronecker deltas, which implies that the sum over permutations reduces to just the identity permutation. In the sum over $n = 1, \ldots, N$, the derivative must act on the normal ordered overlap; if it instead acts on any of the anticommutators, then setting $\lambda = \lambda$ removes the bar over the normal ordered overlap, yielding zero according to normal ordered formula 1 (2.75). Thus, we can remove the bar over the anticommutators, which forces the sum to be diagonal.
\((m' = m, \sigma = \text{identity})\). We obtain:

\[
\frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda_0} \langle \Psi_{\alpha_N, \beta}(t) | \overline{\Psi}_{\alpha_N, \beta}(t) \rangle = \sum_{\sigma \in \text{Sym}(N)} (\text{sgn} \sigma) \left( \prod_{j=1}^{N} \delta_{\alpha_j \alpha_{\sigma(j)}} \right) \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda} \langle \beta(t) | \overline{\beta}(t) \rangle \\
+ \sum_{\sigma \in \text{Sym}(N)} (\text{sgn} \sigma) \sum_{j=1}^{N} \left( \prod_{q=1, q \neq j}^{N} \delta_{\alpha_q \alpha_{\sigma(q)}} \right) \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda} \{c_{\alpha_{\sigma(j)}}(t), \overline{c}_{\alpha_j}(t)\} \langle \beta(t) | \overline{\beta}(t) \rangle \\
+ \sum_{n=1}^{N} \sum_{m \in \mathcal{I}_n(N)} (\text{sgn} m) \sum_{m' \in \mathcal{I}_n(N)} (\text{sgn} m') \sum_{\sigma \in \text{Sym}(N-n)} (\text{sgn} \sigma) \left( \prod_{j=1}^{N-n} \delta_{(N/m)(j) \alpha_{(N'/m')(\sigma_j)}} \right) \frac{\partial}{\partial \lambda} \bigg|_{\lambda = \lambda} \langle m_{\alpha_{m'}}, \beta(t) | \overline{\Psi}_{m_{\alpha_{m'}}, \beta}(t) \rangle \bigg|_{\lambda = \lambda} \\
= \sum_{m \in \mathcal{I}_n(N)} \langle m_{\alpha_{m}}, \beta(t) | \overline{\Psi}_{m_{\alpha_{m}}, \beta}(t) \rangle : = \frac{1}{n!} \sum_{m_1, \ldots, m_n = 1}^{N} \langle m_{\alpha_{m}}, \beta(t) | \overline{\Psi}_{m_{\alpha_{m}}, \beta}(t) \rangle : .
\]

Applying \(i \frac{\partial}{\partial t}\) to both sides then yields the third normal ordered formula (2.77), once we use the symmetry property of the overlap to rewrite the sum with unordered summation indices:

\[
\sum_{m \in \mathcal{I}_n(N)} \langle m_{\alpha_{m}}, \beta(t) | \overline{\Psi}_{m_{\alpha_{m}}, \beta}(t) \rangle : = \frac{1}{n!} \sum_{m_1, \ldots, m_n = 1}^{N} \langle m_{\alpha_{m}}, \beta(t) | \overline{\Psi}_{m_{\alpha_{m}}, \beta}(t) \rangle :
\]

**Proof of Eq. (2.78)** (normal ordered formula 4).

Setting the quantum numbers equal in the second off-diagonal identity (2.105), we obtain:

\[
\langle \Psi_{\alpha_N, \beta}(t) | \mathcal{O}_{1}^\dagger \mathcal{O}_{2} \mathcal{O}_{\text{imp}} | \Psi_{\alpha_N, \beta}(t) \rangle = \sum_{n=1}^{N} \sum_{m \in \mathcal{I}_n(N)} \left[ \langle \Psi_{m_{\alpha_{m}}, \beta}(t) | \mathcal{O}_{1}^\dagger \mathcal{O}_{2} \mathcal{O}_{\text{imp}} | \Psi_{m_{\alpha_{m}}, \beta}(t) \rangle : + \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \ell) \{ \mathcal{O}, c_{\alpha_{m(1)}}(t) \} : + \sum_{\ell' \in \mathcal{I}_1(m)} (\text{sgn} \ell') \{ c_{\alpha_{m(1)}}(t), \mathcal{O}_{1} \} : \right] (2.127)
\]
We again wish to rewrite the sum over increasing sequences as an unrestricted sum. For the first term in brackets, this proceeds exactly as in the previous two sections – changing to the unrestricted sum just introduces a factor of $\frac{1}{n!}$. The remaining terms are slightly more complicated, since the indices are not all equivalent; for instance $\ell(1)$ must be treated differently from the remaining indices (in two of the terms). To arrive at the fourth normal ordered formula (2.78), we need to show the following three equations:

\[
\sum_{m \in \mathcal{I}_n(N)} \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \ell) \{ \mathcal{O}_2, c_{\alpha_{\ell(1)}}^{\dagger}(t) \} : (\Psi_{\alpha_{m},\beta}(t)|\mathcal{O}_1^{\dagger}\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m/\ell},\beta}(t)) : =
\]

\[
\sum_{m \in \mathcal{I}_n(N)} \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \ell) \{ c_{\alpha_{\ell(1)}}^{\dagger}(t), \mathcal{O}_1^{\dagger} \} : (\Psi_{\alpha_{m},\beta}(t)|\mathcal{O}_2^{\dagger}\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m},\beta}(t)) : =
\]

\[
\sum_{m \in \mathcal{I}_n(N)} \sum_{\ell,\ell' \in \mathcal{I}_1(m)} (\text{sgn} \ell) (\text{sgn} \ell') \{ c_{\alpha_{\ell(1)}}, \mathcal{O}_1^{\dagger} \} \{ \mathcal{O}_2, c_{\alpha_{\ell'(1)}}^{\dagger}(t) \}
\]

\[
: (\Psi_{\alpha_{m/\ell'},\beta}(t)|\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m/\ell},\beta}(t)) :
\]

\[
\sum_{m \in \mathcal{I}_n(N)} \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \ell) \{ c_{\alpha_{\ell(1)}}^{\dagger}(t), \mathcal{O}_1^{\dagger} \} \{ \mathcal{O}_2, c_{\alpha_{\ell(1)}}^{\dagger}(t) \}
\]

\[
\times : (\Psi_{\alpha_{m/\ell(n)},\beta}(t)|\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m/\ell},\beta}(t)) :
\]

For the first of these, we proceed as follows:

\[
\sum_{m \in \mathcal{I}_n(N)} \sum_{\ell \in \mathcal{I}_1(m)} (\text{sgn} \ell) \{ \mathcal{O}_2, c_{\alpha_{\ell(1)}}^{\dagger}(t) \} : (\Psi_{\alpha_{m},\beta}(t)|\mathcal{O}_1^{\dagger}\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m/\ell},\beta}(t)) :
\]

\[
= \sum_{m \in \mathcal{I}_n(N)} \sum_{\ell \in \mathcal{I}_1(m)} \{ \mathcal{O}_2, c_{\alpha_{\ell(1)}}^{\dagger}(t) \} : (\Psi_{\alpha_{\ell(1)}}^{\perp}(\ell)\alpha_{m},\beta(t)|\mathcal{O}_1^{\dagger}\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m/\ell},\beta}(t)) :
\]

\[
= \sum_{p=1}^{n} \sum_{m_1 < \cdots < m_p < m_{p+1} < \cdots < m_N} \{ \mathcal{O}_2, c_{\alpha_{m(n)}}(t) \} : (\Psi_{\alpha_{m},\beta}(t)|\mathcal{O}_1^{\dagger}\mathcal{O}_{\text{imp}}|\Psi_{\alpha_{m/\ell(n)},\beta}(t)) :
\]
where the first equality follows from the symmetry property (reordering the indices in the bra vector eliminates the $\text{sgn} \ell$ term), and the next equality from relabelling $\mathbf{m} \to \overline{\text{perm}}[\ell]^{-1} \circ \mathbf{m}$ (note that $m_p = \ell(1)$). The normal ordered matrix element is unaffected by any permutation of the indices $\mathbf{m}/m(n)$; thus, we can replace the sum over the $m_j$ indices by $\sum m_{\sigma(1)} < \cdots < m_{\sigma(n)}$, where $\sigma \in \text{Sym}(n)$ is any permutation with $\sigma_p = n$. We sum over all such permutations at the cost of a factor of $\frac{1}{(n-1)!}$, and then note that $\sum_{p=1}^n \sum_{\sigma \in \text{Sym}(n), \sigma_p = n} \sum m_{\sigma(1)} < \cdots < m_{\sigma(n)}$ is equivalent to the unrestricted sum $\sum_{m_1, \ldots, m_n = 1}^N$. This takes care of the first of the three equations; the second is essentially the complex conjugate, and the third follows from similar arguments.

2.4 The thermodynamic limit

The main focus in this work is on quantum impurity models with a linearized spectrum. This means in particular that one must take the number of electrons $N$ to be large in order to get an answer that is equivalent (in the low energy limit) to what would obtained in a calculation starting from the full spectrum (i.e. without linearizing about the Fermi level).

To specialize to quantum impurity models, we take the generic quantum number $\alpha$ to stand for $\alpha = (\gamma, k, a)$, where $\gamma$ is a lead index, $k$ is momentum, and $a$ is spin ($\gamma = 1, \ldots, N_{\text{leads}}, a = \pm 1/2$ or $\uparrow, \downarrow$). In the previous section, we showed that expectation values in a time-evolving state become (normal ordered) sums over all possible subsets of the quantum numbers in the initial state. These sums over abstract quantum numbers $\alpha$ thus correspond to sums over lead indices, momenta, and spins. Our main goal here is to deal with the momentum summations, showing that they become integrals in the thermodynamic limit (i.e. $N \to \infty$ with a fixed density of particles; see below).

The calculations below are essentially just generalizations of the following manipulation
involving some function \( X(k) \):

\[
\frac{1}{L} \sum_{-D < k < \mu} X(k) \xrightarrow{\text{therm. limit}} \int_{-D}^{D} \frac{dk}{2\pi} X(k) \int_{-D}^{D} \frac{dk}{2\pi} f(k) \frac{1}{e^{(k-\mu)/T} + 1} X(k),
\]

(2.130)

where \( f(k) = [e^{(k-\mu)/T} + 1]^{-1} \) is the Fermi function. The logic is the following. The sum over discrete momenta includes all momenta in a Fermi sea, filling up from the cutoff up to the chemical potential \( \mu \), at zero temperature. (Such a sum would arise in the calculation of some expectation value following the quench of the Fermi sea state.) Since the momenta are spaced by \( 2\pi/L \), we obtain an integral in the thermodynamic limit. (We can also think of this integral as \( \int_{-D}^{D} d\epsilon \rho_{\text{per length}}(\epsilon) f(\epsilon) \), where the density of states per unit length is \( \rho_{\text{per length}}(\epsilon) = \frac{1}{2\pi} \) in the linearized models we consider). To generalize to the case of arbitrary temperature \( T \), we allow the integration to go over the full bandwidth region and put in the Fermi function. This generalization can be justified by calculating the expectation value with the zero temperature initial state replaced by a density matrix (the Boltzmann distribution cutoff by bandwidth). It is often easier in practice to do the zero temperature calculation first and then generalize, rather than doing the density matrix calculation. For completeness, we show the density matrix calculation in Sec. 2.4.3.

### 2.4.1 Simplest case: one lead, no spin

As a warm-up, we suppose that the only quantum number of the field operators is momentum (i.e. \( \alpha = k \)). To be precise, we are considering the free Hamiltonian with chemical potential \( \mu \) and bandwidth \( D \):

\[
H_{\text{initial}} = \sum_{|k| < D} (k - \mu) c_{k}^{\dagger} c_{k}.
\]

(2.131)

The initial state of the quench is the ground state of \( H_{\text{initial}} \); it can be written as \( |\Psi_{k_N,\beta}\rangle = c_{k_N}^{\dagger} |\beta\rangle \), with \( k_N = (-D + \frac{2\pi}{L}, \ldots, -D + \frac{2\pi N}{L}) \) and \( \frac{2\pi N}{L} = D + \mu \) (that is, a Fermi sea filled up to \( \mu \)). The thermodynamic limit consists of taking the system size \( L \) to infinity with
fixed density:

\[
\lim_\text{thermodynamic} = \lim_{L \to \infty, N \to \infty} \lim_{\frac{E}{N} = \mu + D}. 
\] (2.132)

Generically, the fixed \( N \) expectation value of some operator \( O \) [see Eqs. (2.76), (2.77), and (2.78)] take the form (leaving aside any simple terms that are independent of \( N \)):

\[
\langle \Psi_{k\beta}(t) | O | \Psi_{k\beta}(t) \rangle = \sum_{n=1}^{N} \frac{1}{L^n} \sum_{m_1, \ldots, m_n = 1}^{N} X_{n,\beta}(t; k_m), 
\] (2.133)

where the function \( X_{n,\beta} \) appears to depend on \( L \), but will soon be seen to be \( L \)-independent. For example, normal ordered formula 2 (2.76) for the expectation value of a fixed impurity operator contains a sum of the above form with:

\[
X_{n,\beta}(t; k_m) = \frac{L^n}{n!} \langle \Psi_{k_m,\beta}(t) | O_{\text{imp}} | \Psi_{k_m,\beta}(t) \rangle. 
\] (2.134)

It is important that the function \( X_{n,\beta} \) is independent of the system size \( L \). We will verify this explicitly in every case; however, it is also possible to give the following general argument. The momentum operators, in order to be unit normalized, have a prefactor of \( \frac{1}{\sqrt{L}} \). The \( A(t) \) operators then have a prefactor of \( \frac{1}{\sqrt{L}} \), which leads each crossing state \( |\Phi_{k_1,\ldots,k_m,\beta}(t)\rangle \) to have a prefactor of \( L^{-m/2} \). Simple counting of the powers of \( L \) in each state means that the normal ordered expectation value gets a prefactor of \( L^{-n} \); the only question is if any more powers of \( L \) will appear from evaluating the overlap integral, which in principle extends over the full system size (in position space). In every model we can solve, the Fermi sea is linearized, which means that the effect of the quench travels at the Fermi velocity (which we set to 1); this means that the crossing states, which contain the entire interacting part of the problem, must vanish if any position variable is outside the “lightcone” from \( x = 0 \) to \( x = t \). This in turn means that the normal ordered overlap can be written as an integral of many position variables all from 0 to \( t \) (seeing as the normal ordering forces the momentum operators to contract with crossing states and never with each other). Since we always keep \( t \) fixed while taking \( L \) to be large, this implies that the integral cannot produce any factors of \( L \).
The thermodynamic limit then proceeds as follows:

\[
\sum_{n=1}^{N} \frac{1}{L^n} \sum_{m_1,\ldots,m_n=1}^{N} X_{n,\beta}(t; k_m) = \sum_{n=1}^{N} \frac{1}{L^n} \sum_{k_1,\ldots,k_n \in \mathcal{K}_1} X_{n,\beta}(t; k_n) \tag{2.135a}
\]

where \( f(k) \equiv \left( e^{\frac{k}{T(k-\mu)} + 1} \right)^{-1} \) is the Fermi function with temperature \( T \) and chemical potential \( \mu \). The first equation is just a rewriting of the sums over indices as sums over quantum numbers (in this case, momentum only). We then observe that the \( n \)th term of the series is a Riemann sum approximation which becomes a multiple integral in the thermodynamic limit. Taking the thermodynamic limit of the series term-by-term yields the second line above. Before discussing the third line above (the generalization to include temperature), let us consider the term-by-term limit more carefully.

The question is whether we can bring the limit inside the sum in the following manner:

\[
\lim_{N \to \infty} \sum_{n=1}^{N} a_n(N) = \sum_{n=1}^{\infty} \lim_{N \to \infty} a_n(N), \tag{2.136}
\]

where we have temporarily defined \( a_n(N) = \sum_{k_n} X_{n,\beta}(t; k_n) \), and where \( N \to \infty \) stands for the thermodynamic limit. This manipulation is not always valid.\(^6\) It frequently occurs in practice, however, that each \( X_{n,\beta} \) is of order \( g^n \) in some parameter \( g \) (e.g. a coupling constant). Then the \( N \)-particle answer truncated to a fixed order \( M \) in powers of \( g \) becomes \( \sum_{n=1}^{M} a_n(N) \). The \( N \to \infty \) limit can certainly be brought inside the sum, seeing as \( M \) is independent of \( N \); thus,

\[
\lim_{N \to \infty} \sum_{n=1}^{M} a_n(N) = \sum_{n=1}^{M} \lim_{N \to \infty} a_n(N). \tag{2.137}
\]

Taking \( M \to \infty \) then yields the right-hand side of Eq. (2.136). This is not a proof of that equation, but rather a way of interpreting the right-hand side: it corresponds to expanding

\(^6\)Consider \( a_n(N) = \delta_{n,N} \), for example.
the $N$-particle answer in powers of $g$ before taking the thermodynamic limit. This is what we will always do in calculations in this thesis, since the correct order of limits – taking the thermodynamic limit first, then expanding – is too difficult at present. The resulting answer is necessarily a series in powers of $g$. In particular, any part of the true answer that depends non-analytically on $g$ will not be detected. We must bear in mind, then, that while we continue to use the notation of infinite sums, they may be asymptotic rather than convergent.

In the last line of (2.135c), we generalize to the case of arbitrary temperature (rather than zero temperature) by including Fermi functions. This is the same answer that would be obtained had we started with the quench with the density matrix $\rho = e^{-H_{\text{initial}}/T}$, instead of the zero temperature ground state. We show this in Sec. 2.4.3.

2.4.2 Including lead and spin indices

Let us suppose the quantum numbers of the field operators consist not only of momenta, but also some discrete indices. We focus in particular on allowing a lead index $\gamma = 1, \ldots, N_{\text{leads}}$ and a spin index $a = \downarrow, \uparrow$; it is not difficult to allow higher spins or other discrete quantum numbers.

We start the quench with the ground state of:

$$H_{\text{initial}} = \sum_{\gamma=1}^{N_{\text{leads}}} \sum_{|k|<D} (k - \mu_\gamma) c_{\gamma ka}^d c_{\gamma ka},$$

(2.138)
in which lead $\gamma$ has chemical potential $\mu_\gamma$. In this ground state, the momenta in lead $\gamma$ are:

$$K_\gamma \equiv \{-D + \frac{2\pi}{L} j \mid 1 \leq j \leq N_\gamma\} \equiv \{K_1, \ldots, K_{N_\gamma}\},$$

(2.139)

where we have assumed that $H_{\text{initial}}$ has periodic boundary conditions with system size $L$. The thermodynamic limit consists of taking $L$ to infinity with the density fixed, in such a
way that the leads have the specified chemical potentials:

$$
\lim_{L \to \infty, N_\gamma \to \infty} \lim_{\mu_\gamma \to \infty} \frac{N_\gamma}{N} = \mu_\gamma + D \quad \text{for each } \gamma.
$$

(2.140)

Allowing for spin degeneracy, the total number $N$ of electrons in the initial state is

$$
N = 2 \sum_{\gamma=1}^{N_{\text{leads}}} N_\gamma.
$$

Writing $\gamma_N k_N a_N$ for the full list of $N$ quantum numbers, we have that the initial state is $|\Psi_{\gamma_N k_N a_N, \beta} \rangle = c^\dagger_{\gamma_N k_N a_N} |\beta\rangle$. The type of sum we encounter in the $N$-particle expectation value of an operator $O$ is:

$$
\langle \Psi_{\gamma_N k_N a_N, \beta}(t)|O|\Psi_{\gamma_N k_N a_N, \beta}(t)\rangle = \sum_{n=1}^{N} \frac{1}{L^n} \sum_{m_1, \ldots, m_n=1}^{N_{\text{leads}}} X_{n,\beta}(t; \gamma_m k_m a_m).
$$

(2.141)

Taking the thermodynamic limit and generalizing to include temperatures proceeds in the same manner as in Eq. (2.135c) – with the same caveat regarding the term-by-term limit discussed there – including some discrete summations:

$$
\sum_{n=1}^{N} \frac{1}{L^n} \sum_{m_1, \ldots, m_n=1}^{N_{\text{leads}}} X_{n,\beta}(t; \gamma_m k_m a_m) = \sum_{n=1}^{N} \frac{1}{L^n} \sum_{\gamma_1, \ldots, \gamma_n=1}^{N_{\text{leads}}} \sum_{k_j \in K_{\gamma_j}} \sum_{a_1 \ldots a_n} X_{n,\beta}(t; \gamma_n k_n a_n)
$$

(2.142a)

$$
\mathop{\text{therm. limit}}\limits_{\rightarrow} \sum_{n=1}^{\infty} \sum_{\gamma_1, \ldots, \gamma_n=1}^{N_{\text{leads}}} \left( \prod_{j=1}^{n} \int_{-D}^{\mu_{\gamma_j}} \frac{dk_j}{2\pi} \right) \sum_{a_1 \ldots a_n} X_{n,\beta}(t; \gamma_n k_n a_n)
$$

(2.142b)

$$
\mathop{\text{include temp.}}\limits_{\rightarrow} \sum_{n=1}^{\infty} \sum_{\gamma_1, \ldots, \gamma_n=1}^{N_{\text{leads}}} \int_{-D}^{D} \frac{dk_1}{2\pi} \cdots \frac{dk_n}{2\pi} \left( \prod_{j=1}^{n} f_\gamma(k_j) \right) \sum_{a_1 \ldots a_n} X_{n,\beta}(t; \gamma_n k_n a_n),
$$

(2.142c)

where $f_\gamma(k) \equiv \left( e^{\frac{\gamma}{T} (k - \mu_\gamma)} + 1 \right)^{-1}$ is the Fermi function of lead $\gamma$.

In models with even interaction only [see Sec. 2.5], it frequently occurs that the function $X_{n,\beta}$ depends on the lead indices in a very simple way, allowing us to carry out the summation over lead indices explicitly. To take the simplest example, suppose that $X_{n,\beta}$ is independent of lead indices entirely; then Eq. (2.142c) simplifies when we can commute the sum with the product:

$$
\mathop{\text{therm. limit}}\limits_{\rightarrow} \sum_{\gamma_1, \ldots, \gamma_n=1}^{N_{\text{leads}}} \prod_{j=1}^{n} f_\gamma(k_j) = \prod_{j=1}^{n} \sum_{\gamma=1}^{N_{\text{leads}}} f_\gamma(k_j).
$$

(2.143)
2.4.3 Including temperature

In this section, we justify the “include temperature” step in the previous two sections. For simplicity, we consider the one lead case with no spin indices. With $H_{\text{initial}} = \sum_{|k| < D} (k - \mu) c_k^\dagger c_k$, the initial density matrix prior to the quench is $\rho = e^{-H_{\text{initial}}/T}$. We consider the expectation value of an operator $O$ in the time-evolving density matrix $\rho(t) = e^{-iHt} \rho e^{iHt}$:

$$\langle O \rangle \equiv \frac{\text{Tr}[\rho(t)O]}{Z} = \frac{1}{Z} \sum_E e^{-E/T} \langle E(t)|O|E(t) \rangle,$$

where the $|E\rangle$ states are a complete set of energy eigenstates for $H_{\text{initial}}$, $|E(t)\rangle = e^{-iHt}|E\rangle$, and $Z = \sum_E e^{-E/T}$ is the partition function. We set up the calculation with a fixed system size $L$ at first, so that the full set of allowed momenta $|k| < D$ that appear in $H_{\text{initial}}$ is $K_1, \ldots, K_{N_{\text{modes}}}$, with $K_j = -D + \frac{2\pi j}{L}$. The products and sums over momenta that appear in the calculation below are all over this set of allowed momenta. The thermodynamic limit is:

$$\lim_{\text{thermodynamic}} \equiv \lim_{L \to \infty, N_{\text{modes}} \to \infty, \frac{2\pi}{L} N_{\text{modes}} = 2D}.$$

The eigenstates $|E\rangle$ take the form $|E\rangle = c_{kN}^\dagger |\beta\rangle$, where the momenta are arbitrary and the total number of particles can range from $N = 0$ up to $N = N_{\text{modes}}$. It is convenient to use the usual approach of denoting the states by their occupation numbers; thus, $|E\rangle \leftrightarrow \{s_k\}_k$, where $s_k$ indicates whether the mode $k$ is unoccupied ($s_k = 0$) or occupied ($s_k = 1$). Starting from the generic form Eq. (2.133), we obtain:

$$\langle E(t)|O|E(t) \rangle = \sum_{n=1}^{N_{\text{modes}}} \frac{1}{L^n} \sum_{k_1, \ldots, k_n} s_{k_1} \cdots s_{k_n} X_{n,\beta}(t;k_n).$$

(2.146)
The calculation of $\langle \mathcal{O} \rangle$ then proceeds in much the same manner as the usual derivation of the Fermi function:

$$
\langle \mathcal{O} \rangle = \frac{1}{Z} \left( \prod_k \sum_{s_k=0,1} \right) e^{-\frac{1}{T} \sum_{k'=(k'-\mu)s_{k'}}} \sum_{n=1}^{N_{\text{modes}}} \frac{1}{L^n} \sum_{k_1,\ldots,k_n} s_{k_1} \ldots s_{k_n} X_{n,\beta}(t;k_n)
$$

(2.147a)

$$
= \frac{1}{Z} \sum_{n=1}^{N_{\text{modes}}} \frac{1}{L^n} \sum_{k_1,\ldots,k_n} e^{-\frac{1}{T}(k_1-\mu)} \ldots e^{-\frac{1}{T}(k_n-\mu)} \left( \prod_{k \neq k_1,\ldots,k_n, s_k=0,1} e^{-\frac{1}{T}(k-\mu)s_k} \right)
\times X_{n,\beta}(t;k_n)
$$

(2.147b)

$$
= \sum_{n=1}^{N_{\text{modes}}} \frac{1}{L^n} \sum_{k_1,\ldots,k_n} f(k_1) \ldots f(k_n) X_{n,\beta}(t;k_n),
$$

(2.147c)

where we have noted that $f(k) = \frac{e^{-\frac{1}{T}(k-\mu)}}{\sum_{s_k=0,1} e^{-\frac{1}{T}(k-\mu)s_k}}$. The thermodynamic limit now proceeds just as in the zero temperature case, since we have arrived at a sum of the same form. We thus arrive at the same result (2.135c) that we obtained earlier by generalizing the zero temperature calculation. Including lead and spin indices is straightforward.

2.5 Two lead models with even interaction

2.5.1 Overview and many-body wavefunction

This is an important special case which will be used later in this thesis. Our goal in this section is to specialize the results of the general formalism to the case of Hamiltonian of the general form of a two lead impurity model – in particular, a Hamiltonian that separates into two sectors (lead 1 and lead 2), with an interaction term that only involves a certain linear combination of the two sectors. By a rotation of the lead 1/lead 2 basis, the Hamiltonian decouples into a non-interacting sector and an interacting sector. Our objective will be to reduce this as much as possible to the problem of solving the interacting sector only. Many of the results carry through to the case of an arbitrary number of leads.

The general problem can be formulated as follows. The generic quantum number $\alpha$ is replaced by $(\gamma, \alpha)$, where $\gamma = 1, 2$ is the lead index and the additional quantum numbers $\alpha$ are arbitrary. Thus, the field operators of the model are $c_{1\alpha}^\dagger$ and $c_{2\alpha}^\dagger$, acting as usual
on a set of fixed impurity states $|\beta\rangle$. We assume that the Hamiltonian decouples into a non-interacting and an interacting sector upon unitary rotation to an “odd/even” basis. That is:

$$H = H_o + H_e, \quad [H_o, H_e] = 0, \quad [H_o, c_{e\alpha}] = [H_e, c_{o\alpha}] = 0,$$

(2.148)

where the odd/even operators are given by:

$$\begin{pmatrix} c_{o\alpha} \\ c_{e\alpha} \end{pmatrix} = U \begin{pmatrix} c_{1\alpha} \\ c_{2\alpha} \end{pmatrix}, \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad U^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

(2.149)

We assume that $H_o$ is non-interacting; in particular, we assume that the time-evolving field operators $c_{o\alpha}^\dagger(t) = e^{-iH_ot} c_{o\alpha}^\dagger e^{iH_ot}$ are known (for instance, $c_{o\alpha}^\dagger(t) = e^{-i\alpha t} c_{o\alpha}^\dagger$) and that $H_o$ annihilates any fixed impurity state: $H_o |\beta\rangle = 0$. Then the time evolution of any set of odd quantum numbers is immediately given by:

$$e^{-iH_ot} c_{o\alpha N}^\dagger |\beta\rangle = c_{o\alpha N}^\dagger(t) |\beta\rangle.$$

(2.150)

We further assume that we can solve the quench problem for $H_e$, as well; that is we assume that the crossing states are known, and that we can therefore write down the answer for the time evolution of any number of even quantum numbers:

$$|\Psi_{e\alpha N, \beta}(t)\rangle = e^{-iH_e t} c_{e\alpha N}^\dagger |\beta\rangle,$$

(2.151)

where $H_e = H_e^{(0)} + H_e^{(1)}$ has both a non-interacting part and an interacting part, with the field operators evolve as usual only by the non-interacting part: $c_{e\alpha}^\dagger(t) = e^{-H_e^{(0)} t} c_{e\alpha}^\dagger e^{iH_e^{(0)} t}$. In making this assumption, we are continuing on with the general theme of this chapter, which is to reduce the problem as much as possible to the core difficulty (which we then solve in particular models in later chapters); in this case, the core difficulty is the solution for the crossing states of the even sector. Our goal here is to see how, once we have the even crossing states, we can use them to solve another problem: the time evolution of quantum numbers in the lead 1/lead 2 basis. Our goal is to calculate:

$$|\Psi_{\gamma N o N, \beta}(t)\rangle = e^{-iH t} c_{\gamma N o N, \beta} |\beta\rangle.$$

(2.152)
The difficulty is that the initial state is simple in the lead 1/lead 2 basis, but the time evolution is only known in the odd/even basis. A laborious way to proceed would be to write each $c_{\alpha}^{\dagger}$ operator as a linear combination of $c_{o\alpha}^{\dagger}$ and $c_{e\alpha}^{\dagger}$; then, expanding the product, we would find a sum of initial states that are all simple in the odd/even basis. We could then evolve these individually via:

$$e^{-iH_{t}}c_{o\alpha}^{\dagger}c_{e\alpha}^{\dagger}c_{o\alpha}|\beta\rangle = e^{-iH_{t}}c_{o\alpha}^{\dagger}e^{iH_{t}}c_{e\alpha}^{\dagger}e^{-iH_{t}}c_{e\alpha}^{\dagger}e^{-iH_{t}}|\beta\rangle = c_{o\alpha}^{\dagger}(t)|\Psi_{o,\alpha}(t)\rangle. \quad (2.153)$$

The full solution would be a large sum of such terms. There is, however, a simpler way to proceed – we instead use the crossing states $|\Phi_{o,\alpha}\rangle$ (which are known by assumption) to construct the solution in the lead 1/lead 2 basis directly.

We consider the case of a type A model first. The problem is to find the (unsymmetrized) crossing states:

$$\left(H - i\frac{d}{dt}\right)|\chi_{\gamma_{1}\alpha_{1}...\gamma_{n}\alpha_{n},\beta}(t)\rangle = -A_{\gamma_{n}\alpha_{n}}(t)|\chi_{\gamma_{1}\alpha_{1}...\gamma_{n-1}\alpha_{n-1}\beta}(t)\rangle, \quad (2.154a)$$

$$|\chi_{\beta}(t)\rangle = |\beta(t)\rangle, \quad (2.154b)$$

$$|\chi_{\gamma_{1}\alpha_{1}...\gamma_{n}\alpha_{n},\beta}(t=0)\rangle = 0. \quad (2.154c)$$

By assumption, we already know the crossing states for the even sector only:

$$\left(H - i\frac{d}{dt}\right)|\chi_{e\alpha_{1}...e\alpha_{n}\beta}(t)\rangle = -A_{e\alpha_{n}}(t)|\chi_{e\alpha_{1}...e\alpha_{n-1}\beta}(t)\rangle, \quad (2.155a)$$

$$|\chi_{\beta}(t)\rangle = |\beta(t)\rangle, \quad (2.155b)$$

$$|\chi_{e\alpha_{1}...e\alpha_{n},\beta}(t=0)\rangle = 0. \quad (2.155c)$$

(Note that the time-evolving fixed impurity state is the same in either case: $|\beta(t)\rangle = e^{-iH_{o}(0)_{t}}|\beta\rangle = e^{-iH_{o}(0)_{t}}|\beta\rangle$.) The key point is that the $A(t)$ operators are related in a simple way:

$$A_{\gamma\alpha}(t) \equiv [H, c_{\gamma\alpha}^{\dagger}] - i\frac{\partial}{\partial t} c_{\gamma\alpha}^{\dagger}(t) = \frac{1}{\sqrt{2}}A_{e\alpha}(t) \quad \text{(independent of } \gamma = 1, 2). \quad (2.156)$$

We can therefore read off the relation between the lead 1/lead 2 crossing states and the
even crossing states:

\[ |\chi_{\gamma m\alpha,\beta}(t)\rangle = 2^{-n/2} |\epsilon_{\epsilon_{\alpha},\beta}(t)\rangle, \quad |\Phi_{\gamma m\alpha,\beta}(t)\rangle = 2^{-n/2} |\Phi_{\epsilon_{\epsilon_{\alpha}},\beta}(t)\rangle \]  

(2.157)

The general expression for the time-evolving wavefunction [Eqs. (2.39) and (2.40)] then becomes:

\[ |\Psi_{\gamma N\alpha,\beta}(t)\rangle = \sum_{n=0}^{N} \sum_{m \in \mathcal{I}_n(N)} (\hat{\text{sgn}} m) c_{\gamma N/m\alpha N/m}(t) |\Phi_{\gamma m\alpha,\beta}(t)\rangle \]  

(2.158a)

\[ = \sum_{n=0}^{N} 2^{-n/2} \sum_{m \in \mathcal{I}_n(N)} (\hat{\text{sgn}} m) c_{\gamma N/m\alpha N/m}(t) |\Phi_{\epsilon\epsilon_{\alpha},\beta}(t)\rangle. \]  

(2.158b)

In this way, we have shown that solving the quench problem in the even basis (i.e. finding the even crossing states) yields, in a simple way, the solution of the quench problem in the lead 1/lead 2 basis. (Certainly this must be the same answer that would be obtained using the more laborious approach, mentioned earlier, of summing over the odd/even basis.)

While we did the calculation for type A models only, the final result also holds for type B models; one only needs the relation between \( B(t) \) operators:

\[ B_{\gamma_1\alpha_1\gamma_2\alpha_2}(t) \equiv \{ A_{\gamma_2\alpha_2}(t), c_{\gamma_1\alpha_1}(t) \} = \frac{1}{2} B_{\epsilon\alpha_1\epsilon\alpha_2} \quad (\text{independent of } \gamma_1, \gamma_2 \in \{1, 2\}). \]  

(2.159)

### 2.5.2 N-particle expectation values

The fact that the crossing states are built from even sector operators only leads to a significant simplification of the latter three normal ordered formulas [Eqs. (2.76), (2.77), and (2.78)]. The general rule is that, inside the normal ordering symbol, any lead 1/lead 2 indices can be replaced by an even index, with a factor of \( 1/\sqrt{2} \) for each index replaced.

Let us illustrate this by considering the normal ordered expectation value of an impurity operator:

\[ :\langle \Psi_{\gamma m\alpha,\beta}(t)|O_{\text{imp}}|\Psi_{\gamma m\alpha,\beta}(t)\rangle : = \sum_{p,p'=1}^{n} 2^{-p/2} 2^{-p'/2} \sum_{\ell \in \mathcal{I}_p(m)} \hat{\text{sgn}} \ell \sum_{\ell' \in \mathcal{I}_{p'}(m)} \hat{\text{sgn}} \ell' \]  

\[ \times :\langle \Phi_{\epsilon\epsilon_{\alpha},\beta}(t)|c_{\gamma m/\ell' \epsilon m/\ell}(t)O_{\text{imp}}c_{\gamma m/\ell' \epsilon m/\ell}(t)|\Phi_{\epsilon\epsilon_{\alpha},\beta}(t)\rangle : \quad (n = |m|). \]  

(2.160)
The crossing states are annihilated by any odd field operator. We can therefore replace:

\[ c_{N/\ell}^\dagger(t) \rightarrow 2^{-(n-p)/2} c_{eN/\ell}^\dagger(t), \quad c_{N/\ell}^\dagger(t) \rightarrow 2^{-(n-p')/2} c_{eN/\ell'}^\dagger(t), \]  

which, with the previous equation, yields:

\[ : \langle \Psi_{\gamma_m\alpha_{m,\beta}}(t) | \mathcal{O}_{\text{imp}} | \Psi_{\gamma_m\alpha_{m,\beta}}(t) \rangle : = 2^{-n} : \langle \Psi_{e\alpha_{m,\beta}}(t) | \mathcal{O}_{\text{imp}} | \Psi_{e\alpha_{m,\beta}}(t) \rangle : . \]  

Then, replacing the general index \( \alpha \) by \( (\gamma, \alpha) \) in normal ordered formula 2 (2.76), we find the following simplified version:

\[ \langle \Psi_{\gamma_N\alpha_{N,\beta}}(t) | \mathcal{O}_{\text{imp}} | \Psi_{\gamma_N\alpha_{N,\beta}}(t) \rangle = \langle \beta(t) | \mathcal{O}_{\text{imp}} | \beta(t) \rangle + \sum_{n=1}^{N} \frac{1}{2^{n} n!} \sum_{m_1,\ldots,m_n=1}^{N} : \langle \Psi_{e\alpha_{m_{n},\beta}}(t) | \mathcal{O}_{\text{imp}} | \Psi_{e\alpha_{m_{n},\beta}}(t) \rangle : . \]  

Let us turn next to the fourth normal ordered formula (the expectation value of \( \mathcal{O}_1^\dagger \mathcal{O}_2 \mathcal{O}_{\text{imp}} \)). The simplification that occurs depends on the inserted operators \( \mathcal{O}_1 \) and \( \mathcal{O}_2 \); one useful case is when one is odd and the other even:

\[ \mathcal{O}_1 = \mathcal{O}_o, \quad \mathcal{O}_2 = \mathcal{O}_e. \]  

Any normal ordered product that contains an odd operator is zero, seeing as the odd operator must annihilate a crossing state on one side or the other (i.e., \( \mathcal{O}_o | \Phi(t) \rangle \) is always zero). Therefore, in normal ordered formula 4 (2.78), we need only keep the two terms in which \( \mathcal{O}_o^\dagger \) is contracted. We can also replace the lead 1/lead 2 quantum numbers by even quantum numbers inside the normal ordering symbol (the calculation is very similar to the one done above):

\[ : \langle \Psi_{\gamma_{m/m_{n}}\alpha_{m/m_{n},\beta}}(t) | \mathcal{O}_e \mathcal{O}_{\text{imp}} | \Psi_{\gamma_{m/m_{n}}\alpha_{m/m_{n},\beta}}(t) \rangle : = 2^{-n+1/2} : \langle \Psi_{e\alpha_{m/m_{n},\beta}}(t) | \mathcal{O}_e \mathcal{O}_{\text{imp}} | \Psi_{e\alpha_{m,\beta}}(t) \rangle : . \]  

---

\( ^8 \)That is, \( \mathcal{O}_o \) is a linear combination of \( c_{o\alpha} \) operators and \( \mathcal{O}_e \) is a linear combination of \( c_{e\alpha} \) operators. We emphasize that in the earlier section, the \( \mathcal{O}_1 \) and \( \mathcal{O}_2 \) operators are arbitrary – the 1 and 2 labels are not necessarily lead indices.
where \( n = |m| \). Then, noting that \( \{c_\alpha(t), O_o^\dagger\} = \frac{1}{\sqrt{2}}(-1)^{\gamma-1}\{c_\alpha(t), O_o^\dagger\} \), we find that normal ordered formula 4 simplifies to:

\[
\langle \Psi_{\gamma N\alpha N, \beta}(t) | O_o^\dagger O_e O_{\text{imp}} | \Psi_{\gamma N\alpha N, \beta}(t) \rangle = \sum_{n=1}^{N} \frac{1}{2^n(n-1)!} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{m_n-1}\{c_{\alpha m_n}(t), O_o^\dagger\} : \langle \Psi_{e_{\alpha m/m_n, \beta}}(t) | O_e O_{\text{imp}} \rangle \Psi_{e_{\alpha m, \beta}}(t) : \\
+ \sum_{\ell \in \ell_1(m)} (\text{sgn } \ell) \{O_e, c_{\alpha \ell(1)}^\dagger(t)\} : \langle \Psi_{e_{\alpha m/m_n, \beta}}(t) | O_{\text{imp}} \rangle \Psi_{e_{\alpha m, \beta}}(t) : \quad (2.166)
\]

A further specialization of setting \( O_{\text{imp}} = 1 \) is also useful. In this case, the second term is a normal ordered overlap between two states and therefore vanishes unless \( n = 1 \) [so that \( m = (m_1) = \ell \), and \( m/m_n \) and \( m/\ell \) are each the empty list – see the identity (2.79)]. We thus obtain:

\[
\langle \Psi_{\gamma N\alpha N, \beta}(t) | O_o^\dagger O_e | \Psi_{\gamma N\alpha N, \beta}(t) \rangle = \frac{1}{2} \sum_{m=1}^{N} (-1)^{m_n-1}\{c_{\alpha m}(t), O_o^\dagger\} \{O_e, c_{\alpha m}(t)\} \\
+ \sum_{n=1}^{N} \frac{1}{2^n(n-1)!} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{m_n-1}\{c_{\alpha m_n}(t), O_o^\dagger\} : \langle \Psi_{e_{\alpha m/m_n, \beta}}(t) | O_e \rangle \Psi_{e_{\alpha m, \beta}}(t) : \
\]

\[
(2.167)
\]

There remains only the second normal ordered formula. In this case, we must first recapitulate the basic setup of the problem, now with the barred degrees of freedom.

To calculate a generic observable using the derivative formula, we may need the varying Hamiltonian \( \Pi \) to be such that there is no decoupling into a non-interacting and an interacting sector; we will consider only the special case in which the decoupling does occur:

\[
\Pi = \Pi_o + \Pi_e, \ [\Pi_o, \Pi_e] = 0, \ [\Pi_o, \varepsilon_{\alpha \alpha}] = [\Pi_e, \varepsilon_{\alpha \alpha}] = 0, \quad (2.168)
\]

where the odd/even operators are given by:

\[
\begin{pmatrix}
\varepsilon_{\alpha \alpha} \\
\varepsilon_{\alpha \alpha}
\end{pmatrix} = \mathcal{U} \begin{pmatrix}
c_{\alpha 1} \\
-c_{\alpha 2}
\end{pmatrix}, \quad \mathcal{U}^\dagger \mathcal{U} = 1. \quad (2.169)
\]

The unitary matrix \( \mathcal{U} \) depends, in general, on the varying parameter \( \chi \); removing the bar recovers Eq. (2.149). We assume that the time-evolving operators in the odd sector,
\( \overline{c}_{\alpha}(t) \equiv e^{-iH^{(0)}_t}c_{\alpha}e^{iH^{(0)}_t} \), are known, and that the odd sector decouples from the fixed impurity states: \( \overline{H}_o|\beta\rangle = 0 \). The even Hamiltonian has a non-interacting and an interacting part (\( H_e = H^{(0)}_e + H^{(1)}_e \)), and the field operators evolve via the non-interacting part (\( \overline{c}_{\alpha}(t) \equiv e^{-iH^{(0)}_t}c_{\alpha}e^{iH^{(0)}_t} \)); the full time evolution problem for the even sector is assumed to be solved (i.e. we have the crossing states \( \overline{\Phi}_{e\alpha m, \beta}(t) \)).

At this point we have not defined any \( \overline{c}_{1\alpha}, \overline{c}_{2\alpha} \) operators. For reasons we will soon explain, it is convenient to define:

\[
\begin{pmatrix}
\overline{c}_{1\alpha} \\
\overline{c}_{2\alpha}
\end{pmatrix} \equiv \mathcal{U} \begin{pmatrix}
c_{1\alpha} \\
c_{2\alpha}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} c_{1\alpha} \\
c_{2\alpha}
\end{pmatrix}. \tag{2.170}
\]

Removing the bar recovers Eq. \( (2.149) \), so our notation is consistent.\(^9\) Inverting, we find:

\[
\begin{pmatrix}
c_{1\alpha} \\
c_{2\alpha}
\end{pmatrix} = \mathcal{U}^\dagger \begin{pmatrix}
\overline{c}_{1\alpha} \\
\overline{c}_{2\alpha}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} , \tag{2.171}
\]

which is precisely the same as Eq. \( (2.149) \), just with a bar over all of the operators. In other words, the problem of finding \( e^{-iH_t\overline{c}_{\gamma N\alpha N}^\dagger}|\beta\rangle \) given the even crossing states \( |\overline{\Phi}_e(t)\rangle \) is exactly the same as the problem of finding \( e^{-iH_tc_{\gamma N\alpha N}^\dagger}|\beta\rangle \) given the even crossing states \( |\Phi_e(t)\rangle \). By putting bars on Eq. \( (2.158b) \), we can read off the solution:

\[
|\overline{\Phi}_{\gamma N\alpha N, \beta}(t)\rangle \equiv e^{-iH_t\overline{c}_{\gamma N\alpha N}^\dagger}|\beta\rangle = \sum_{n=0}^{N} 2^{-n/2} \sum_{m \in \mathcal{I}_n(N)} (\delta_{\text{sgn}} m) \overline{c}_{\gamma N/m\alpha N/m}^\dagger(t)|\overline{\Phi}_{e\alpha m, \beta}(t)\rangle. \tag{2.172}
\]

With this setup complete, we can now proceed with simplifying the second normal ordered formula, Eq. \( (2.77) \). We have:

\[
\frac{\partial}{\partial \lambda} \bigg|_{\lambda=\lambda} :\langle \Psi_{\gamma m\alpha m, \beta}(t)|\overline{\Phi}_{\gamma m\alpha m, \beta}(t)\rangle: = \sum_{p, p' = 1}^{n} 2^{-p/2} 2^{-p'/2} \sum_{\ell \in \mathcal{I}_p(m)} (\delta_{\text{sgn}} \ell) \sum_{\ell' \in \mathcal{I}_{p'}(m)} (\delta_{\text{sgn}} \ell') \overline{c}_{\gamma m/\ell \alpha m/\ell}^\dagger(t) \overline{c}_{\gamma m/\ell' \alpha m/\ell'}(t)|\overline{\Phi}_{e\alpha \ell, \beta}(t)\rangle : \quad (n = |m|). \tag{2.173}
\]

\(^9\) Eq. \( (2.170) \) defines a function of \( \lambda \) which outputs \( c_{\alpha} \) when we set \( \lambda = \lambda; \) thus, writing this function as \( \overline{c}_{\gamma \alpha} \) is consistent with our convention for the meaning of the bar. Using \( \mathcal{U}^\dagger \) instead of \( \mathcal{U}^\dagger \) would also be consistent, but not as useful.
We cannot necessarily replace the $\gamma$ quantum numbers inside the inner product by $e$, since an unbarred odd operator does not necessarily annihilate a crossing state in the barred even sector. Further simplification depends on anticommutation relations between unbarred and barred operators. We will consider only a special case in which we have the following relations:

$$\frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \{ c_{\alpha}(t), \overline{c}_{\alpha}^\dagger(t) \} = \frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \{ c_{\alpha}(t), \overline{c}_{\alpha}^\dagger(t) \} = 0 \quad (2.174a)$$

$$\frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \{ c_{\alpha}(t), \overline{c}_{\alpha}^\dagger(t) \} = - \left( \frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \{ c_{\alpha}(t), \overline{c}_{\alpha}^\dagger(t) \} \right)^* \quad (2.174b)$$

In view of this assumption, we have:

$$\frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \langle \Phi_{\gamma \alpha \epsilon \beta}^\alpha(t) | c_{m/\ell ' \gamma_m /\ell '}(t) \overline{c}_{m/\ell \gamma_m /\ell}(t) \rangle_{\gamma \alpha \epsilon \beta} = 2^{-(n-p)/2} 2^{-(n-p')/2} \frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \langle \Phi_{\gamma \alpha \epsilon \beta}^\alpha(t) : = \right. \right.$$

$$\times \left( \sum_{s' \in \lambda_s} (\text{sgn} s)(-1)^{\gamma s} \sum_{s \in \lambda_s} (\text{sgn} s)(-1)^{\gamma s} \langle \Phi_{\gamma \alpha \epsilon \beta}^\alpha(t) | c_{m/\ell ' \gamma_m /\ell '}(t) \overline{c}_{m/\ell \gamma_m /\ell}(t) \rangle_{\gamma \alpha \epsilon \beta} : \right.$$ 

$$+ \sum_{s' \in \lambda_s} (\text{sgn} s')(1)^{\gamma s'} \langle \Phi_{\gamma \alpha \epsilon \beta}^\alpha(t) | c_{m/\ell ' \gamma_m /\ell '}(t) \overline{c}_{m/\ell \gamma_m /\ell}(t) \rangle_{\gamma \alpha \epsilon \beta} : \right). \quad (2.175)$$

Returning to Eq. (2.173) and doing the $s$ ($s'$) sum before the $\ell$ ($\ell'$) sum, we find:

$$\frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \langle \Psi_{\gamma \alpha \epsilon \beta}^\alpha(t) | \overline{\Psi}_{\gamma \alpha \epsilon \beta}^\alpha(t) \rangle =

2^{-n} \frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \sum_{s \in \lambda_s} (\text{sgn} s)(-1)^{\gamma s} \left( \langle \Psi_{\gamma \alpha \epsilon \beta}^\alpha(t) | c_{\alpha \gamma}(t) \overline{\Psi}_{\gamma \alpha \epsilon \beta}^\alpha(t) \rangle : \right.$$

$$+ \langle \Psi_{\gamma \alpha \epsilon \beta}^\alpha(t) | \overline{c}_{\alpha \gamma}(t) \overline{\Psi}_{\gamma \alpha \epsilon \beta}^\alpha(t) \rangle : \right). \quad (2.176)$$

Normal ordered formula 3 thus becomes:

$$i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \langle \Psi_{\gamma \alpha \epsilon \beta}^\alpha(t) | \overline{\Psi}_{\gamma \alpha \epsilon \beta}^\alpha(t) \rangle = i \frac{\partial}{\partial \lambda} \frac{\partial}{\partial \lambda} \left|_{\lambda=\lambda_s} \right. \langle \beta(t) | \overline{\beta}(t) \rangle$$

$$- \frac{1}{2} \sum_{m=1}^N \left( \{ c_{\alpha \gamma}(t) \overline{c}_{\alpha \gamma}(t) \} + \{ c_{\alpha \gamma}(t) \overline{c}_{\alpha \gamma}(t) \} \right)$$

$$+ \sum_{n=1}^N \frac{1}{2 n(n!)} \sum_{m_1, \ldots, m_n=1}^N \sum_{s \in \lambda_s} (\text{sgn} s)(-1)^{\gamma s} \left( \langle \Psi_{\gamma \alpha \epsilon \beta}^\alpha(t) | c_{\alpha \gamma}(t) \overline{\Psi}_{\gamma \alpha \epsilon \beta}^\alpha(t) \rangle : \right.$$

$$+ \langle \Psi_{\gamma \alpha \epsilon \beta}^\alpha(t) | \overline{c}_{\alpha \gamma}(t) \overline{\Psi}_{\gamma \alpha \epsilon \beta}^\alpha(t) \rangle : \right) \right). \quad (2.177)$$
Recall that we can use fermionic symmetries inside the normal ordering symbol [see Sec 2.3.4]; thus, we can replace $|\psi_{m}^{(a)}(t)\rangle \rightarrow (\text{sgn } s)|\psi_{m_{1}a_{1}}^{(a)}(t)\rangle$. Then, relabelling summation indices yields:

$$i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \langle \psi_{\alpha N_{N},\beta}(t) | \bar{\psi}_{\alpha N_{N},\beta}(t) \rangle = i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \left( \langle \beta(t) | \bar{\beta}(t) \rangle \right)$$

$$- \frac{1}{2} \sum_{m=1}^{N} (-1)^{\gamma_{m}} \left( \{c_{\alpha_{m}}(t), \bar{\tau}_{\alpha_{m}}^{i}(t)\} + \{c_{\alpha_{m}}(t), \bar{\tau}_{\alpha_{m}}^{j}(t)\} \right)$$

$$+ \sum_{n=1}^{N} \frac{1}{2^{n}(n-1)!} \sum_{m_{1},\ldots,m_{n}=1}^{N} (-1)^{\gamma_{m_{n}}-1} \left( : \langle \psi_{\alpha_{m_{n}}}(t) | c_{\alpha_{m_{n}}}(t) \bar{\psi}_{\alpha_{m_{n}}}(t) : \right)$$

$$+ : \langle \psi_{\alpha_{m_{n}}}(t) | \bar{\tau}_{\alpha_{m_{n}}}^{i}(t) \rangle : \right).$$

(2.178)

Final simplification:

$$i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \langle \psi_{\alpha_{N_{N}},\beta}(t) | \bar{\psi}_{\alpha_{N_{N}},\beta}(t) \rangle = i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \left( \langle \beta(t) | \bar{\beta}(t) \rangle \right)$$

$$+ \text{Re} \left[ i \frac{\partial}{\partial t} \frac{\partial}{\partial \lambda} \left( \sum_{m=1}^{N} (-1)^{\gamma_{m}} \{c_{\alpha_{m}}(t), \bar{\tau}_{\alpha_{m}}^{i}(t)\} \right) \right]$$

$$+ \sum_{n=1}^{N} \frac{1}{2^{n}(n-1)!} \sum_{m_{1},\ldots,m_{n}=1}^{N} (-1)^{\gamma_{m_{n}}-1} : \langle \psi_{\alpha_{m_{n}}}(t) | c_{\alpha_{m_{n}}}(t) \bar{\psi}_{\alpha_{m_{n}}}(t) : \right).$$

(2.179)

2.6 Time-independent formalism

It is convenient in some problems to solve for the infinite time limit of the wavefunction directly, without following the detailed time evolution. The formalism we have developed in this chapter applies, with minor modifications, to the time-independent case.

Although it is not strictly necessary, we formulate the entire discussion in terms of scattering theory. The passage from the time-dependent to the time-independent picture results in the initial condition in time (at $t = 0$ in our setup, usually $t = -\infty$ in scattering theory) becoming a time-independent boundary condition in space (e.g. incoming plane waves).

We write the Hamiltonian as $H = H^{(0)} + H^{(1)} = h + V$, where $h$ is the non-interacting Hamiltonian from the point of view of scattering theory. That is, $h$ is the “completely
The Lippmann-Schwinger equation for scattering “in” states is:

$$|\Psi_{\alpha N, \beta, \text{in}}\rangle = |\Psi_{\alpha N, \beta}\rangle + \frac{1}{E - \hbar + i\eta} \mathcal{V}|\Psi_{\alpha N, \beta, \text{in}}\rangle,$$

where $|\Psi_{\alpha N, \beta}\rangle \equiv c_{\alpha N}^\dagger |\beta\rangle$ is an eigenstate of $h$ with energy $E \equiv E_{\alpha 1} + \cdots + E_{\alpha N}$. This is equivalent to the time-independent Schrödinger equation:

$$(H - E)|\Psi_{\alpha N, \beta, \text{in}}\rangle = 0,$$

with the scattering boundary condition of plane waves with quantum numbers $\alpha_1, \ldots, \alpha_N$ (with the fixed impurity state having quantum number $\beta$). The non-interacting Hamiltonian $H^{(0)}$, which includes quadratic terms such as impurity tunneling and potential scattering, has a set of scattering operators $c_{\alpha, \text{in}}^\dagger$ that satisfy:

$$[H, c_{\alpha, \text{in}}^\dagger] - E_{\alpha} c_{\alpha, \text{in}}^\dagger = 0,$$

and that create scattering “in” states corresponding to $c_{\alpha}^\dagger$. The solution to the Lippman-Schwinger equation in the special case of no interaction ($H^{(1)} = 0$) is given by a product of these operators:

$$|\Psi_{\alpha N, \beta, \text{in}}^0\rangle = c_{\alpha N, \text{in}}^\dagger |\beta\rangle.$$

Let us note also the Lippmann-Schwinger equation can also be formulated with $H^{(0)}$, rather than $h$, as the “free” part:

$$|\Psi_{\alpha N, \beta, \text{in}}\rangle = |\Psi_{\alpha N, \beta}^0\rangle + \frac{1}{E - \hbar + i\eta} H^{(1)} |\Psi_{\alpha N, \beta, \text{in}}\rangle.$$

In other words, the scattering boundary condition can be encoded either by the state $|\Psi_{\alpha N, \beta}\rangle$ or the state $|\Psi_{\alpha N, \beta}^0\rangle$. 

free” part that describes the propagation of plane waves, not including any tunneling to the impurity or scattering off a potential. For instance, $h = -i \int dx \, \psi^\dagger(x) \frac{d}{dx} \psi(x)$ in the IRL (Chapter 5). Note that we work in infinite volume. We write $h = \int d\alpha \, E_{\alpha} c_{\alpha}^\dagger c_{\alpha}$, where the field operators are Dirac normalized.
To include the interaction term $H^{(1)}$, we proceed in much the same way as in the time-dependent case. The main point is to isolate the core difficulty of the interacting problem, which is in this case to find time-independent crossing states satisfying the appropriate conditions. We begin by defining time-independent versions of the $A$ and $B$ operators:

$$A_{\alpha,\text{in}} = [H, c_{\alpha,\text{in}}] - E_{\alpha} c_{\alpha,\text{in}}, \quad (2.185a)$$
$$B_{\alpha_1\alpha_2,\text{in}} = \{ A_{\alpha_2,\text{in}}, c_{\alpha_1,\text{in}} \} = B^{(\text{red})}_{\alpha_1\alpha_2,\text{in}} - B^{(\text{red})}_{\alpha_2\alpha_1,\text{in}}, \quad (2.185b)$$

As in the time-dependent case, we assume that $H^{(0)}|0\rangle = H^{(1)}|0\rangle = A_{\alpha,\text{in}}|0\rangle = 0$ and that $B_{\alpha_1\alpha_2,\text{in}}$ commutes with any $c_{\alpha,\text{in}}$. The same manipulations result in the time-independent version of the general form [Eqs. (2.39) and (2.40)] for the wavefunction:

$$|\Psi_{\alpha_N,\beta,\text{in}}\rangle = \sum_{n=0}^{N} \sum_{m \in I_n(N)} (\text{sgn } m) c_{\alpha_n/m,\text{in}}^\dagger |\Phi_{\alpha_m,\beta,\text{in}}\rangle, \quad (2.186)$$

where the crossing states are given in terms of unsymmetrized crossing states differently for type A and type B models. In a type A model, we have:

$$|\Phi_{\alpha_m,\beta,\text{in}}\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) |\chi_{\alpha_m,\sigma,\beta,\text{in}}\rangle, \quad (2.187)$$

where the unsymmetrized crossing states must satisfy:

$$\left( H - \sum_{\ell=1}^{n} E_{\ell} \right) |\chi_{\alpha_1...\alpha_n,\beta,\text{in}}\rangle = -A_{\alpha_n,\text{in}} |\chi_{\alpha_1...\alpha_{n-1},\beta,\text{in}}\rangle, \quad (2.188a)$$
$$|\chi_{\beta,\text{in}}\rangle = |\beta\rangle. \quad (2.188b)$$

Also, each $|\chi_{\alpha_n,\beta,\text{in}}\rangle$ must satisfy the boundary condition of having no plane waves coming in from infinity (since the incoming $\alpha_N$ quantum numbers are already accounted for in $|\Psi^{0}_{\alpha_N,\beta,\text{in}}\rangle$). This last condition is the time-independent analog of Eq. (2.42b) (namely, that the unsymmetrized crossing states do not disturb the initial condition in time; here the initial condition is replaced by a time-independent boundary condition).

In a type B model, we have:

$$|\Phi_{\alpha_m,\beta,\text{in}}\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{p \in P(m)} |\chi_{\alpha_{p\sigma},\beta,\text{in}}\rangle, \quad (2.189)$$
where the unsymmetrized crossing states satisfy a more complicated condition than in the type A case, which we now state. Given a partition $\mathbf{p}$ of $(1, \ldots, n)$, the crossing state condition is:

$$
(H - \sum_{\ell=1}^{n} E_{\ell}) |\chi_{\alpha_{\mathbf{p}}, \beta, \text{in}}\rangle = \begin{cases} 
-B_{\alpha_{n-1} \alpha_{n}, \text{in}} |\chi_{\alpha_{\mathbf{p}/(n-1,n)}, \beta, \text{in}}\rangle & q = 2 \\
-A_{\alpha_{n}, \text{in}} |\chi_{\alpha_{\mathbf{p}/n}, \beta, \text{in}}\rangle & 3 \leq q \leq n
\end{cases},
$$

(2.190a)

$$
|\chi_{\alpha, \beta, \text{in}}\rangle = |\beta\rangle.
$$

(2.190b)

As in the type A case, each $|\chi_{\alpha, \beta, \text{in}}\rangle$ must satisfy the boundary condition of having no plane waves coming in from infinity.

While we have specified incoming boundary conditions, the entire procedure carries through with any other choice of boundary conditions (e.g. outgoing). Indeed, the entire formalism could in principle be applied to find eigenstates satisfying any boundary condition, even one in a finite volume system and unrelated to scattering theory. However, as in the time-dependent case, the only applications so far are in quantum impurity models.

The formalism presented in earlier sections for calculating expectation values also carries through straightforwardly. The derivative approach of Sec. 2.3.2 requires some modification, as we now describe.

Suppose we wish to find the expectation value $\langle \Psi(E)|\mathcal{O}|\Psi(E)\rangle$, where $H|\Psi(E)\rangle = E|\Psi(E)\rangle$. We assume that $E$ varies continuously (as it does if $|\Psi(E)\rangle$ is a scattering state in an infinite volume system), so that there is a family of nearby states $|\Psi(E')\rangle$ with $E'$ later set to $E$. Let $|\overline{\Psi}(E)\rangle$ be a $\lambda$-dependent family of states satisfying $\overline{H}|\overline{\Psi}(E)\rangle = E|\overline{\Psi}(E)\rangle$. Then, with $\overline{H}$ of the same form as in Eq. (2.68), we have the following result:

$$
\langle \Psi(E)| \left( \sum_{j=1}^{n} \frac{dh_{j}(\lambda)}{d\lambda} |_{\lambda=\lambda} \right) |\Psi(E)\rangle = \lim_{E' \to E} (E - E') \frac{\partial}{\partial \lambda} |_{\lambda=\lambda} \langle \Psi(E')|\overline{\Psi}(E)\rangle.
$$

(2.191)

Naively, the right-hand side appears to be zero; however, we find in applications that the $\lambda$ derivative produces a $1/(E - E')$ pole that cancels the prefactor. Let us note also that the varying states $|\overline{\Psi}(E)\rangle$ do not need to satisfy any special boundary conditions – even
if $|\psi(E)\rangle$ is a scattering “in” state, $|\overline{\psi}(E)\rangle$ need not be, as long as $|\overline{\psi}(E)\rangle|_{\lambda=\lambda} = |\psi(E)\rangle$ holds.

We now provide the proof of the simplest case of Eq. (2.191), in which $\mathcal{H} = H + \overline{\lambda}\mathcal{O}$. Notice that $\langle\Psi(E')\rangle$ is a function of $E'$ and $|\overline{\psi}(E)\rangle$ is a function of $E$ and $\overline{\lambda}$; the key point is that $E$, $E'$ and $\overline{\lambda}$ are all independent parameters. Then we have:

$$\langle\psi(E)|\mathcal{O}|\psi(E)\rangle = \lim_{E'\to E} \left. \frac{\partial}{\partial \overline{\lambda}} \right|_{\lambda=\lambda} \langle\psi(E')|\mathcal{O}|\overline{\psi}(E)\rangle = \langle\psi(E)|\mathcal{O}|\psi(E)\rangle.$$  \hspace{1cm} (2.192a)

$$\lim_{E'\to E} \left. \frac{\partial}{\partial \overline{\lambda}} \right|_{\lambda=\lambda} \langle\psi(E')|\mathcal{H} - H|\overline{\psi}(E)\rangle = \lim_{E'\to E} (E - E') \left. \frac{\partial}{\partial \overline{\lambda}} \right|_{\lambda=\lambda} \langle\psi(E')|\overline{\psi}(E)\rangle. \hspace{1cm} (2.192b)$$

The more general case (2.191) can be shown similarly.
Chapter 3
Two non-interacting models

The new approach developed in the previous chapter is mainly of interest for its application to interacting problems. However, it is often a useful starting point to turn off the interactions, both as a check and as a way of presenting, in a simple setting, some points that also arise in a more complicated fashion in interacting problems. To this end, we apply a wavefunction approach to two free models: the potential scattering model and the resonant level model (RLM). The first serves as a warm-up or toy version of the Kondo model, and the second serves the same purpose for the interacting resonant level model and Anderson impurity model.

Our approach is to present the solution directly, then indicate how it is a special case of the more powerful technology developed in the previous chapter.

3.1 Potential scattering model – one lead

3.1.1 Wavefunction

The one lead potential scattering model (making the usual linearization and reduction to one dimension) is:

\[ H = -i \int_{-L/2}^{L/2} dx \psi^\dagger(x) \frac{d}{dx} \psi(x) + J^\prime \psi^\dagger(0) \psi(0). \]  

(3.1)

The \( J^\prime \) term is an external delta function potential at \( x = 0 \) (compare to the Kondo model, in which the impurity at \( x = 0 \) has quantum degrees of freedom). The model meets the
general conditions described in Sec. 2.2. The field operators are:

\[ c^\dagger_k \equiv c^\dagger = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \, e^{ikx} \psi^\dagger(x), \]  

(3.2)

with \( k \) quantized to integer multiples of \( \frac{2\pi}{L} \) due to the periodic boundary conditions. The only fixed impurity state \(|\beta\rangle\) is the empty state \(|0\rangle\), so we will drop the index \( \beta \) entirely. As for the separation of \( H \) into \( H^{(0)} + H^{(1)} \), there are two ways to proceed. In this chapter, we set \( H^{(0)} = H \) and \( H^{(1)} = 0 \), which is simpler; later, we set \( H^{(1)} = J' \psi^\dagger(0)\psi(0) \) in order to see what the solution looks like if the potential scattering is treated as an interaction.

The initial state at \( t = 0 \) is taken to be a free product state with arbitrary momenta: \(|\Psi_{kN}\rangle = c^\dagger_{kN}|0\rangle\). The quench consists of turning on the \( J' \) term at \( t = 0 \):

\[ |\Psi_{kN}(t)\rangle = e^{-iHt}|\Psi_{kN}\rangle = c^\dagger_{kN}(t)|0\rangle, \]  

(3.3)

where \( c^\dagger_k(t) = e^{-iHt}c^\dagger_k e^{iHt} \). It is straightforward to solve for the \( c^\dagger(t) \) operators. Time evolution will keep the momentum operators within the single particle sector:

\[ c^\dagger_k(t) = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \, g_k(t, x) \psi^\dagger(x), \]  

(3.4)

where the function \( g_k(t, x) \) is determined by the equation of motion \([H, c^\dagger_k(t)] - \frac{d}{dt}c^\dagger_k(t) = 0\) with the initial condition \( c^\dagger_k(t = 0) = c^\dagger_k \). These translate to the following requirements on \( g_k(t, x) \):

\[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) g_k(t, x) + J' g_k(t, 0) \delta(x) = 0, \]  

(3.5a)

\[ g_k(0, x) = e^{ikx}. \]  

(3.5b)

The delta function comes from the local nature of the scattering potential. It follows that the function \( g_k(t, x) \) must have a discontinuity at \( x = 0 \) so that the derivative can generate another delta function.

The solution is:

\[ g_k(t, x) = e^{-ik(t-x)} \left[ 1 + M\Theta(0 < x < t) + M^*\Theta(t < x < 0) \right], \]  

(3.6)
where:

\[ M = \frac{-iJ'}{1 + i\frac{J'}{2}} \]  

(3.7)

To see this, we make the following ansatz (focusing on the case of positive time for now):

\[ c_k^\dagger(t) = e^{-ikt}c_k^\dagger + \frac{1}{\sqrt{L}} \int dx \, F_k(t-x)\Theta(0 < x < t)\psi^\dagger(x), \]  

(3.8)

where \( F_k \) is a single variable function to be determined. This ansatz puts all of the discontinuity explicitly in Heaviside functions (we take \( F_k \) to be continuous), satisfies the initial condition at \( t = 0 \), and has the effect of the quench contained within the “light cone” \( x < t \).

Taking \( F_k \) to depend on \((t, x)\) only through the difference guarantees the cancellation of certain unwanted terms in the calculation; in particular, we have:

\[
\left[-i \int_{-L/2}^{L/2} dx \, \frac{d}{dx} \psi^\dagger(x), c_k^\dagger(t)\right] - i \frac{\partial}{\partial t} c_k^\dagger(t) = \\
\frac{1}{\sqrt{L}} \int dx \, F_k(t-x) \left[ \left(-i \frac{\partial}{\partial x} - i \frac{\partial}{\partial t}\right) \Theta(0 < x < t) \right] \psi^\dagger(x) = \frac{1}{\sqrt{L}} F_k(t)(-i)\Theta(0 < t)\psi^\dagger(0).
\]  

(3.9)

The first equation uses the fact that \( F_k \) only depends on the difference of coordinates (the differential operators together yield zero on \( F_k \)). With a generic function \( F_k \) of both \( t \) and \( x \), we would have obtained an additional unwanted term of the form of an integral \( \psi^\dagger(x) \) (multiplied by a non-singular function of \( x \)). In the second equation, we have used \( \Theta(0 < x < t) = \Theta(0 < x)\Theta(x < t) \) to obtain \((-i \frac{\partial}{\partial t} - i \frac{\partial}{\partial x}) \Theta(0 < x < t) = -i\delta(x)\Theta(0 < t)\), noting that \( \Theta(x < t) = \Theta(t - x) \) is a function only of the difference of coordinates.

The other term in the Schrodinger equation also involves \( \psi^\dagger(0) \):

\[ [J'\psi^\dagger(0)\psi(0), c_k^\dagger(t)] = \frac{J'}{\sqrt{L}} e^{-ikt}\psi^\dagger(0) + \frac{J'}{\sqrt{L}} \int dx \, F_k(t-x)\delta(x)\Theta(0 < x < t)\psi^\dagger(x) \]  

(3.10a)

\[ = \frac{J'}{\sqrt{L}} e^{-ikt}\psi^\dagger(0) + \frac{J'}{\sqrt{L}} F_k(t)\frac{1}{2} \Theta(0 < t)\psi^\dagger(0). \]  

(3.10b)

Here, we have made the replacement \( \delta(x)\Theta(x) \to \frac{1}{2}\delta(x) \), which is equivalent to saying that under multiplication by \( \delta(x) \), a function (ultimately \( g_k(t, x) \) from above) that is discontinuous at \( x = 0 \) can be replaced by the average of its left and right limits as \( x \to 0 \). This
“averaging prescription” is used in all of the explicit wavefunctions in the main text of this thesis. See Sec. 3.4 for more detail.

Collecting terms, we find that the equation of motion for $c_k^\dagger(t)$ reduces to:

$$-iF_k(t) + J' \left[ e^{-ikt} + \frac{1}{2} F_k(t) \right] = 0,$$

hence: $F_k(t) = \mathcal{M} e^{-ikt}$, \hspace{1cm} (3.11a)

in agreement with Eq. (3.6).

Strictly speaking, the above calculation works for $0 < t < L/2$. Exactly at the point $t = 0$, we appear to have a difficulty, since we have implicitly set $\Theta(0 < t) = 1$ for $t = 0$ (rather than, say, 0 or 1/2). To remove this doubt, we generalize the initial ansatz to include negative times:

$$c_k^\dagger(t) = e^{-ikt} c_k^\dagger + \frac{1}{\sqrt{L}} \int dx \ [F_k(t-x)\Theta(0 < x < t) + G_k(t-x)\Theta(t < x < 0)] \psi^\dagger(x).$$

Repeating the above calculation, we find:

$$[H, c_k^\dagger(t)] - i \frac{\partial}{\partial t} c_k^\dagger(t) = \frac{J'}{\sqrt{L}} e^{-ikt} \psi^\dagger(0) + \frac{1}{\sqrt{L}} \left[ -iF_k(t)\Theta(0 < t) + iG_k(t)\Theta(t < 0) \right] \psi^\dagger(0)$$

$$+ \frac{J'}{\sqrt{L}} \left[ F_k(t)\frac{1}{2}\Theta(0 < t) + G_k(t)\frac{1}{2}\Theta(t < 0) \right] \psi^\dagger(0).$$

The trick is to write $\frac{J'}{\sqrt{L}} e^{-ikt} \psi^\dagger(0) = \frac{J'}{\sqrt{L}} e^{-ikt} \psi^\dagger(0) [\Theta(0 < t) + \Theta(t < 0)]$ and then separately cancel the $\Theta(0 < t)$ and $\Theta(t < 0)$ parts. This leads to the same condition on $F_k$ as found previously, and also:

$$iG_k(t) + J' \left[ e^{-ikt} + \frac{1}{2} G_k(t) \right] = 0.$$

We then conclude that $G_k(t) = F_k^*(t)$, in agreement with Eq. (3.6). In using $1 = \Theta(0 < t) + \Theta(t < 0)$, we are being deliberately vague about which Heaviside function makes up the unity at $t = 0$; we could instead write it as $1 = \Theta(0 \leq t) + \Theta(t < 0)$ (declaring that the positive branch is 1 at $t = 0$), or $1 = \Theta(t) + \Theta(-t)$ with $\Theta(0) = 1/2$. The boundary point does not matter unless the Heaviside is multiplied by a delta function (in which case we need some prescription such as the averaging discussed in Sec. 3.4).
The constant $\mathcal{M}$ (3.7) satisfies the following identity:

$$\mathcal{M} + \mathcal{M}^* + |\mathcal{M}|^2 = 0. \quad (3.15)$$

This is a statement of the optical theorem of scattering theory; $\mathcal{M}$ is related to the $S$-matrix (which must be a pure phase, on general grounds) via:

$$S = 1 + \mathcal{M} = \frac{1 - iJ' / 2}{1 + iJ' / 2}. \quad (3.16)$$

To see this, we take the long time limit – in a precise sense now to be defined – of the operator $c^\dagger_k(t)$. It is important to remove the overall phase factor and to take the limit in a pointwise sense: we find the limit reached at each point $x$ without requiring that the limit is reached uniformly for all $x$. To do this for all $x$, we send $L \to \infty$, removing the prefactor $1/\sqrt{L}$ to convert from Kronecker delta normalization to Dirac delta normalization. The result is the scattering “in” operator:

$$c^\dagger_{k,\text{in}} = \int dx \lim_{t \to \infty} e^{ikt} \lim_{L \to \infty} \sqrt{L} \{ \psi(x), c^\dagger_k(t) \} = \int dx \ e^{ikx} [\Theta(-x) + (1 + \mathcal{M}) \Theta(x)] \psi^\dagger(x). \quad (3.17)$$

Thus, the quantity $S = 1 + \mathcal{M}$ is the phase shift for an electron crossing the potential. The scattering “out” operator can be found similarly by taking $t \to -\infty$, instead. To match the usual convention, we introduce the $T$-matrix, given by $T = i\mathcal{M}$. Note that to leading order in $J'$, we have $T = J'$, in agreement with the Born approximation.

We have seen that the exact solution for $N$ particles follows easily once we have the $c^\dagger(t)$ operators. To put this in the language of the previous chapter, we note that the $A_k(t)$ operators of this model are identically zero, which implies that the crossing states all vanish and $|\Psi_{kN}(t)\rangle = |\Psi_{kN}^0(t)\rangle$ is the full solution. We can also solve this model with the potential scattering term treated as an interaction (see Sec. A.1 and set the Kondo coupling $J$ to zero). This leads to non-vanishing crossing states and therefore a more complicated form of the wavefunction. Calculating observables, we find simplifications that reflect the fact that the wavefunction is ultimately a product of single particle operators.
3.1.2 Evaluation of an observable

We evaluate the density of electrons at the origin:

\[ \langle \psi^\dagger(0)\psi(0) \rangle_t \equiv \langle \Psi_{kN}(t) | \psi^\dagger(0)\psi(0) | \Psi_{kN}(t) \rangle. \tag{3.18} \]

We will see below that this observable is unphysical; still, it serves as a first example application of the derivative formula from Chapter 2. This observable can be found by differentiating with respect to \( J' \). Following the notation introduced in Sec. 2.3.2, we denote the varying parameter by \( J' \), its corresponding Hamiltonian by \( H' \), etc. Recall that we have some freedom in defining the \( \phi \)-dependent family of initial states – any states can be chosen as long as removing the bar yields the initial state \( |\Psi_{kN}\rangle \) that we are interested in. For this calculation, we make the simplest choice, \( |\Psi_{kN}\rangle = |\Psi_{kN}\rangle \), whose time evolution is described by \( \overline{c}^\dagger_k(t) \) operators:

\[ |\Psi_{kN}(t)\rangle = e^{-iH't} |\Psi_{kN}\rangle = \overline{c}^\dagger_{kN}(t) |0\rangle, \tag{3.19} \]

where:

\[ \overline{c}^\dagger_k(t) = e^{-iH't}c^\dagger_k e^{iH'} = e^{-ikt}c^\dagger_k + \frac{1}{\sqrt{L}} \int dx J_k(t-x)\Theta(0 < x < t)\psi^\dagger(x), \tag{3.20a} \]

\[ J_k(t) = Me^{-ikt}, \quad M = \frac{-iJ'}{1 + \frac{i}{2}J'} \tag{3.20b} \]

The derivative formula (2.66) then yields:

\[ \langle \psi^\dagger(0)\psi(0) \rangle_t = i \frac{\partial}{\partial t} \frac{\partial}{\partial J'} \bigg|_{J' = J} \langle 0 | c_{kN}(t)\overline{c}^\dagger_{kN}(t) |0\rangle \tag{3.21a} \]

\[ = i \frac{\partial}{\partial t} \frac{\partial}{\partial J'} \bigg|_{J' = J} \sum_{\sigma} (\text{sgn } \sigma) \prod_{j=1}^N \{ c_{k\sigma(j)}(t), \overline{c}^\dagger_{kj}(t) \} \tag{3.21b} \]

\[ = \sum_{j=1}^N i \frac{\partial}{\partial t} \frac{\partial}{\partial J'} \bigg|_{J' = J} \{ c_{kj}(t), \overline{c}^\dagger_{kj}(t) \}, \tag{3.21c} \]

where we have noted that each anticommutator becomes a Kronecker delta if the bar is removed. (We are assuming that there are no repeats in the list \( (k_1, \ldots, k_N) \) of initial momenta, since the wavefunction would just be zero otherwise.) The last line also be
reached directly via normal ordered formula 3 (2.77) (recall that all crossing states are zero in this simple case). The derivatives of the anticommutator are easily evaluated:

\[
\left. i \frac{\partial}{\partial t} \frac{\partial}{\partial J'} \right|_{J=J'} \{ c_k(t), c_k^\dagger(t) \} = \left. i \frac{\partial}{\partial t} \frac{\partial}{\partial J} \right|_{J=J'} \left[ 1 + \frac{t}{L} (\mathcal{M} + \mathcal{M}^* + \mathcal{M}^* \mathcal{M}^*) \right] \\
= \left. i \frac{1}{L} \frac{\partial}{\partial J} \right|_{J=J'} (S^* \mathcal{S} - 1) = \left. i \frac{1}{L} S^* \frac{\partial}{\partial J} \right|_{J=J'} \mathcal{S} = \frac{1}{L} \frac{1}{1 + \frac{1}{4} J'^2},
\]

where we have taken \( t > 0 \) throughout. We have written the answer in terms of \( S \)-matrices using the optical identity (3.15), which is not really necessary here but will more useful in the case of the Kondo model. We have found that there no dependence on the momenta, so the sum over \( j \) yields:

\[
\langle \psi^\dagger(0) \psi(0) \rangle_t = \frac{N}{L} \frac{1}{1 + \frac{1}{4} J'^2}.
\]

We can take the initial \( N \) quantum numbers to describe a Fermi sea (though it makes no difference). Setting \( J' = 0 \) recovers the free density \( N/L \), as expected. Surprisingly, it seems that the density decreases (relative to the \( J' = 0 \) model) even if \( J' < 0 \), i.e. an attractive potential. For reasons explained below, this is an artifact of our having calculated the density precisely at the point \( x = 0 \); in fact, the density of electrons is completely unaffected by the potential.

Let us do the same calculation directly – that is, without using the derivative formula. We find:

\[
\langle \psi^\dagger(0) \psi(0) \rangle_t = \langle 0 | c_{kN}(t) \psi^\dagger(0) \psi(0) c_{kN}^\dagger(t) | 0 \rangle \\
= \sum_{j=1}^{N} \{ c_{k_j}(t), \psi^\dagger(0) \} \{ \psi(0), c_{k_j}(t) \} = \sum_{j=1}^{N} | \{ \psi(0), c_{k_j}(t) \} |^2.
\]

The anticommutator is easily evaluated:

\[
\{ \psi(0), c_k(t) \} = \frac{1}{\sqrt{L}} e^{-ikt} \left( 1 + \frac{1}{2} \mathcal{M} \right),
\]

(where we have assumed \( t > 0 \), and, using the optical identity (3.15), we obtain the same
We could also find this using normal ordered formula 4 (2.78) with $O_1^\dagger = \psi^\dagger(0)$, $O_2 = \psi(0)$, and $O_{\text{vac}} = 1$. As in the derivative case, the calculation is greatly simplified due to the fact that the crossing states all vanish. All normal ordered products vanish except for $(0|0) := 1$, which can only be obtained in the last term in brackets in (2.78), and only for $n = 1$.

Since the derivative formula relies on the fact that the time evolving state satisfies the Schrodinger equation, we can view the agreement with the direct calculation as a consistency check that we have found the time evolving state correctly. Still, the physical meaning of what we have calculated in this case is in doubt.

The problem we are running into is generic to wavefunctions with discontinuities. What we have been calculating corresponds to declaring the value of the wavefunction at $x = 0$ to be the average of its value on either side of zero, then taking the modulus squared; the more physically correct procedure would be to find the modulus of the wavefunction on both sides and then average. The most correct approach of all would be to say that the density at any single point has no meaning, seeing as we only get physical answers by integrating the density over some set.\footnote{A set of measure greater than zero, to be precise.}

As a simple example to illustrate the problem, suppose we wish to calculate the density in the following state:

$$|\Psi\rangle = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ (\Theta(-x) - \Theta(x)) \psi^\dagger(x).$$

In other words, the wavefunction is $\frac{1}{\sqrt{L}}$ to the left of zero and $-\frac{1}{\sqrt{L}}$ to the right. The density, or modulus squared of the wavefunction, is plainly equal to $\frac{1}{L}$ for every non-zero $x$; if we insist on finding the value for the density strictly at $x = 0$, the most sensible choice
is $\frac{1}{L}$ (the average value from the left and right). On the other hand, the average of the wavefunction on either side yields zero strictly at the origin, which would lead us to say that the density is zero at the origin and $\frac{1}{L}$ everywhere else. While this is still correct – since changing the density at a single point has no effect if the density is integrated with any reasonable function – it does indicate that our calculation of the density strictly at zero could give a misleading impression.

The ambiguity is resolved if we calculate the $x$-dependent density:

$$\langle \psi^\dagger(x)\psi(x) \rangle_t = \sum_{j=1}^{N} |\{\psi(x), c_{kj}(t)\}|^2 = \sum_{j=1}^{N} \frac{1}{L} |1 + \mathcal{M}|^2 = \frac{N}{L},$$

(3.28)

where we have taken $0 < x < t$, and where the last equality follows from the optical identity (3.15). The same answer is obtained if instead $0 < t < x$, since then the wavefunction is a pure plane wave. Thus, the potential has no effect at all on the density. The answer we obtained for the point $x = 0$ (averaging the wavefunction before taking the modulus) does not give an accurate picture for what is happening in the system.

In interacting problems such as the Kondo model, we will not find it so easy to calculate $x$-dependent observables; indeed, it is much easier if the operator we are evaluating is exactly at $x = 0$, since this often means we can calculate it using the derivative method. One procedure is to calculate the observable strictly at zero using the derivative formula, then also using direct calculation; if the results agree, then it is straightforward to modify the direct calculation so that the observable is evaluated at $0^+$ (that is, approaching zero from the right) rather than strictly at zero, which removes any difficulties of averaging. While the observable is then still just at single point (and hence meaningless), it is more likely to be a representative point than $x = 0$ obtained by averaging.

Let us note here that this subtlety only occurs because we considered a product of field operators at the same position. The current operator of the two lead model (see next section, or next chapter) has two fields both at $x = 0$, but they are not the same type of field (one is from lead 1 and the other from lead 2). Thus, the issue discussed above that arises in calculating the density does not arise in calculating the current.
3.2 Potential scattering – two leads

3.2.1 Wavefunction

As a warm-up to the calculation of the current in the Kondo model, we consider the two lead version of this free model:

\[
H = -i \int_{-L/2}^{L/2} dx \: \psi_1^\dagger(x) \frac{d}{dx} \psi_1(x) - i \int_{-L/2}^{L/2} dx \: \psi_2^\dagger(x) \frac{d}{dx} \psi_2(x) + \frac{1}{2} J' (\psi_1^\dagger(0) + \psi_2^\dagger(0)) (\psi_1(0) + \psi_2(0)).
\] (3.29a)

The field operators \( c_\alpha^\dagger \) now depend on a lead index \( \gamma \) in addition to momentum \( k \):

\[
c_\alpha^\dagger \equiv c_{\gamma k}^\dagger = \frac{1}{\sqrt L} \int_{-L/2}^{L/2} dx \: e^{ikx} \psi_\gamma^\dagger(x).
\] (3.30)

Note that the potential scattering part of the Hamiltonian includes two types of terms: potential scattering within the same lead, and hopping between the leads. A more general version of this model would allow an arbitrary Hermitian matrix of couplings in the lead 1/lead 2 basis; we have made the simplest choice, so that the model separates into an “odd” part with no potential and an “even” part that is identical to the one lead model.

The unitary change of variables to the odd/even basis is given by:

\[
\begin{pmatrix}
\psi_o(x) \\
\psi_e(x)
\end{pmatrix} = U \begin{pmatrix}
\psi_1(x) \\
\psi_2(x)
\end{pmatrix}, \quad U = \frac{1}{\sqrt 2} \begin{pmatrix}
1 & -1 \\
1 & 1
\end{pmatrix}.
\] (3.31)

In the odd/even basis, the Hamiltonian separates into two independent (commuting) parts:

\[
H_o = -i \int_{-L/2}^{L/2} dx \: \psi_0^\dagger(x) \frac{d}{dx} \psi_0(x),
\] (3.32a)

\[
H_e = -i \int_{-L/2}^{L/2} dx \: \psi_e^\dagger(x) \frac{d}{dx} \psi_e(x) + J' \psi_e^\dagger(0) \psi_e(0),
\] (3.32b)

\[
H = H_o + H_e.
\] (3.32c)
Since the odd sector consists of free fermions, the time-dependent operators evolve by phases:
\[ c_{ok}^\dagger(t) \equiv e^{-iH_t} c_{ok}^\dagger e^{iH_t} = e^{-ikt} c_{ok}^\dagger, \]  
(3.33)
while the time-dependent operators in the even sector can be read off from the solution of the one lead model (we focus on \( t \geq 0 \) from now on):
\[ c_{ek}^\dagger(t) \equiv e^{-iH_t} c_{ek}^\dagger e^{iH_t} = e^{-ikt} c_{ek}^\dagger + \frac{1}{\sqrt{L}} \int dx F_k(t-x) \Theta(0 < t < x) \psi_e^\dagger(x). \]  
(3.34)
Then the time dependent operators in the original basis can be found by rotating back:
\[
\begin{pmatrix}
    c_{1k}(t) \\
    c_{2k}(t)
\end{pmatrix} = U(t) \begin{pmatrix}
    c_{ok}(t) \\
    c_{ek}(t)
\end{pmatrix}, \quad U(t) = \frac{1}{\sqrt{2}} \begin{pmatrix}
    1 & 1 \\
    -1 & 1
\end{pmatrix}. 
\]  
(3.35)

We can gain some insight into these operators by writing them in position space and taking the long time limit [as in Eq. (3.17)] to get scattering “in” operators:
\[
c_{\gamma k}^\dagger(t) = e^{-ikt} c_{\gamma k}^\dagger + \frac{1}{\sqrt{L}} \int dx \ e^{-ik(t-x)} \frac{1}{2} M \Theta(0 < x < t) [\psi_1^\dagger(x) + \psi_2^\dagger(x)] \quad (\gamma = 1, 2),
\]  
(3.36a)
\[
c_{\gamma k,\text{in}}^\dagger = \int dx \ e^{ikx} \left\{ \Theta(-x) + \left( 1 + \frac{1}{2} M \right) \Theta(x) \right\} \psi_\gamma^\dagger(x) + \frac{1}{2} M \Theta(x) \psi_\gamma^\dagger(x) \} \quad (\gamma = 1, 2),
\]  
(3.36b)
where \( \gamma = 2 \) if \( \gamma = 1 \) and vice-versa. The operator \( c_{\gamma k,\text{in}}^\dagger \) creates a state in which a plane wave comes in from the left in lead \( \gamma \) only, with subsequent scattering into both leads as the plane wave crosses the potential at the origin (Fig. 3.1b).

It is important to distinguish between the \( S \)-matrix of the even sector (or one lead model), which is a phase shift \( S = 1 + M = 1 - iT \), and the full \( S \)-matrix of the two lead model given as follows:
\[
S_{\text{two leads}} = \begin{pmatrix}
    1 & 0 \\
    0 & 1
\end{pmatrix}, \quad \text{where:} \quad T_{\text{two leads}} = \begin{pmatrix}
    T/2 & T/2 \\
    T/2 & T/2
\end{pmatrix}.
\]  
(3.37)
Even sector (i.e. one lead model)

Two lead model

Figure 3.1: Single-particle scattering picture. We use the notation $M = -i\mathcal{T}$, with $\mathcal{M}$ given in Eq. (3.7). (a) In the even sector – which is a copy of the one lead model – an electron comes in from the left and scatters off the potential with a phase shift $S = 1 - i\mathcal{T}$. This process is described by the scattering operator $c_{\gamma k,\text{in}}^\dagger$ [Eq. (3.17) with $\psi^\dagger \rightarrow \psi^\dagger_{\gamma k}$]. (b) In the two lead model, an electron in lead 1 comes in from the left and scatters off the potential into both leads. This process is described by the scattering operator $c_{1k,\text{in}}^\dagger$ [Eq. (3.36b)]. A similar diagram can be drawn with an incoming electron in lead 2, instead, and the full $S$-matrix is $S_{\text{two leads}}$ [Eq. (3.37)]. Note that when $\mathcal{T} = -2i$, there is perfect transmission – the electron from lead 1 goes completely into lead 2.

Generally speaking, we find the even sector quantities to be more useful (once we transition to interacting problems).

The operator $c_{\gamma k}^\dagger(t)$ describes a finite time, finite volume process following the quench of turning on the potential scattering at $t = 0$. Since model is non-interacting, these time dependent operators are sufficient to solve for the time evolution of an initial state with arbitrary momenta and lead indices:

$$|\Psi_{\gamma NkN}\rangle \equiv c_{\gamma NkN}^\dagger|0\rangle, \quad |\Psi_{\gamma NkN}(t)\rangle \equiv e^{-iHt}|\Psi_{\gamma NkN}\rangle = c_{\gamma NkN}^\dagger(t)|0\rangle.$$  \tag{3.38}

Many of the calculations below will be made easier by going to the odd/even basis, even though the quantum numbers in the initial state we are ultimately interested in (two Fermi seas) are in the lead 1/lead 2 basis. For later reference, we note the following anticommutation relations:

$$\{\psi_\alpha(x), c_{\alpha k}^\dagger(t)\} = \frac{1}{\sqrt{L}}e^{-ikt},$$  \tag{3.39a}

$$\{\psi_\alpha(x), c_{\alpha k}(t)\} = \frac{1}{\sqrt{L}}\left[e^{-ik(t-x)} + F_k(t-x)\Theta(0 < x < t)\right],$$  \tag{3.39b}

$$\{\psi_\alpha(x), c_{\alpha k}^\dagger(t)\} = \{\psi_\alpha(x), c_{\alpha k}^\dagger(t)\} = 0.$$  \tag{3.39c}
from which we also obtain (for $\gamma = 1, 2$):

\[
\{\psi_\alpha(x), c_{\gamma k}^\dagger(t)\} = \frac{1}{\sqrt{2L}} (-1)^{\gamma-1} e^{-ik(t-x)}, \tag{3.40a}
\]

\[
\{\psi_\epsilon(x), c_{\gamma k}^\dagger(t)\} = \frac{1}{\sqrt{2L}} \left[ e^{-ik(t-x)} + F_k(t-x) \Theta(0 < x < t) \right]. \tag{3.40b}
\]

### 3.2.2 Evaluation of the current

With two leads, we can calculate a more interesting quantity – the charge current between the leads. We define this quantity precisely, then calculate it in several equivalent forms, finding the same answer each time.

The Hamiltonian conserves the total number of electrons $N_1 + N_2$. We therefore define the average current flowing from lead 1 to lead 2 to be the rate of electrons leaving lead 1:

\[
I(t) = -\frac{d}{dt} \langle \Psi_{\gamma kN}(t) | \hat{N}_1 | \Psi_{\gamma kN}(t) \rangle \tag{3.41}
\]

where $\hat{N}_1 = \int_{-L/2}^{L/2} dx \, \psi_1^\dagger(x) \psi_1(x)$. Since this calculation involves the integral of a density (rather than the density at the single point $x = 0$), there should be none of the ambiguities found in Sec. 3.1.2. To have a way of checking the answer, it is useful to write the current in another form. Following standard steps, we obtain:

\[
I(t) = -\langle \Psi_{\gamma kN}(t) | i[H, \hat{N}_1] | \Psi_{\gamma kN}(t) \rangle \tag{3.42a}
\]

\[
= \langle \Psi_{\gamma kN}(t) | \left( \int_{-L/2}^{L/2} dx \frac{d}{dx} \left[ \psi_1^\dagger(x) \psi_1(x) \right] + \hat{I} \right) | \Psi_{\gamma kN}(t) \rangle, \tag{3.42b}
\]

where: $\hat{I} = \frac{1}{2} J'[\psi_1^\dagger(0) \psi_2(0) + \text{h.c.}} \tag{3.42c}$

The total derivative term is usually dropped because of the periodic boundary conditions; one then identifies $\hat{I}$ as the current operator. We will refer to $\hat{I}$ as the “local form” of the current, as opposed to the original form defined as the rate of change of $N_1$.

While we do indeed find that the expectation value of this operator agrees with the definition of $I(t)$ given previously, the ignoring of the boundary term should be examined more closely. Consider the state $|\Psi\rangle = \int_{-L/2}^{L/2} dx \, g(x) \psi^\dagger(x) |0\rangle$ in the one lead model, for
some function $g(x)$. The expectation value of the boundary term is:

$$\int_{-L/2}^{L/2} dx \langle \Psi | \frac{d}{dx} \left[ \psi^+(x) \psi(x) \right] | \Psi \rangle = \sum_j \left( |g(x_j^+)|^2 - |g(x_j^-)|^2 \right)$$

(3.43a)

$$= \sum_j (\langle \Psi | \left( \psi^+(x_j^+) \psi(x_j^+) - \psi^+(x_j^-) \psi(x_j^-) \right) | \Psi \rangle)$$

(3.43b)

where the sum is over points of discontinuity in the function $g(x)$.

Since the wavefunction in the present case has discontinuities, it is not clear that we can drop the boundary term. To be precise, the discontinuities are to be found at $x = 0$ and $x = t$, and the contribution of the boundary term is therefore:

$$\langle \Psi_{\gamma_N} | \int_{-L/2}^{L/2} dx \frac{d}{dx} \left[ \psi^+_1(x) \psi_1(x) \right] | \Psi_{\gamma_N} \rangle =$$

$$\langle \Psi_{\gamma_N} | \left( \psi^+_1(0^+) \psi_1(0^+) - \psi^+_1(0^-) \psi_1(0^-) \right) | \Psi_{\gamma_N} \rangle$$

$$+ \langle \Psi_{\gamma_N} | \left( \psi^+_1(t^+) \psi_1(t^+) - \psi^+_1(t^-) \psi_1(t^-) \right) | \Psi_{\gamma_N} \rangle.$$  (3.44)

A short calculation shows that the contribution from $x = 0^\pm$ is exactly cancelled by the contribution from $x = t^\pm$; furthermore, each individually yields the same answer (up to a sign) as the expectation value of the local operator $\hat{T}$ given above, which in turn is identical to the original form of the current.

In the remainder of this section, we evaluate the current in several different ways, obtaining the same answer each time. First, we use the original definition. Then we calculate the local form via the derivative formula, and also by direct calculation. Once these calculations are all shown to agree, we set the arbitrary quantum numbers to describe two Fermi seas and take the thermodynamic limit to obtain a physical answer.

**Original form.**

The original form (3.41) reduces to the evaluation of the bilinear $\psi^+_1 \psi_1$. It proves convenient to switch the calculation to the odd/even basis. Note that the lead 1 number operator can be written as:

$$\hat{N}_1 = \frac{1}{2} \hat{N} + \frac{1}{2} \left( \int_{-L/2}^{L/2} dx \ psi^+_\alpha(x) psi_\alpha(x) + \text{h.c.} \right).$$  (3.45)
Then, since $N$ is conserved, we obtain:

$$I(t) = -\text{Re} \left[ \frac{d}{dt} \int_{-L/2}^{L/2} dx \langle \Psi_{\gamma N k_N}(t) | \psi_o^\dagger(x) \psi_e(x) | \Psi_{\gamma N k_N}(t) \rangle \right]. \quad (3.46)$$

Thus, we can examine the bilinear $\psi_o^\dagger(x) \psi_e(x)$, instead. We find:

$$\langle \Psi_{\gamma N k_N}(t) | \psi_o^\dagger(x) \psi_e(x) | \Psi_{\gamma N k_N}(t) \rangle = \sum_{j=1}^{N} \{ c_{\gamma j}^\dagger(t), \psi_o^\dagger(x) \} \{ \psi_e(x), c_{\gamma j}^\dagger(t) \} \quad (3.47a)$$

$$= \frac{1}{L} \sum_{j=1}^{N} \frac{1}{2} (-1)^{\gamma_j-1} (1 + \mathcal{M} \Theta(0 < x < t)), \quad (3.47b)$$

where have used the anticommutation relations found earlier. It is then straightforward to obtain:

$$I(t) = -\text{Re} \left[ \frac{1}{L} \sum_{j=1}^{N} \frac{1}{2} (-1)^{\gamma_j-1} \mathcal{M} \right] \quad (3.48a)$$

$$= \frac{1}{L} \sum_{j=1}^{N} (-1)^{\gamma_j-1} \frac{1}{4} |\mathcal{M}|^2 \quad (3.48b)$$

where we used the optical identity (3.15). We have found that the current is independent of time for $t > 0$. Repeating the calculation with negative time, one finds that the current is a signum function in time. With a Keldysh calculation, we can show that the time scale on which the current turns on is of order $1/D_H$, where $D_H$ is the cutoff on the Hamiltonian; we have implicitly set $D_H = \infty$, resulting in an instantaneous jump in the current after the quench. The same occurs in the leading contribution to the Kondo current (Sec. 4.3.1).

**Local form, direct calculation.**

A similar calculation can be done using the local form (3.42c). First, we change to the odd/even basis, finding:

$$\tilde{I} = i \frac{1}{2} J' \psi_o^\dagger(0) \psi_e(0) + \text{h.c.} \quad (3.49)$$

Evaluating the bilinear, we find:

$$\langle \Psi_{\gamma N k_N}(t) | \psi_o^\dagger(0) \psi_e(0) | \Psi_{\gamma N k_N}(t) \rangle = \sum_{j=1}^{N} \{ c_{\gamma j}^\dagger(t), \psi_o^\dagger(0) \} \{ \psi_e(0), c_{\gamma j}^\dagger(t) \} \quad (3.50a)$$

$$= \frac{1}{L} \sum_{j=1}^{N} \frac{1}{2} (-1)^{\gamma_j-1} \left( 1 + \frac{1}{2} \mathcal{M} \right), \quad (3.50b)$$
where we have again used the anticommutation relations (3.39a)-(3.39c). The factor of 1/2 multiplying $\mathcal{M}$ comes from the averaging prescription for the delta function. The current is then:

$$\langle \Psi_{\gamma N k N}(t) | i \hat{I} | \Psi_{\gamma N k N}(t) \rangle = \frac{1}{L} \sum_{j=1}^{N} \frac{1}{2} (-1)^{\gamma_j} \text{Re} \left[ i J' \left( 1 + \frac{1}{2} \mathcal{M} \right) \right], \quad (3.51a)$$

which is the same answer as before, due to the identity $\text{Re}[i J' \mathcal{M}] = |\mathcal{M}|^2$.

**Local form, derivative calculation.**

To use the derivative formula of Sec. 2.3.2, we generalize the Hamiltonian to a one-parameter family of Hamiltonians:

$$\mathcal{H} = -i \int_{-L/2}^{L/2} dx \left( \frac{d}{dx} \psi_1^\dagger(x) \frac{d}{dx} \psi_1(x) - i \int_{-L/2}^{L/2} dx \psi_2^\dagger(x) \frac{d}{dx} \psi_2(x) \right) + \frac{1}{2} J'(e^{i \phi} - 1) \psi_1^\dagger(0) \psi_2(0) + \frac{1}{2} J'(e^{-i \phi} - 1) \psi_2^\dagger(0) \psi_1(0). \quad (3.52)$$

Here, $\phi$ is a real parameter (recall that the bar has nothing to do with complex conjugation), and the value of this parameter for the original model is $\phi = \phi = 0$. We can write the varying Hamiltonian as:

$$\mathcal{H} = H + \frac{1}{2} J'(e^{i \phi} - 1) \psi_1^\dagger(0) \psi_2(0) + \frac{1}{2} J'(e^{-i \phi} - 1) \psi_2^\dagger(0) \psi_1(0). \quad (3.53)$$

Hence, the general formula (2.68) yields:

$$\langle \Psi_{\gamma N k N}(t) | \left( \frac{1}{2} J' \psi_1^\dagger(0) \psi_2(0) - i \frac{1}{2} J' \psi_2^\dagger(0) \psi_1(0) \right) | \Psi_{\gamma N k N}(t) \rangle = \left. i \frac{\partial}{\partial \phi} \right|_{\phi=0} \frac{\partial}{\partial t} \langle \Psi_{\gamma N k N}(t) | \overline{\Psi}(t) \rangle, \quad (3.54)$$

where $|\overline{\Psi}(t)\rangle = e^{-i \mathcal{H}t} |\Psi\rangle$ and $|\overline{\Psi}\rangle$ is any $\phi$-dependent family of states that reduces to $|\Psi_{\gamma N k N}\rangle$ for $\phi = 0$. The left-hand side of Eq. (3.54) is exactly the expectation value of $\hat{I}$ at time $t$, and the right-hand side is what we need to evaluate.
Let us bring the Hamiltonian $H$ to an odd/even basis with a $\phi$-dependent unitary matrix $U$:

$$
\begin{pmatrix}
c_{ok} \\
c_{ek}
\end{pmatrix} = U
\begin{pmatrix}
c_{1k} \\
c_{2k}
\end{pmatrix},
$$

where $U = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\frac{\phi}{2}} & e^{i\frac{\phi}{2}} \\
e^{-i\frac{\phi}{2}} & e^{i\frac{\phi}{2}} \end{pmatrix}$. \hspace{1cm} (3.55)

Note that removing the bar yields the matrix $U$ from before. The Hamiltonian separates into two (commuting) parts:

$$
\begin{align*}
H_o &= -i \int_{-L/2}^{L/2} dx \overline{\psi}_o(x) \frac{d}{dx} \psi_o(x), \\
H_e &= -i \int_{-L/2}^{L/2} dx \overline{\psi}_e(x) \frac{d}{dx} \psi_e(x) + J \overline{\psi}_e(0) \psi_e(0), \\
H &= H_o + H_e,
\end{align*}
$$

where $\overline{\psi}_i(x) = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{-ikx} \overline{c}_{jk}$ with $\gamma = o$ or $e$. The odd and even components are identical to $H_o$ and $H_e$ from earlier with the unbarred fields relabeled as barred; hence the time dependent operators can be obtained by relabeling Eq. (3.33) and Eq. (3.34):

$$
\begin{align*}
\overline{c}_{ok}^\dagger(t) &\equiv e^{-\mathcal{M}_t} \overline{c}_{ok} e^{\mathcal{M}_t} = e^{-ikt} \overline{c}_{ok}, \\
\overline{c}_{ek}^\dagger(t) &\equiv e^{-\mathcal{M}_t} \overline{c}_{ek} e^{\mathcal{M}_t} = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ F_k(t, x) \overline{\psi}_e(x).
\end{align*}
$$

We now use the freedom we have in defining the family of states $|\Psi\rangle$ to make the calculation easier. This makes little difference in the present case – the potential scattering model being rather simple – but the same choice will be useful in interacting models. We set $|\Psi\rangle = \overline{c}_{\gamma N k N}^\dagger |0\rangle$, where the barred creation operators $\overline{c}_{1k}^\dagger$ and $\overline{c}_{2k}^\dagger$ are defined below; we verify that $\overline{c}_{\gamma k}^\dagger |\phi = 0\rangle = c_{\gamma k}^\dagger$, justifying the use of the bar notation. Then the time evolution is given by $|\Psi(t)\rangle = \overline{c}_{\gamma N k N}^\dagger(t) |0\rangle \equiv |\overline{\Psi}_{\gamma N k N}(t)\rangle$, where the barred operators evolve in time via $\overline{c}_{\gamma k}^\dagger(t) = e^{-\mathcal{M}_t} \overline{c}_{\gamma k} e^{\mathcal{M}_t}$.

To motivate the definition of $\overline{c}_{1k}^\dagger$ and $\overline{c}_{2k}^\dagger$, let us imagine for a moment that the potential scattering model is a difficult, interacting problem which we have solved in the one lead case (i.e. we have found the crossing states). We know from Sec. 2.5 that the time evolution of
the two lead model follows easily due to the relation of the creation operators in the lead 1/lead 2 basis to the operators in the odd/even basis:

\[
\begin{pmatrix}
  c_{1k}(t) \\
  c_{2k}(t)
\end{pmatrix} = U^\dagger \begin{pmatrix}
  c_{ok}(t) \\
  c_{ek}(t)
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  1 & 1 \\
  -1 & 1
\end{pmatrix} \begin{pmatrix}
  c_{ok}(t) \\
  c_{ek}(t)
\end{pmatrix}.
\] (3.58)

The important point about this relation is that both \(c_{1k}(t)\) and \(c_{2k}(t)\) have the same even part; this is what guarantees that \(A_{1k}(t) = A_{2k}(t) = \frac{1}{\sqrt{2}} A_{ek}(t)\), which makes it easy to reuse the same crossing states from the one lead model to find \(e^{-iHt}c_{\gamma NkN}^\dagger |0\rangle\) (with lead indices \(\gamma_N\) in the lead 1/lead 2 basis). We would like the same relation to hold with the time-dependent barred creation operators:

\[
\begin{pmatrix}
  \bar{c}_{1k}(t) \\
  \bar{c}_{2k}(t)
\end{pmatrix} = U^\dagger \begin{pmatrix}
  \bar{c}_{ok}(t) \\
  \bar{c}_{ek}(t)
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  1 & 1 \\
  -1 & 1
\end{pmatrix} \begin{pmatrix}
  \bar{c}_{ok}(t) \\
  \bar{c}_{ek}(t)
\end{pmatrix}.
\] (3.59)

If this relation holds, then the problem of finding \(e^{-i\Pi t}c_{\gamma NkN}^\dagger |0\rangle\) is exactly the same as the problem of finding \(e^{-iHt}c_{\gamma NkN}^\dagger |0\rangle\) with unbarred fields relabeled as barred; hence the solution is also obtained by the same relabelling. We therefore define:

\[
\begin{pmatrix}
  \bar{c}_{1k} \\
  \bar{c}_{2k}
\end{pmatrix} = U^\dagger \begin{pmatrix}
  \bar{c}_{ok} \\
  \bar{c}_{ek}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  1 & 1 \\
  -1 & 1
\end{pmatrix} \begin{pmatrix}
  \bar{c}_{ok} \\
  \bar{c}_{ek}
\end{pmatrix},
\] (3.60a)

and:

\[
\bar{c}_{\gamma}^\dagger (x) = \frac{1}{\sqrt{L}} \sum_k e^{-ikx} c_{\gamma k}^\dagger \quad (\gamma = 1, 2),
\] (3.60b)

so that the desired relation (3.59) follows from evolving in time with \(\Pi\). It is clear that the barred operators reduce to \(c_{1k}\) and \(c_{2k}\) if the bar is removed, so the definition is consistent.

With the setup complete, the calculation is straightforward:

\[
i \frac{\partial}{\partial \phi} \bigg|_{\phi = 0} \frac{\partial}{\partial t} \langle \Psi_{\gamma NkN}(t) | \bar{\Psi}_{\gamma NkN}(t) \rangle = i \frac{\partial}{\partial \phi} \bigg|_{\phi = 0} \frac{\partial}{\partial t} \langle 0 | c_{\gamma NkN}(t) c_{\gamma NkN}^\dagger (t) | 0 \rangle
\]

\[
= i \frac{\partial}{\partial \phi} \bigg|_{\phi = 0} \frac{\partial}{\partial t} \sum_{\sigma \in \text{Sym}(N)} (\text{sgn } \sigma) \prod_{j=1}^{N} \{ c_{\gamma(j)k\sigma(j)}(t), \bar{c}_{\gamma(j)k\sigma(j)}^\dagger (t) \}
\]

\[
= \sum_{j=1}^{N} i \frac{\partial}{\partial \phi} \bigg|_{\phi = 0} \frac{\partial}{\partial t} \{ c_{\gamma(j)k_j}(t), \bar{c}_{\gamma(j)k_j}^\dagger (t) \}.
\] (3.61c)
It is straightforward to show the following anticommutation relations (e.g. by rotating back to the unbarred fields in the lead 1/lead 2 basis, whose anticommutation relations are canonical):

\[
\{\psi_o(x'), \overline{\psi}_o(x)\} = \{\psi_e(x'), \overline{\psi}_e(x)\} = \cos \left(\frac{1}{2} \phi\right) \delta(x-x'),
\]

(3.62a)

\[
\{\psi_o(x'), \overline{\psi}_e(x)\} = \{\psi_e(x'), \overline{\psi}_o(x)\} = i \sin \left(\frac{1}{2} \phi\right) \delta(x-x').
\]

(3.62b)

These allow us to find the anticommutation relations of field operators at the same time but evolving with different Hamiltonians:

\[
\{c_{ok}(t), \overline{c}_{ok}(t)\} = \{c_{ek}(t), \overline{c}_{ek}(t)\} = \cos \left(\frac{1}{2} \phi\right),
\]

(3.63a)

\[
\{c_{ok}(t), \overline{c}_{ek}(t)\} = i \sin \left(\frac{1}{2} \phi\right) \left(1 + \frac{t}{L \mathcal{M}}\right),
\]

(3.63b)

\[
\{c_{ek}(t), \overline{c}_{ok}(t)\} = i \sin \left(\frac{1}{2} \phi\right) \left(1 + \frac{t}{L \mathcal{M}^*}\right).
\]

(3.63c)

While we could use these relations to find \(\{c_{\gamma k}(t), \overline{c}_{\gamma k}(t)\}\), we instead take a simpler path, noting the action of the derivative operator of interest on each of the equations above:

\[
i \frac{\partial}{\partial \phi} \bigg|_{\phi=\phi_0} \frac{\partial}{\partial t} \{c_{ok}(t), \overline{c}_{ok}(t)\} = i \frac{\partial}{\partial \phi} \bigg|_{\phi=\phi_0} \frac{\partial}{\partial t} \{c_{ek}(t), \overline{c}_{ek}(t)\} = 0,
\]

(3.64a)

\[
i \frac{\partial}{\partial \phi} \bigg|_{\phi=\phi_0} \frac{\partial}{\partial t} \{c_{ok}(t), \overline{c}_{ek}(t)\} = \left[i \frac{\partial}{\partial \phi} \bigg|_{\phi=\phi_0} \frac{\partial}{\partial t} \{c_{ek}(t), \overline{c}_{ok}(t)\}\right]^* = -\frac{1}{2} \frac{1}{L \mathcal{M}}.
\]

(3.64b)

Then, in view of the relation (3.59), we obtain:

\[
i \frac{\partial}{\partial \phi} \bigg|_{\phi=\phi_0} \frac{\partial}{\partial t} \{c_{\gamma k}(t), \overline{c}_{\gamma k}(t)\} = \left.i \frac{\partial}{\partial \phi} \bigg|_{\phi=\phi_0} \frac{\partial}{\partial t} \left\{\frac{1}{\sqrt{2}} \gamma^{-1} c_{ok}(t), \frac{1}{\sqrt{2}} \overline{c}_{ek}(t)\right\}\right. + \text{c.c.}
\]

(3.65a)

\[
= \text{Re} \left[\left(-1\right)^{-1} \frac{1}{2} \frac{1}{L \mathcal{M}}\right].
\]

(3.65b)

Returning to Eq. (3.54) and Eq. (3.61c), we see:

\[
\langle \Psi_{\gamma N k N}(t) | \mathcal{I} | \Psi_{\gamma N k N}(t) \rangle = \sum_{j=1}^{N} \text{Re} \left[\left(-1\right)^{-1} \frac{1}{2} \frac{1}{L \mathcal{M}}\right],
\]

(3.66)

which agrees precisely with the expression (3.48a) found earlier for \(I(t)\).
The thermodynamic limit.

So far, we have taken the initial quantum numbers $\gamma_{\mathbf{N}}k_{\mathbf{N}}$ of the state before the quench to be arbitrary. Let us now specialize to the case of two Fermi seas. We take:

$$\mathbf{N} \rightarrow \widetilde{\mathbf{N}} = (1, \ldots, N_1 + N_2)$$

$$K_j = -D + \frac{2\pi}{L}(j - 1), \ K_\gamma = \{K_j \mid 1 \leq j \leq N_\gamma\} \quad (\gamma = 1, 2)$$

The particle numbers $N_1$ and $N_2$ encode the chemical potentials of each lead via:

$$\mu_\gamma - (-D) = \frac{2\pi}{L}N_\gamma \quad (\gamma = 1, 2)$$

Since the momenta are spaced by $\frac{2\pi}{L}$, the answer we obtained can be recognized as a Riemann approximation to a single integral:

$$I(t) = \frac{1}{L} \sum_{j=1}^{N_1} \frac{1}{4} |M|^2 + \frac{1}{L} \sum_{j=1}^{N_2} (-1) \frac{1}{4} |M|^2$$

$$\xrightarrow{\text{therm. limit}} \int_{\mu_1}^{\mu_2} \frac{1}{2\pi} \frac{1}{4} |M|^2 = \frac{e^2}{h} V \frac{\frac{1}{4} J^2}{1 + \frac{1}{4} J^2}$$

where we have written $V \equiv \mu_1 - \mu_2$ and restored physical units (see Sec. 1.5). We see here that the sum over momenta in lead 1 is mostly cancelled by the sum over momenta in lead 2 (which contribute with opposite sign); in particular, the entire range of momenta from the lower cutoff $-D$ up to $\mu_2$ makes no contribution. This is a consequence of the problem being non-interacting.

Writing the sums in another form makes it clear how to generalize the above to allow both leads to be at arbitrary temperatures:

$$I(t) = \frac{1}{L} \sum_{j \in K_1} \frac{1}{4} |M|^2 + \frac{1}{L} \sum_{j \in K_2} (-1) \frac{1}{4} |M|^2$$

$$\xrightarrow{\text{therm. limit}} \int_{-D}^{D} \frac{dk}{2\pi} \left[ f_1(k) - f_2(k) \right] \frac{1}{4} |M|^2 \xrightarrow{D \rightarrow \infty} e^2 \frac{\frac{1}{4} J^2}{h} V \frac{\frac{1}{4} J^2}{1 + \frac{1}{4} J^2}$$

Here, $f_\gamma(k) = [e^{(k-\mu_\gamma)/T_\gamma} + 1]^{-1}$ is the Fermi function with temperature $T_\gamma$ and chemical potential $\mu_\gamma$ ($\gamma = 1, 2$). Evidently, temperature has no effect whatsoever in the large
bandwidth limit; this is a consequence of the $S$-matrix of the model being independent of momentum.

This answer agrees exactly with Ref. [53], in which this model is presented as a simple check in a larger calculation (though the authors do not evaluate the final integral for arbitrary temperature for some reason). Note also that the steady state conductance can be written as:

$$\lim_{t \to \infty} \frac{\partial}{\partial V} I(t) = \frac{e^2}{h} \frac{1}{4} |\mathcal{M}|^2.$$  

(3.72)

This agrees with the Landauer formula; to see this, note from Eq. (3.37) that the transmission coefficient is $| - iT/2|^2 = |T|^2/4$ (and recall that $\mathcal{M} = -iT$).

**Large coupling and the unitarity limit.**

Since the $S$-matrix is a phase, the modulus of the $T$-matrix (which is equal to $|\mathcal{M}|$) is at most equal to 2; therefore there is an absolute upper bound of $e^2/\hbar$ on the conductance. This is known as the unitarity limit since it comes ultimately from the unitarity of the $S$-matrix. (More generally, the maximal value is $e^2/\hbar$ times the number of channels; there are usually two channels due to spin degeneracy, but here we are considering spinless electrons.) This maximal value is reached if we consider an infinitely strong potential:

$$\frac{\partial I}{\partial V} = \frac{e^2}{\hbar} \frac{\frac{1}{4} J'^2}{1 + \frac{1}{4} J'^2} \xrightarrow{J' \to \infty} \frac{e^2}{\hbar}.$$  

(3.73)

Let us see why this occurs at the level of the wavefunction. For $J' \to \infty$, the constant $\mathcal{M}$ goes to $-2$. We can then see from Eq. (3.36b) that there is perfect transmission – e.g., an plane wave comes from the left in lead 1 and completely hops into lead 2 (with an overall minus sign), with no outgoing wave in lead 1 at all. See also Fig. 3.1. We will see in the next chapter that much of this discussion also applies in the Kondo model in the limit of large coupling ($J \to \pm \infty$).
3.3 Resonant level model

The one lead resonant level model (making the usual reduction to one dimension) is:

\[ H^{(0)} = -i \int_{-L/2}^{L/2} dx \psi^\dagger(x) \frac{d}{dx} \psi(x) + \epsilon d^\dagger d + \left[ v \psi^\dagger(0) d + \text{h.c.} \right]. \] (3.74)

The field operators consist of the same operators \( c^\dagger_k = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{ikx} \psi^\dagger(x) \) that appeared in the potential scattering model, and also the \( d^\dagger \) operator. The only “fixed impurity state” is \( |0\rangle \). The hopping term \( v \psi^\dagger(0) d \) neither annihilates \( d^\dagger |0\rangle \) nor maps it into a linear combination of \( |0\rangle \) and \( d^\dagger |0\rangle \); thus we do not count \( d^\dagger |0\rangle \) as a second “fixed impurity state.”

We will also consider the simplest multi-lead version of the model:

\[ H^{(0)} = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^{N_{\text{leads}}} \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \psi^\dagger_\gamma(x) \frac{d}{dx} \psi^\dagger_\gamma(x) + \epsilon d^\dagger d + \left[ \frac{v}{\sqrt{N_{\text{leads}}}} \sum_{\gamma=1}^{N_{\text{leads}}} \psi^\dagger_\gamma(0) d + \text{h.c.} \right]. \] (3.75)

3.3.1 Wavefunction

We solve for the time-evolving operators of the one lead model. Then, we take the long time limit to arrive at scattering operators. Finally, we present the generalization to the multilead case.

One lead model – time evolution.

Since the model is non-interacting, the field operators should stay in the single particle sector under time evolution:

\[ c^\dagger_k(t) \equiv e^{-iH^{(0)}t} c^\dagger_k e^{iH^{(0)}t} = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ g_k^{(c)}(t, x) \psi^\dagger(x) + \frac{1}{\sqrt{L}} g_k^{(d)}(t) d^\dagger, \] (3.76a)

\[ d^\dagger(t) \equiv e^{-iH^{(0)}t} d^\dagger e^{iH^{(0)}t} = \int_{-L/2}^{L/2} dx \ g^{(c)}(t, x) \psi^\dagger(x) + g^{(d)}(t) d^\dagger, \] (3.76b)

where the functions \( g_k^{(c)}(t, x), g_k^{(d)}(t, x), g^{(c)}(t, x), \) and \( g^{(d)}(t) \) are constrained by the operator equations of motion \([H, c^\dagger_k(t)] = -i \frac{d}{dt} c^\dagger_k(t) = [H, d^\dagger(t)] = -i \frac{d}{dt} d^\dagger(t) = 0\), with the initial conditions \( c^\dagger_k(t = 0) = c^\dagger_k \) and \( d^\dagger(t = 0) = d^\dagger \). These translate to the following differential equations
for the functions:

\[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) g_k^{(c)}(t, x) + v g_k^{(d)}(t) \delta(x) = 0, \quad (3.77a) \]

\[ \left( -i \frac{d}{dt} + \epsilon \right) g_k^{(d)}(t) + v^* g_k^{(c)}(t, 0) = 0, \quad (3.77b) \]

with the same equations for \( g^{(c)}(t, x) \) and \( g^{(d)}(t, x) \); the initial conditions become \( g_k^{(c)}(t = 0, x) = e^{ikx}, g_k^{(d)}(t = 0) = 0, g^{(c)}(t = 0, x) = 0, \) and \( g^{(d)}(t = 0) = 1. \)

We obtain a finite list of functions to solve before because the model is quadratic and conserves particle number. (The situation is similar to solving for the Green’s functions via the equations of motion method.) We can solve for these functions in a simple closed form due to the tunneling term being particularly simple (i.e. a delta function in position space, or uniform in momentum space). In the regime of interest \(-L/2 < t < L/2,\) so that the quench has not reached the (artificial) periodic boundary – the solution is:

\[ g_k^{(c)}(t, x) = e^{-ik(t-x)} - i \mathcal{T}(k) \Theta(x) \Theta(t-x) \left( e^{-ik(t-x)} - e^{-iz(t-x)} \right) \]

\[ + i \mathcal{T}^*(k) \Theta(-x) \Theta(t-x) \left( e^{-ik(t-x)} - e^{-iz^*(t-x)} \right), \quad (3.78a) \]

\[ g_k^{(d)}(t) = \frac{1}{v} \left( \mathcal{T}(k) \Theta(t) (e^{-ikt} - e^{-izt}) + \mathcal{T}^*(k) \Theta(-t) (e^{-ikt} - e^{-iz^*t}) \right), \quad (3.78b) \]

\[ g^{(c)}(t, x) = -iv \left( \Theta(x) \Theta(t-x) e^{-iz(t-x)} - \Theta(-x) \Theta(x-t) e^{-iz^*(t-x)} \right), \quad (3.78c) \]

\[ g^{(d)}(t) = \Theta(t) e^{-izt} + \Theta(-t) e^{-iz^*t}, \quad (3.78d) \]

where we have defined three quantities that appear throughout the rest of this chapter (and also in Chapters 5 and 6):

\[ \mathcal{T}(k) \equiv \frac{2\Delta}{k - z}, \quad \Delta \equiv \frac{1}{2} |v|^2, \quad z \equiv \epsilon - i\Delta. \quad (3.79) \]

The same averaging prescription \( \delta(x) \Theta(x) = \frac{1}{2} \delta(x) \) discussed in more detail in the potential scattering case, and in Sec. 3.4, has been used again. Note that the \( \mathcal{T} - \)matrix \( \mathcal{T}(k), \) which is a momentum-independent matrix in the Kondo model, is in this case a momentum-dependent complex number. The \( S - \)matrix \( S(k) = 1 - i\mathcal{T}(k) \) is a pure phase, as is easily verified. Equivalently, we have the following statement of the optical theorem:

\[ -2\text{Im} \left[ \mathcal{T}(k) \right] = |\mathcal{T}(k)|^2. \quad (3.80) \]
The quantity $\Delta$ is called the resonance width. It is more common in the literature to find the tunneling term in the Hamiltonian written as $\sum_k \mathcal{V}_k c_k^\dagger d + \text{h.c.}$, and the resonance width is usually defined as $\Delta(w) = \pi \rho |\mathcal{V}_w|^2$, where $\rho$ is the density of states. Here, we have $\mathcal{V}_k = v/\sqrt{L}$ and $\rho = L/(2\pi)$, so $\Delta(w) = \frac{1}{2} |v|^2$.

We have included negative times in the calculation, even though these are not relevant to the quench setup. This is done so that we can take $t \to \pm \infty$ to generate two different kinds of scattering operators (creating “in” and “out” states), as we discuss in more detail below. Also, the negative time part of the solution can resolve any possible doubt that the Schrödinger equation is satisfied at all times, including the point $t = 0$.

A more convenient way of writing the $c_k^\dagger(t)$ operators is the following (focusing on the $0 \leq t < L/2$ regime):

$$c_k^\dagger(t) = e^{-ikt} c_k^\dagger + \frac{1}{\sqrt{L}} \int dx \ F_k(t-x) \left[ \Theta(0 < x < t) \psi^\dagger(x) + \frac{i}{v} \delta(x) \Theta(0 < t)d^\dagger \right], \quad (3.81a)$$

where: $F_k(t) = -iT(k) \left( e^{-ikt} - e^{-izt} \right)$. \quad (3.81b)

This is a form that will generalize to the interacting case, so we explain it in some detail.

The first term is the time evolution for the fully free model with no tunneling ($v = 0$), and takes the correct value $c_k^\dagger$ at $t = 0$. The second term, which includes the effect of the tunneling, should therefore vanish at $t = 0$, as we now verify. For $t = 0$, the electron contribution is an integration over $\Theta(0 < x < 0)$, which represents a set of measure 0, and the impurity contribution is zero due to $F_k(t = 0) = 0$. These statements hold regardless of what values we assign to the quantities $\Theta(0 < 0 < 0)$ and $\Theta(0 < 0)$. The boundary points do not matter, and writing $\leq$ instead of $<$ in the Heaviside functions would make no difference.

In addition to making the initial condition hold automatically, Eq. (3.81a) is also set up in such a way as to make it easy to solve for the function $F_k(t-x)$. To see this, let us
calculate $[H, c_k^\dagger(t)] - i \frac{\partial}{\partial t} c_k^\dagger(t)$. We split up the calculation in parts as follows:

$$
\left[ -i \int_{-L/2}^{L/2} dx \, \psi^\dagger(x) \frac{d}{dx} \psi(x) + \epsilon \delta d, c_k^\dagger(t) \right] - i \frac{\partial}{\partial t} c_k^\dagger(t) =
$$

$$
\frac{1}{\sqrt{L}} \int dx \, F_k(t - x) \left[ \left( -i \frac{\partial}{\partial x} - i \frac{\partial}{\partial t} \right) \Theta(0 < x < t) \right] \psi^\dagger(x)
$$

$$
+ \frac{i}{\sqrt{Lv}} \left[ -i \delta(t) F_k(t) + \left( -i \frac{\partial}{\partial t} + \epsilon \right) F_k(t) \Theta(0 < t) \right] d^\dagger,
$$

(3.82a)

$$
[v \psi^\dagger(0)d, c_k^\dagger(t)] = i \frac{1}{\sqrt{L}} F_k(t) \Theta(0 < t) \psi^\dagger(0),
$$

(3.82b)

$$
[v^* d^\dagger \psi(0), c_k^\dagger(t)] = \frac{1}{\sqrt{L}} v^* e^{-ikt} d^\dagger + \frac{1}{\sqrt{Lv}} v^* \int dx \, F_k(t - x) \Theta(0 < x < t) \delta(x) d^\dagger.
$$

(3.82c)

Note that in writing the first equation, we have already used the fact that $F_k$ is a function only of the difference $t - x$. Also, there is a partial cancellation between the first and second equations. Writing $\Theta(0 < x < t) = \Theta(0 < x) \Theta(x < t)$, we obtain $\left( -i \frac{\partial}{\partial t} - i \frac{\partial}{\partial x} \right) \Theta(0 < x < t) = -i \delta(x) \Theta(0 < t)$, so this term cancels with the second equation once integrated over $x$.

In the third equation, we use the averaging prescription: $\theta(0 < x < t) \delta(x) \rightarrow \frac{1}{2} \Theta(0 < t)$.

All together, we find:

$$
[H^{(0)}, c_k^\dagger(t)] - i \frac{\partial}{\partial t} c_k^\dagger(t) = \frac{1}{\sqrt{L}} v^* e^{-ikt} d^\dagger + \frac{1}{\sqrt{Lv}} \left( -i \frac{\partial}{\partial t} + \epsilon - i \Delta \right) F_k(t) \Theta(0 < t) d^\dagger
$$

$$
+ \frac{1}{\sqrt{Lv}} \delta(t) F_k(t) d^\dagger.
$$

(3.83)

The delta function term must cancel separately from the others. It then suffices to find $F_k(t)$ satisfying:

$$
\left( -i \frac{\partial}{\partial t} + z \right) F_k(t) = 2i \Delta e^{-ikt},
$$

(3.84a)

$$
F_k(t = 0) = 0,
$$

(3.84b)

from which we obtain Eq. (3.81b).

Strictly speaking, the above works for $0 < t < L/2$. Exactly at the point $t = 0$, we appear to have a difficulty, since we have implicitly set $\Theta(0 < t) = 1$ for $t = 0$ (rather than, say, 0 or 1/2). To remove this doubt, we generalize the calculation to include negative
times:
\[
c_k^\dagger(t) = e^{-ikt}c_k^\dagger + \frac{1}{\sqrt{L}} \int dx \left[ F_k(t-x)\Theta(0 < x < t)\psi^\dagger(x) + \frac{i}{v}\delta(x)\Theta(0 < t)d^\dagger \right] \\
+ \frac{1}{\sqrt{L}} \int dx \left[ G_k(t-x)\Theta(t < x < 0)\psi^\dagger(x) - \frac{i}{v}\delta(x)\Theta(0 < t)d^\dagger \right]. \tag{3.85}
\]

Repeating the above calculation, one finds:
\[
[H^{(0)}, c_k^\dagger(t)] - i\frac{\partial}{\partial t}c_k^\dagger(t) = \frac{1}{\sqrt{L}} v^* e^{-ikt}d^\dagger + \frac{1}{\sqrt{L}} v \left( -i\frac{\partial}{\partial t} + \epsilon - i\Delta \right) F_k(t)\Theta(0 < t)d^\dagger \\
+ \frac{1}{\sqrt{L}} v e^{-ikt}d^\dagger - \frac{1}{\sqrt{L}} v \left( -i\frac{\partial}{\partial t} + \epsilon + i\Delta \right) G_k(t)\Theta(t < 0)d^\dagger + \frac{1}{\sqrt{L}} \delta(t) G_k(t)d^\dagger. \tag{3.86}
\]

We must have \( F_k(t = 0) + G_k(t = 0) = 0 \) for the delta terms to cancel. (This is equivalent to the statement that the impurity part of the operator, which is \( \frac{i}{v} F_k(t) \) for \( t > 0 \) and \( -\frac{i}{v} G_k(t) \) for \( t < 0 \), must be continuous at \( t = 0 \).) For the remaining terms, we write
\[
\frac{1}{\sqrt{L}} v^* e^{-ikt}d^\dagger = \frac{1}{\sqrt{L}} v^* e^{-ikt}d^\dagger [\Theta(0 < t) + \Theta(t < 0)] \text{ and then separately cancel the } \Theta(0 < t) \text{ and } \Theta(t < 0) \text{ parts. This leads to the same condition } Eq. \ (3.84a) \text{ on } F_k \text{ as found previously, and also:}
\]
\[
\left( -i\frac{\partial}{\partial t} + z^* \right) G_k(t) = -2i\Delta e^{-ikt}. \tag{3.87}
\]

We then conclude that \( G_k(t) = F_k^*(-t) \), with \( F_k \) given by Eq. \ (3.81b). In using \( 1 = \Theta(0 < t) + \Theta(t < 0) \), we are again being vague about which Heaviside function makes up the unity at \( t = 0 \); see the corresponding discussion in the potential scattering case 3.1.1.

The long time limit.

The steady state regime we are interested in has \( t \to \infty \) and \( L \to \infty \) with \( t \ll L \). Since we take the infinite volume limit, the Kronecker-normalized momentum operators become Dirac normalized. The prescription for obtaining a scattering operator is the following [see also Eq. \ (3.17)]:
\[
c_{k,\text{in}}^\dagger \equiv \lim_{t \to \infty} e^{ikt} \lim_{L \to \infty} \sqrt{L} \left( \int dx \{\psi(x), c_{k}^\dagger(t)\} \psi^\dagger(x) + \{d, c_{k}^\dagger(t)\}d^\dagger \right), \tag{3.88}
\]
with $c_{k,\text{out}}^\dagger$ being the same expression with $t \to -\infty$. To see this, consider the single particle wavefunction $c_k^\dagger(t)|0\rangle$. This wavefunction does not approach any limit at large time as a state; the transient $e^{-iz(t-x)}$ terms cannot, in general, be neglected, since $x$ can be close to $t$. However, the projection of the wavefunction onto any given position ket $|x\rangle = (0|\psi(x)$ does approach a limit (though not all $x$ reach the limit uniformly). The idea is to build a time-independent wavefunction whose value at each $x$ is the value obtained by taking the long time limit of the time-evolving wavefunction at that $x$. The factor of $\sqrt{L}$ is just a conversion to Dirac delta normalization.

Taking the limit, we find:

$$
c_{k,\text{in}}^\dagger = c_k^\dagger + \int dx \ F_{k,\text{in}}(x) \left( \Theta(0 < x)\psi^\dagger(x) + \frac{i}{v}d^\dagger \right), \quad (3.89a)
$$

where:

$$
F_{k,\text{in}}(x) = -i\mathcal{T}(k)e^{ikx} \quad \text{and} \quad c_k^\dagger = \int dx \ e^{ikx}\psi^\dagger(x). \quad (3.89b)
$$

We use the same symbol $c_k^\dagger$ even in the infinite volume case, noting that these operators are now Dirac normalized: $\{c_k, c_k^\dagger\} = 2\pi\delta(k - k')$. Using the “optical” identity (3.80), we can verify that $\{c_{k',\text{in}}, c_{k,\text{in}}^\dagger\} = 2\pi\delta(k - k')$, as well.

The $c_{k,\text{in}}^\dagger$ operator creates a scattering “in” state, meaning one in which the only incoming plane wave is $e^{ikx}$. Since we have a linear spectrum with only right-movers, any plane wave on the left is incoming and any plane wave on the right is outgoing, regardless of the sign of $k$. (More generally, a scattering “in” state would be one in which the only incoming plane wave from any direction is the one with the specified momentum in the operator.) Furthermore, since the scattering event (i.e. tunneling to the dot) occurs only at $x = 0$, the “in” requirement translates to the wavefunction being $e^{ikx}$ for all $x < 0$. Similarly, a scattering “out” state for the momentum $k$ is one in which the wavefunction is $e^{ikx}$ for $x > 0$.

It is also possible to find the scattering operators directly, without taking a long time limit. The defining equation is:

$$
[H, c_{k,\text{in}}^\dagger] - kc_{k,\text{in}}^\dagger = 0, \quad (3.90)
$$
subject to the boundary condition that $c_{k,\text{in}}^\dagger|0\rangle$ is a state with an incoming plane wave $e^{ikx}$ on the left. We can write down Eq. (3.89a) as an ansatz – note that the incoming boundary condition is satisfied automatically, due to the $\Theta(0 < x)$ term – and then solve for $F_{k,\text{in}}(x)$ in much the same way as in the time-dependent case. The “out” operators can be found similarly.

Note that the electron part of the “in” wavefunction $c_{k,\text{in}}^\dagger|0\rangle$ is $e^{ikx}[1 - i\mathcal{T}(k)\Theta(0 < x)] = e^{ikx}[\Theta(x < 0) + (1 - i\mathcal{T}(k))\Theta(0 < x)]$. Then the $S$-matrix is $1 - i\mathcal{T}(k) = \frac{k - e^{i\Delta}}{k - e^{-i\Delta}}$, in agreement with Bethe Ansatz. Indeed, the $c_{k,\text{in}}^\dagger$ operators are exactly the starting point of the Bethe Ansatz construction of eigenstates in models in which the non-interacting part is the RLM.

Let us comment here on the relation of these scattering operators to the Lippmann-Schwinger equation. The RLM Hamiltonian can be written as $H^{(0)} = h + \mathcal{V}$, where $h = -i\int dx \psi^\dagger(x)\frac{d}{dx}\psi(x)$ has the reservoir degrees of freedom only, and $\mathcal{V}$ has the dot energy and tunneling. As opposed to a quench problem, in which the given information is the initial state at $t = 0$, the given information in the scattering problem is an eigenstate $|\Psi\rangle_{kN} \equiv c_{kN}^\dagger|0\rangle$ of $h$ – or equivalently, the set of quantum numbers $k_N$ for $N$ incoming plane waves.\footnote{We consider incoming plane waves, but the generalization to outgoing plane waves is straightforward.} The RLM scattering “in” state $|\Psi_{kN,\text{in}}^0\rangle$ is then defined by the Lippman-Schwinger equation:

$$|\Psi_{kN,\text{in}}^0\rangle = |\Psi_{kN}\rangle + \frac{1}{E - h + i\eta}\mathcal{V}|\Psi_{kN,\text{in}}^0\rangle.$$  

(3.91)

This equation is equivalent to the time-independent Schrödinger equation (for $H^{(0)}$) with the boundary condition of incoming plane waves with momenta $k_N$. By construction, the $c_{k,\text{in}}^\dagger$ operator creates a single electron state with incoming plane wave $e^{ikx}$. Thus, since the RLM is non-interacting, the solution to the Lippmann-Schwinger equation is given by a product of these operators:

$$|\Psi_{kN,\text{in}}^0\rangle = c_{kN,\text{in}}^\dagger|0\rangle.$$  

(3.92)

In chapter 5, we consider adding an interaction term $H^{(1)}$ to the RLM Hamiltonian. Let us...
consider $H^{(1)}$ as part of $\mathcal{V}$, i.e. $H = H^{(0)} + H^{(1)} = h + \mathcal{V}$, with $h = -i \int dx \psi^\dagger(x) \frac{d}{dx} \psi(x)$ as before. The Lippmann-Schwinger equation for the full Hamiltonian, including the interaction term, can be written either with respect to $h$ or with respect to the RLM Hamiltonian $H^{(0)}$:

\begin{align}
|\Psi_{kN,\text{in}}\rangle &= |\Psi_{kN}\rangle + \frac{1}{E - h + i\eta} \mathcal{V} |\Psi_{kN,\text{in}}\rangle \\
&= |\Psi^0_{kN,\text{in}}\rangle + \frac{1}{E - H^{(0)} + i\eta} H^{(1)} |\Psi_{kN,\text{in}}\rangle.
\end{align}

Both forms are equivalent to the time-independent Schrödinger equation (now for the interacting Hamiltonian $H$) with the boundary condition of incoming plane waves with momenta $k_N$. The second form makes a clearer connection with our general wavefunction formalism (Sec. 2.6), which is a method for systematically adding corrections (built from $c_{k,\text{in}}^\dagger$ operators and crossing states) to the non-interacting answer $|\Psi^0_{kN,\text{in}}\rangle$ to arrive at the full answer in the form $|\Psi_{kN,\text{in}}\rangle = \sum_{n=0}^N |\Psi^n_{kN,\text{in}}\rangle$.

While we have presented this discussion in the spinless one lead RLM, it is straightforward to include lead and spin indices.

**Multilead model.**

Returning to the time-dependent case, we proceed to the multilead version of the model, given by Eq. (3.75). The model separates, under a unitary rotation of the fields, into a copy of the one lead RLM and $N_{\text{leads}} - 1$ free fermion fields. We can then find the time evolution of fields in the original basis by rotating, using the RLM time evolution given above (and the fact that the free fermion fields all evolve by the same $e^{-ikt}$ phase factor), and rotating
back. The result, which we derive in more detail below, is the following:

\[ c_{\gamma k}^\dagger(t) \equiv e^{-iH(0)t}c_{\gamma k}^\dagger e^{iH(0)t} \tag{3.94a} \]

\[ = e^{-ikt}c_{\gamma k}^\dagger + \frac{1}{N_{\text{leads}}} \int dx F_k(t - x) \left[ \Theta(0 < x < t) \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma}^\dagger(x) + \frac{i\sqrt{N_{\text{leads}}}}{v} \delta(x)\Theta(0 < t)d^\dagger \right]. \tag{3.94b} \]

To see this, we define a new set of fields (which we will write with a dotted lead index) as:

\[ c_{\tilde{\gamma} k} = \sum_{\gamma=1}^{N_{\text{leads}}} U_{\gamma\tilde{\gamma}} c_{\gamma k} \quad (\tilde{\gamma} = \tilde{1}, \ldots, \tilde{N}_{\text{leads}}), \tag{3.95} \]

where \( U \) is any \( N_{\text{leads}} \times N_{\text{leads}} \) unitary matrix with \( U_{\tilde{\gamma}\gamma} = 1/\sqrt{N_{\text{leads}}} \) for all \( \gamma \). Written in terms of these fields, \( H(0) \) becomes:

\[ H(0) = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma}^\dagger(x) \frac{d}{dx} \psi_{\gamma}(x) + \epsilon d^\dagger d + \left[ v\psi_{N_{\text{leads}}}^\dagger(0)d + \text{h.c.} \right], \tag{3.96} \]

in which the tunneling term only evolves the last field \( c_{\tilde{N}_{\text{leads}} k} \) (and its conjugate). We then find the time evolution in the original basis as follows. First, we note:

\[ c_{\gamma k}(t) = \sum_{\gamma=1}^{N_{\text{leads}}} U_{\gamma\tilde{\gamma}}^\dagger c_{\tilde{\gamma} k}(t), \tag{3.97} \]

where:

\[ c_{\tilde{\gamma} k}(t) \equiv e^{-iH(0)t}c_{\tilde{\gamma} k}^\dagger e^{iH(0)t} \tag{3.98a} \]

\[ = \begin{cases} 
  e^{ikt}c_{\tilde{\gamma} k} 
  & \tilde{1} \leq \tilde{\gamma} \leq \tilde{N}_{\text{leads}} - \tilde{1} \\
  e^{ikt}c_{\tilde{\gamma} k} + \left( \frac{1}{\sqrt{L}} \int dx F_k(t - x) \left[ \Theta(0 < x < t)\psi_{N_{\text{leads}}}^\dagger(x) \right. \\
  & + \left. \left. \frac{i}{v}\delta(x)\Theta(0 < t)d^\dagger \right] \right)^\dagger 
  & \tilde{\gamma} = \tilde{N}_{\text{leads}} 
\end{cases} \tag{3.98b} \]

We then carry out the sum in Eq. (3.97) to obtain:

\[ c_{\gamma k}(t) = e^{ikt}c_{\gamma k} 
+ \mathcal{U}_{\gamma\tilde{N}_{\text{leads}}}^\dagger \frac{1}{\sqrt{L}} \left( \int dx F_k(t - x) \left[ \Theta(0 < x < t)\psi_{N_{\text{leads}}}^\dagger(x) + \frac{i}{v}\delta(x)\Theta(0 < t)d^\dagger \right] \right)^\dagger, \tag{3.99} \]
which is exactly the adjoint of Eq. (3.94b) once we note that $\mathcal{U}_{\gamma N_{\text{leads}}}^\dagger = 1/\sqrt{N_{\text{leads}}}$ and
\[
\psi_{N_{\text{leads}}}^\dagger (x) = \sum_{\beta=1}^{N_{\text{leads}}} \mathcal{U}_{N_{\text{leads}}\beta} \psi_{\beta} (x) = \frac{1}{\sqrt{N_{\text{leads}}}} \sum_{\beta=1}^{N_{\text{leads}}} \psi_{\beta} (x).
\]

The time-independent scattering operators of the multilead model can be found similarly.

One case we will study in particular is the two lead model ($N_{\text{leads}} = 2$), in which refer to the two dotted fields as “odd” ($o$) and “even” ($e$):
\[
\begin{pmatrix}
c_{ok} \\
c_{ek}
\end{pmatrix} = \mathcal{U} \begin{pmatrix}
c_{1k} \\
c_{2k}
\end{pmatrix}, \quad \text{where: } \mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & -1 \\
1 & 1
\end{pmatrix}.
\]

### 3.3.2 Dot occupancy

We calculate the expectation value of the dot as a function of time following the quench in the multilead model. We consider an initial state in which the dot is unoccupied, $|\Psi_{\gamma Nk_N}\rangle = c_{\gamma Nk_N}^\dagger |0\rangle$, with the quantum numbers $\gamma Nk_N$ describing filled Fermi seas in each lead (at zero temperature at first, later to be generalized to arbitrary temperature in each lead). The Fermi sea momenta in lead $\gamma$ are $K_{\gamma} \equiv \{ -D + \frac{2\pi}{L} (j-1) | 1 \leq j \leq N_{\gamma} \}$ with $N_{\gamma} \frac{2\pi}{L} = \mu_{\gamma} + D$.

Then we find:
\[
\langle n_d \rangle(t) \equiv \langle \Psi_{\gamma Nk_N} (t) | d^\dagger d | \Psi_{\gamma Nk_N} (t) \rangle = \langle 0 | c_{\gamma Nk_N} (t) d^\dagger d_{\gamma Nk_N}^\dagger (t) | 0 \rangle = \sum_{j=1}^{N} \langle \{ d, c^\dagger_{kj} (t) \} \rangle^2
\]
\[
= \frac{1}{L} \sum_{j=1}^{N} \left| \frac{i}{v \sqrt{N_{\text{leads}}}} F_{kj} (t) \right|^2 = \frac{1}{L} \sum_{\gamma=1}^{N_{\text{leads}}} \sum_{k_j \in K_{\gamma}} \left| \frac{i}{v \sqrt{N_{\text{leads}}}} F_{kj} (t) \right|^2
\]
\[
\xrightarrow{\text{therm. limit, including temperature}} \frac{1}{N_{\text{leads}}} \sum_{\gamma=1}^{N_{\text{leads}}} \int_{-D}^{D} \frac{dk}{2\pi} f_{\gamma} (k) \frac{|F_{k} (t)|^2}{2\Delta}, \quad (3.101)
\]
where $f_{\gamma} (k) = [\exp ((k - \mu_{\gamma})/T_{\gamma}) + 1]^{-1}$ and $F_{k}$ is given by Eq. (3.81b). In Ref. [54], $\langle n_d \rangle(t)$ is calculated in the one lead model at zero temperature; our result agrees in this special case. In the steady state limit, we find:
\[
\lim_{t \to \infty} \langle n_d \rangle(t) = \frac{1}{N_{\text{leads}}} \sum_{\gamma=1}^{N_{\text{leads}}} \int_{-D}^{D} \frac{dk}{2\pi} f_{\gamma} (k) \frac{|T(k)|^2}{2\Delta}, \quad (3.102a)
\]
\[
= \frac{1}{N_{\text{leads}}} \sum_{\gamma=1}^{N_{\text{leads}}} \int_{-D}^{D} \frac{dk}{2\pi} f_{\gamma} (k) \frac{2\Delta}{(k - \epsilon)^2 + \Delta^2}, \quad (3.102b)
\]
This steady state limit can also be found directly using the scattering “in” operators (this was done in the two lead case in Ref. [55] as a check). In the equilibrium limit (equal temperatures and chemical potentials in all leads), we recover the standard occupancy of the RLM.

The calculation can also be done via the derivative approach of Sec. 2.3.2 by letting the dot energy $\epsilon$ vary; the same answer is obtained.

### 3.3.3 Current

We specialize to the two lead model, $N_{\text{leads}} = 2$. As in the potential scattering case, the (charge) current is the rate of change of the number of electrons in one of the reservoirs. The conserved number operator of the RLM is $\hat{N}_1 + \hat{N}_2 + d^\dagger d$, which means that the current from lead 1 ($-\frac{d}{dt} \langle \hat{N}_1 \rangle$) is not always equal to minus the current from lead 2 ($\frac{d}{dt} \langle \hat{N}_2 \rangle$), since the occupancy of the dot can fluctuate. In the steady state limit, the occupancy no longer fluctuates [see Eq. (3.102a)], and the two definitions of the current coincide.

We write the current leaving lead $\gamma$ in a time-evolving state $|\Psi(t)\rangle$ as:

$$I_\gamma(t) \equiv -\frac{d}{dt} \langle \Psi(t) | \hat{N}_\gamma | \Psi(t) \rangle \quad (\gamma = 1, 2).$$

(3.103)

Then a similar calculation as in the potential scattering case yields:

$$I_\gamma(t) = -\langle \Psi(t) | i[H, \hat{N}_\gamma] | \Psi(t) \rangle$$

(3.104a)

$$= \langle \Psi(t) \rangle \left( \int_{-L/2}^{L/2} dx \frac{d}{dx} \left[ \psi_1^\dagger(x) \psi_1(x) \right] + \hat{I}_\gamma \right) |\Psi(t)\rangle,$$

(3.104b)

where: $\hat{I}_\gamma = \frac{i\nu}{\sqrt{2}} \psi_\gamma^\dagger(0) d + \text{h.c.}$

(3.104c)

As in the potential scattering case, we drop the total derivative term. This is standard (see, e.g., Ref. [56]), though in this case we have not explicitly checked that the $x = 0^\pm$ and $x = t^\pm$ contributions to the total derivative term cancel.

The time-dependent current from either lead can be calculated in the same manner as the occupancy (Sec. 3.3.2). We set $|\Psi(t)\rangle = |\Psi_{3NkN}(t)| \equiv e^{-iH(0)t}c_{3NkN}^\dagger |0\rangle = c_{3NkN}^\dagger (t) |0\rangle$. 


We then find:

$$
\langle \Psi_{\gamma NkN}(t) | \hat{I}_\gamma | \Psi_{\gamma NkN}(t) \rangle = \sum_{j=1}^{N} \text{Re} \left[ \sqrt{2}i v \sum_{j=1}^{N} \{ c_{\gamma j k_j}(t), \psi_{\gamma j}(0) \} \{ d, c_{\gamma j k_j}^\dagger(t) \} \right],
$$

(3.105)

and each anticommutator produces a factor of $1/\sqrt{\mathcal{L}}$, so that we have an expression that becomes an integral over $k$ in the thermodynamic limit. The final answer in the steady state limit is the standard expression for the RLM current:

$$
\lim_{t \to \infty} I_1(t) = - \lim_{t \to \infty} I_2(t) = \int_{-D}^{D} \frac{dk}{2\pi} |f_1(k) - f_2(k)| \frac{1}{4} |T(k)|^2.
$$

(3.106)

Let us verify this answer another way, by setting up the calculation directly in the steady state with the scattering “in” operators. We can also take this opportunity to show an application of the time-independent derivative formula.

Since we work directly in the steady state, we can consider the symmetrized current operator:

$$
\hat{I}_{\text{Sym}} = (\hat{I}_1 - \hat{I}_2) = \frac{i}{2\sqrt{2}} v \left( \psi_1^\dagger(0) - \psi_2^\dagger(0) \right) d + \text{h.c.}
$$

(3.107)

Our task is to evaluate:

$$
I_{\text{steady state}} = \frac{\langle \Psi_\text{in}^0 | \hat{I}_{\text{Sym}} | \Psi_\text{in}^0 \rangle}{\langle \Psi_\text{in} | \Psi_\text{in} \rangle},
$$

(3.108)

where $|\Psi_\text{in}^0\rangle = c_{\gamma NkN,\text{in}}^\dagger |0\rangle$ is the scattering “in” state corresponding to the free state $|\Psi\rangle = c_{\gamma NkN}^\dagger |0\rangle$ [see Eq. (3.91)], and where the quantum numbers $\gamma NkN$ are later specialized to describe two Fermi seas. The normalization factor is discussed below. To reduce the calculation of the expectation value to the evaluation of an overlap, we let $\bar{\phi}$ be a varying real number and consider the following $\bar{\phi}$-dependent Hamiltonian (recall from that the overbar is a label and does not signify complex conjugation):

$$
\overline{H} = H + \left[ \frac{v}{\sqrt{2}} \left( e^{i\frac{\bar{\phi}}{2}} - 1 \right) \psi_1^\dagger(0) d + \frac{v}{\sqrt{2}} \left( e^{-i\frac{\bar{\phi}}{2}} - 1 \right) \psi_2^\dagger(0) d + \text{h.c.} \right].
$$

(3.109)

Then we can write the expectation value of $\hat{I}_{\text{Sym}}$ (in any eigenstate $|\Psi(E)\rangle$ of the original $H$ with energy $E$) in terms of an overlap; the derivative formula (2.191) yields:

$$
\langle \Psi(E) | \hat{I}_{\text{Sym}} | \Psi(E) \rangle = \lim_{E' \to E} \left( E - E' \right) \frac{\partial}{\partial \bar{\phi}} \bigg|_{\bar{\phi} = \bar{\phi}} \langle \Psi(E') | \Psi(E) \rangle,
$$

(3.110)
where $|\Psi(E)\rangle$ is any family of states satisfying $H|\Psi(E)\rangle = E|\Psi(E)\rangle$ and $|\Psi(E)\rangle|_{\bar{\phi}=\phi} = |\Psi(E)\rangle$, and $\langle \Psi(E')|\Psi(E)\rangle$ any family of eigenstates of $H$ (with energy $E'$) that reduces to $\langle \Psi(E')|\Psi(E)\rangle$ for $E = E'$. The state of interest is $|\Psi(E)\rangle = |\Psi_{in}\rangle$, which has energy $E = \sum_{j=1}^{N} k_j$. We have a considerable freedom in constructing the families of states. We set $\langle \Psi(E')| = \langle \Psi_{in}|$, meaning the adjoint of $|\Psi_{in}\rangle$ with each momenta $k_j$ replaced by a varying momentum $k'_j$. It is convenient to bring the $\bar{\phi}$-dependent Hamiltonian $(3.109)$ to the same form as the original $H$, allowing us to use the scattering operators already obtained. This is done using defining the same $\bar{\phi}$-dependent fields as we used in the potential scattering calculation, defined via Eqs. (3.55) and (3.60a). In terms of these fields, we have:

$$H = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^{2} \bar{\psi}_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) + e d_a^\dagger d_a + \left[ \frac{v}{\sqrt{2}} \sum_{\gamma=1}^{2} \bar{\psi}_{\gamma a}^\dagger(0) d_a + \text{h.c.} \right] , \quad (3.111)$$

which is the same Hamiltonian already considered, with each unbarred electron field replaced by the corresponding barred field. We know the “in” states of this Hamiltonian provided that the incoming plane waves are in the barred basis. Hence, it is convenient to let the $\bar{\phi}$-dependent family of eigenstates be scattering states defined in the same way:

$$|\Psi(E)\rangle = |\Psi_{in}\rangle = \tau_{\gamma N, m, \text{in}}^\dagger |0\rangle. \quad (3.112)$$

Evaluating the right-hand side of Eq. (3.110), we find:

$$(3.110) = \lim_{\text{all } k'_j \rightarrow k_j} (E - E') \frac{\partial}{\partial \bar{\phi}} |_{\bar{\phi}=\phi} \sum_{\sigma \in \text{Sym}(N)} (\text{sgn } \sigma) \prod_{m=1}^{N} \{ c_{\gamma m, k_m, m, \text{in}}, \tau_{\gamma m, k_m, m, \text{in}}^\dagger \} \quad (3.113a)$$

$$= [2\pi \delta(0)]^{N-1} \sum_{m=1}^{N} \lim_{k'_m \rightarrow k_m} (k_m - k'_m) \frac{\partial}{\partial \bar{\phi}} |_{\bar{\phi}=\phi} \{ c_{\gamma m, k'_m, m, \text{in}}, \tau_{\gamma m, k_m, m, \text{in}}^\dagger \}, \quad (3.113b)$$

where we have noted that the “in” operators are Dirac normalized. If any permutation other than the identity is chosen, then the result is zero in the limit of all $k'_j \rightarrow k_j$. The normalization factor in Eq. (3.108) is $\langle \Psi|\Psi\rangle = [2\pi \delta(0)]^{N}$, so we obtain:

$$I_{\text{steady state}} = \frac{1}{2\pi \delta(0)} \sum_{m=1}^{N} \lim_{k'_m \rightarrow k_m} (k_m - k'_m) \frac{\partial}{\partial \bar{\phi}} |_{\bar{\phi}=\phi} \{ c_{\gamma m, k'_m, m, \text{in}}, \tau_{\gamma m, k_m, m, \text{in}}^\dagger \}. \quad (3.114)$$

The prescription for making sense of this and other answers obtained directly in the infinite volume limit is to identify:

$$2\pi \delta(0) \leftrightarrow L. \quad (3.115)$$
We can see this heuristically by noting that $2\pi\delta(0) = \{c_k, c_k^\dagger\} = \int dx \ e^{iqx}$ for $q = 0$, which is the system size $L = \infty$. The momenta $k_N$, which vary continuously, are (after the limit $k'_m \to k_m$ is taken) chosen to be quantized with spacing $\frac{1}{\pi(0)} = \frac{2\pi}{L}$, and then $L$ is taken to infinity with a fixed density of electrons in the same way as in the time-dependent case. This prescription is used in the work of Nishino et al.

The answer (3.114) is then in the right form for getting an integral in the thermodynamic limit, provided that the quantity being summed is non-singular. We turn next to the calculation of this quantity, which then yields the standard result (3.106) for the current.

As an aside, we mention here that the normalization factor in this case could also have been written as $\langle \Psi^0_{\text{in}} | \Psi^0_{\text{in}} \rangle = [2\pi\delta(0)]^N$, since the “in” operators are Dirac normalized. However, it seems to be the case in some interacting problems that the full overlap $\langle \Psi_{\text{in}} | \Psi_{\text{in}} \rangle$ contains additional terms. By comparing the time-independent calculation with the time-dependent version (in which normalization factor is identically 1 at all times), we can see that the correct normalization is $\langle \Psi | \Psi \rangle$.

We proceed with the evaluation of (3.114). We know the “in” operators in the odd/even basis:

$$\bar{c}^\dagger_{\text{ok}, \text{in}} = \bar{c}^\dagger_{\text{ok}}, \quad \bar{c}^\dagger_{\text{ek}, \text{in}} = \bar{c}^\dagger_{\text{ek}} + \int dx \ F_{k, \text{in}}(x) \left[ \Theta(0 < x) \bar{c}^\dagger_{\text{ek}}(x) + \frac{i}{\nu} \delta(x) d^\dagger \right]. \quad (3.116)$$

We then obtain the “in” operators in the lead 1/lead 2 basis by rotation:

$$\begin{pmatrix} \bar{c}_{1k, \text{in}} \\ \bar{c}_{2k, \text{in}} \end{pmatrix} = U \begin{pmatrix} \bar{c}_{\text{ok}, \text{in}} \\ \bar{c}_{\text{ek}, \text{in}} \end{pmatrix}. \quad (3.117)$$

In particular, we have:

$$c_{\gamma k, \text{in}} = \sum_{\gamma = o,e} U^\dagger_{\gamma \gamma} c_{\gamma k}, \quad \bar{c}^\dagger_{\gamma k, \text{in}} = \sum_{\gamma = o,e} \bar{c}^\dagger_{\gamma k, \text{in}} U_{\gamma \gamma} \quad (\gamma = 1, 2). \quad (3.118)$$
which yields:

\[
\{c_{\gamma k',\text{in}}, \bar{\tau}^\dagger_{\gamma k,\text{in}}\} = \sum_{\gamma',\gamma''=\alpha,\beta} \mathcal{U}_{\gamma'}^{\dagger} \mathcal{U}_{\gamma''} \{c_{\gamma' k',\text{in}}, \bar{\tau}_{\gamma'' k,\text{in}}\} \quad (\gamma = 1, 2)
\]  

(3.119a)

\[
= \frac{1}{2} \left[ \sum_{\gamma=\alpha,\beta} \{c_{\gamma k',\text{in}}, \bar{\tau}_{\gamma k,\text{in}}\} + (-1)^{\gamma-1} \left( \{c_{\alpha k',\text{in}}, \bar{\tau}_{\beta k,\text{in}}\} + \{c_{\beta k',\text{in}}, \bar{\tau}_{\alpha k,\text{in}}\}\right) \right].
\]  

(3.119b)

We proceed to evaluate the necessary anticommutators in the odd/even basis. We note:

\[
\left( \begin{array}{c} \bar{c}_{ok} \\ \bar{c}_{ek} \end{array} \right) = \mathcal{U}^\dagger \left( \begin{array}{c} c_{ok} \\ c_{ek} \end{array} \right) = \left( \begin{array}{cc} \cos(\bar{\phi}/2) & -i \sin(\bar{\phi}/2) \\ -i \sin(\bar{\phi}/2) & \cos(\bar{\phi}/2) \end{array} \right) \left( \begin{array}{c} c_{ok} \\ c_{ek} \end{array} \right),
\]  

(3.120a)

hence:

\[
\left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \left( \begin{array}{c} \bar{c}_{ok} \\ \bar{c}_{ek} \end{array} \right) = -i \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \left( \begin{array}{c} c_{ok} \\ c_{ek} \end{array} \right) = -i \left( \begin{array}{c} c_{ek} \\ c_{ek} \end{array} \right),
\]  

(3.120b)

and:

\[
\left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \bar{\psi}_e(x) = -\frac{i}{2} \psi_0(x).
\]  

(3.120c)

Applying these to Eq. (3.116) yields:

\[
\left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \bar{\tau}_{\gamma k,\text{in}} = -\frac{i}{2} c_{ek},
\]  

(3.121a)

\[
\left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \bar{\tau}_{\gamma k,\text{in}} = -i \left[ c_{ok} + \int dx \; F^*_{k,\text{in}}(x) \Theta(0 < x) \psi_0(x) \right].
\]  

(3.121b)

We have \( \left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \{c_{\gamma k',\text{in}}, \bar{\tau}^\dagger_{\gamma' k,\text{in}}\} = 0 \) (for \( \gamma = o \) or \( e \)), since \( \{c_{ok'}, c^\dagger_{ek}\} = \{c_{ek'}, c^\dagger_{ok}\} = 0 \). Thus, the odd-odd and even-even contributions to Eq. (3.119b) vanish; the non-vanishing anticommutators under the \( \bar{\phi} \) derivative are the odd-even and even-odd combinations. For odd-even, we find:

\[
\left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \{c_{ok',\text{in}}, \bar{\tau}^\dagger_{ek,\text{in}}\} = \frac{i}{2} \left( \{c_{ok'}, c^\dagger_{ek}\} + \int dx \; F_{k,\text{in}}(x) \Theta(0 < x) \{c_{ok'}, \psi^\dagger_0(x)\} \right)
\]  

(3.122a)

\[
= \frac{i}{2} \left[ 2\pi \delta(k - k') - i \mathcal{T}(k) \left( \pi \delta(k - k') + \text{P.V.} \frac{i}{k - k'} \right) \right],
\]  

(3.122b)

where we have recalled that \( F_{k,\text{in}}(x) = -i \mathcal{T}(k) e^{ikx} \); \text{P.V.} indicates the principal value. Only the pole in \( k - k' \) survives in the \( k' \to k \) limit:

\[
\lim_{k' \to k} (k - k') \left. \frac{\partial}{\partial \bar{\phi}} \right|_{\bar{\phi}=0} \{c_{ok',\text{in}}, \bar{\tau}^\dagger_{ek,\text{in}}\} = \frac{i}{2} \mathcal{T}(k).
\]  

(3.123)
The even-odd contribution is found similarly:

\[
\lim_{k' \to k} (k - k') \frac{\partial}{\partial \phi} \bigg|_{\phi=0} \{c_{ek', \text{in}}, \bar{c}_{ek', \text{in}}\} = \lim_{k' \to k} (k - k') \frac{i}{2} \left( \{c_{ek'}, \bar{c}_{ek'}\} + \int dx F_{k', \text{in}} \Theta(0 < x) \{\psi_e(x), \bar{c}_{ek'}\} \right)
\]

\[
= \frac{i}{2} T^*(k).
\]

From Eq. (3.119b), we thus find:

\[
\lim_{k' \to k} (k - k') \frac{\partial}{\partial \phi} \bigg|_{\phi=0} \{c_{\gamma k', \text{in}}, \bar{c}_{\gamma k', \text{in}}\} = \frac{1}{2} (-1)^{\gamma^{-1}} \left( \frac{i}{2} T(k) - \frac{i}{2} T^*(k) \right)
\]

\[
= \frac{1}{4} (-1)^{\gamma^{-1}} |T(k)|^2,
\]

where use the optical identity (3.80). Finally, we return to Eq. (3.114) and choose the quantum numbers \(\gamma_Nk_N\) to describe two Fermi seas, resulting in:

\[
I_{\text{steady state}} = \frac{1}{2\pi \delta(0)} \sum_{m=1}^{N} \frac{1}{4} (-1)^{\gamma m^{-1}} |T(k_m)|^2 = \frac{1}{2\pi \delta(0)} \left( \sum_{k \in K_1} - \sum_{k \in K_2} \right) \frac{1}{4} |T(k)|^2
\]

\[
\overset{\text{therm. limit}}{\longrightarrow} \left( \int_{-D}^{\mu_1} \frac{dk}{2\pi} - \int_{-D}^{\mu_2} \frac{dk}{2\pi} \right) \frac{1}{4} |T(k)|^2.
\]

This agrees with the standard result (3.106) once we generalize to arbitrary lead temperatures.

### 3.4 On the averaging prescription for the delta function

A common feature in all of the quantum impurity models considered in this thesis is that the linearity of the spectrum \((d/dx)\), combined with the localized (Dirac delta) nature of the tunneling between the leads and the dot, results in differential equations that require some extra regularization. The basic issue, which appears already in non-interacting models (as we have seen in the previous sections) is that the differential equations include \(\delta(x)\) multiplying a function (the wavefunction) that is discontinuous at \(x = 0\). Ordinarily, a
function multiplying a delta function can be replaced by its value at zero, but here the left and right limits of the function are different as \( x \) approaches zero.

The prescription we have chosen amounts to *averaging* the left and right limits of the wavefunction as \( x \to 0 \). This same prescription is used in one of the solutions of the Kondo model in equilibrium by Bethe Ansatz, and can thought of as assigning a value of \( 1/2 \) to the quantity \( \Theta(0) \), i.e. \( \Theta(x)\delta(x) = \frac{1}{2}\delta(x) \) (see Ref. [40]). In the Appendix, we do a calculation that partially supports this prescription. In particular, we include a cutoff on the Hamiltonian, so that the potential scattering model (for example) becomes:

\[
H = \sum_{|k|<D} k c^\dagger_k c_k + \frac{J'}{L} \sum_{|k|<D,|k'|<D} c^\dagger_k c_{k'}.
\]  

(3.127)

We solve for the time evolution and show that the following limit yields the same answer as the averaging prescription:

\[
\lim_{D \to \infty} \lim_{L \to \infty} \sqrt{L} e^{-iHt} c^\dagger_k e^{iHt}.
\]  

(3.128)

The factor of \( \sqrt{L} \) is just a conversion from Kronecker delta normalization (for the finite size system) to Dirac delta normalization (for the infinite size system). Strictly speaking, the calculation only supports the averaging prescription in the limits of large system size and large bandwidth – limits that we instead take *after* first using the averaging prescription to solve for the wavefunction.

An alternative to averaging prescription – one that we will call the “integration prescription” – has also been used in the literature. To explain this prescription in the simplest context, we consider the time-independent Schrodinger equation for the potential scattering model:

\[
\left(-i \frac{d}{dx} I + J' \delta(x) - E\right) g(x) = 0.
\]  

(3.129)

Whereas the averaging prescription replaces \( \delta(x)g(x) \to \frac{1}{2} \delta(x) [g(0^-) + g(0^+)] \), the integration prescription proceeds by writing \( g(x) \) as a plane wave times a phase factor:

\[
g(x) = e^{ikx} e^{i\phi(x)}.
\]  

(3.130)
We get a differential equation for \( \phi(x) \) which we then integrate:

\[
\frac{d}{dx} \phi(x) = -J' I \delta(x),
\]

(3.131a)

hence: \( \phi(x) = -J' \Theta(x) \),

(3.131b)

hence: \( g(x) = e^{i k x} \left[ \Theta(-x) + e^{-i J'} \Theta(x) \right] \).

(3.131c)

(We have taken here the boundary condition for a scattering “in” state; the calculation is very similar if we instead consider the time evolution of \( c_k^\dagger \).) Thus, the scattering phase shift in this prescription is given by \( S = e^{-i J'} \), rather than by the averaging prescription answer of \( S = \frac{1 - i \frac{1}{2} J'}{1 + i \frac{1}{2} J'} \).

The integration prescription has been used successfully for a Bethe Ansatz solution of the Kondo model (see Ref. [57]). Indeed, it has been argued in the literature – in the context of the single particle Dirac equation, in which the same considerations occur – that the averaging prescription is simply wrong, and that the integration prescription is correct [58]. The argument is based on regulating the delta function only, and not the kinetic term. In other words, the derivative term is \( d/dx \) (which includes all modes), while the delta function is smoothed out in some way (which means that high energy modes are suppressed, though not necessarily by the sharp cutoff we used above). In quantum impurity models, regulating the whole Hamiltonian – including the kinetic term – seems more aligned with the underlying band theory. As we showed above, this way of regulating the Hamiltonian leads, albeit only in the limit of large bandwidth and large system size, to the same result as the averaging prescription.

It has also been argued in the literature that the two different prescriptions represent different renormalization schemes. In the simple case of the potential scattering model, either prescription leads to a \( J' \)-dependent phase shift of the wavefunction upon crossing the scatterer; the only difference is the scheme-dependent (and thus unphysical) functional form of the phase shift on \( J' \). This argument is further supported by the fact that the same final answers for physical quantities are obtained in the Kondo model (solving in equilibrium
using Bethe Ansatz) using either scheme. It is important that the Kondo calculations in each case were done in the regime of weak bare coupling $J$.

A difference arises, however, when we push these two schemes to strong bare coupling.\(^3\) While we defer further discussion of this point to the next chapter, the main point is that the schemes give different answers for large coupling. We have already seen above that the averaging prescription seems to be better motivated in terms of the underlying band theory; we will see in the next chapter that the strong coupling results obtained via this prescription seem to make more sense. Thus, the conclusion seems to be that the averaging and integration prescriptions give equivalent answers for small bare coupling, but that only the averaging prescription works for large bare coupling.

\(^3\)The particular value of $J$ which is considered the strongest coupling is prescription-dependent. For instance, we can see in the potential scattering model that the value of $J'$ at which $S = -1$ — i.e. a phase shift of $\pi/2$, leading to conductance reaching the unitarity limit — is $J' = \pm \infty$ in the averaging prescription and $J' = \pm \pi$ in the integration prescription. By itself, this difference is of no significance, but we will see that physically different answers are obtained in the two schemes in the Kondo model for strong bare coupling.
Chapter 4
Kondo model

The Kondo model, discussed in more detail in Chapter 1, is the main application so far of the new approach introduced in this thesis. In this chapter, we use the techniques of Chapter 2 to calculate the time-evolving many-body wavefunction of the Kondo model (with one lead or two leads) and the non-equilibrium steady state, or many-body scattering state, that results in the long time limit. We then focus on the electric current (in the two lead model), finding an exact formula for average value in terms of the quantum numbers of an arbitrary number \( N \) of electrons. The case of physical interest has these \( N \) quantum numbers describing two Fermi seas – with a voltage difference and/or temperature difference between the leads to drive the current – with \( N \) taken to infinity in the thermodynamic limit (in which the system size also goes to infinity, with fixed density \( N/L \)).

Taking the thermodynamic limit of the exact expression for the current turns out to be a formidable task. We take the limit order-by-order in an expansion parameter, which can either be the Kondo coupling \( J \) or its inverse, \( 1/J \). The former case covers the same regime accessible by conventional perturbation theory, and the latter case allows us to explore a new regime. We find in particular that the case of strong ferromagnetic (\( J \rightarrow -\infty \)) is a new universal regime, in which the universal conductance curve approaches the unitarity limit \((2e^2/h)\) asymptotically at large voltage or temperature.

We also show that either series, in \( J \) or in \( 1/J \), converges to all orders in the long time limit (note that this limit is taken after the thermodynamic limit, so that \( t \ll L \) always). This confirms that the infinitely-large leads serve as thermal reservoirs, despite the fact that there is no explicit relaxation process in the model. Convergence in time to all orders in \( J \)
has already been established by a Keldysh calculation in the literature [30], but both the 1/J series and its convergence in time to all orders are new results.

4.1 Wavefunction

Our main focus is the two lead Kondo model:

\[
H^{(0)} = -i \sum_{\gamma=1,2} \int_{-L/2}^{L/2} dx \left( \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) - B S^z \right),
\]

\[
H^{(1)} = \frac{1}{2} J \sum_{\gamma,\gamma'=1,2} \psi_{\gamma a}^\dagger(0) \sigma_{aa'} \psi_{\gamma' a'}(0) \cdot \mathbf{S},
\]

\[
H = H^{(0)} + H^{(1)},
\]

in which we have made the usual linearization of the spectrum and reduction to one dimension, with universality in mind (see Chapter 1). We have taken the coupling of the leads to be of the simplest form: the spin flips from one lead to another (\(\psi_1^\dagger \psi_2\) and \(\psi_2^\dagger \psi_1\)) have the same coefficient as the spin flips within each lead (\(\psi_1^\dagger \psi_1\) and \(\psi_2^\dagger \psi_2\)). This means in particular that the Hamiltonian decouples into a non-interacting “odd” (subscript \(o\)) part and an “even” (subscript \(e\)) part that is identical to the one lead model:

\[
\begin{pmatrix}
  c_{oka} \\
  c_{eka}
\end{pmatrix} = \mathcal{U} \begin{pmatrix}
  c_{1ka} \\
  c_{2ka}
\end{pmatrix}, \quad \mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  1 & -1 \\
  1 & 1
\end{pmatrix}, \quad \mathcal{U}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  1 & 1 \\
  -1 & 1
\end{pmatrix}.
\]

After this rotation, we obtain \(H = H_o + H_e\), with \(H_o \equiv H^{(0)}_o = -i \int_{-L/2}^{L/2} dx \psi_{oa}^\dagger(x) \frac{d}{dx} \psi_{oa}(x)\) and:

\[
H^{(0)}_e = -i \int_{-L/2}^{L/2} dx \psi_{e}^\dagger(x) \partial_x \psi_e(x) - B S^z,
\]

\[
H^{(1)}_e = J \psi_{ea}^\dagger(0) \sigma_{aa'} \psi_{ea'}(0) \cdot \mathbf{S},
\]

\[
H_e = H^{(0)}_e + H^{(1)}_e.
\]

As shown in Sec. 2.5, this decoupling means that we can use the crossing states of the even sector (i.e. the one lead model) to construct the solution of the two lead model. We
therefore begin our study with the even sector Hamiltonian $H_e$, dropping the subscript $e$ and considering it as the one lead model.

It is straightforward to verify that that the basic conditions required for the method [see Sec. 2.2] are valid in both the one lead model and the two lead model. The fixed impurity states are the impurity spin states (along the $z$-axis) $|\uparrow\rangle \equiv |1/2\rangle$ and $|\downarrow\rangle \equiv |-1/2\rangle$, which are annihilated by $H^{(1)}$. Since we put a magnetic field on the impurity, the two spin states rotate into each other under evolution by $H^{(0)}$:

$$|a_0(t)\rangle \equiv e^{-iH^{(0)}t}|a_0\rangle = e^{i\alpha_B t}|a_0\rangle.$$ (4.4)

We take the field operators to be the momentum creation operators:

$$c_\uparrow^\dagger \equiv c^\dagger_{\gamma ka} \equiv \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{ikx} \psi^\dagger_{\gamma a}(x),$$ (4.5)

with the momenta $k$ quantized as usual by the periodic boundary conditions, and with a lead index $\gamma = 1, 2$ that can dropped (or replaced by $e$) to consider the one lead model. The interaction term $H^{(1)}$ is of the form $c^\dagger c O_{\text{imp}}$; thus, the $B(t)$ operators vanish [since $c^\dagger(t)$ will be a linear combination of $c^\dagger$ operators], and so the model is type A. Below, we present the exact wavefunction at any time in two equivalent forms. We refer to the first form as the solution in the “$J = 0$ basis,” since the single particle operators in this case will be defined as the time evolution via the $J = 0$ part of the Hamiltonian only:

$$c^\dagger_{ka}(t) \equiv e^{-iH^{(0)}t}c^\dagger_{ka}e^{iH^{(0)}t} = e^{-ikt}c^\dagger_{ka} \quad (J = 0 \text{ basis}).$$ (4.6)

The second form is the solution in the “$|J| = \infty$ basis,” which takes as its starting point the single particle operators corresponding to $H^{(0)}$ plus a potential scattering term of infinite strength:

$$c^\dagger_{ka}(t) \equiv \lim_{|J| \to \infty} e^{-i(H^{(0)}+J^\dagger\psi_{\alpha'}^\dagger(0)\psi_{\alpha'}(0))t} c^\dagger_{ka}e^{i(H^{(0)}+J^\dagger\psi_{\alpha'}^\dagger(0)\psi_{\alpha'}(0))t} \quad (|J| = \infty \text{ basis})$$ (4.7a)

$$= \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{-ik(t-x)} [1 - 2\Theta(0 < x < t) - 2\Theta(t < x < 0)] \psi_a^\dagger(x).$$ (4.7b)
[To obtain the second line, note that the two spin components are independent copies of the potential scattering model, and see Eq. (3.7).] The motivation for this second form becomes clear when we solve the model in the $J = 0$ basis and find that the $|J| \to \infty$ limit of the $S$-matrix is the same as would be obtained had we considered a potential scattering model with infinite $|J'|$.

Infrared pathologies well-known in the literature prevent us from getting sensible answers for observables when the magnetic field on the dot is present in $H$ (see Chapter 7 for more discussion); nevertheless, we can still solve for the exact wavefunction at all times. We present the solution with the magnetic field in the hopes that the methods discussed in the literature for dealing with the infrared problems can be adapted to our method of calculation. In our main results for observables, we set the magnetic field to zero.

Let us specialize the general formalism of Sec. 2.2 to the case of the one lead model (4.3c) (dropping the subscript $e$ for now). The problem is to find the time evolution of a product state with arbitrary momenta and spins:

\[
|\Psi_{kN\sigma N,a_0} \rangle \equiv c_{kN\sigma N}^\dagger |a_0 \rangle, \quad |\Psi_{kN\sigma N,a_0}(t) \rangle \equiv e^{-iHt}|\Psi_{kN\sigma N,a_0} \rangle.
\]

(4.8)

This amounts to solving for the crossing states. The time-evolving wavefunction is given by:

\[
|\Psi_{kN\sigma N,a_0}(t) \rangle = \sum_{n=0}^{N} \sum_{m \in \mathcal{I}_n(N)} (\text{sgn } m) c_{kN/m\sigma N/m}^\dagger (t) |\Phi_{km\sigma m,a_0}(t) \rangle,
\]

(4.9)

where the crossing states $|\Phi(t) \rangle$ are antisymmetrizations of the unsymmetrized crossing states $|\chi(t) \rangle$:

\[
|\Phi_{km\sigma m,a_0}(t) \rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) |\chi_{km\sigma \sigma,a_0}(t) \rangle.
\]

(4.10)

Similarly, in the two lead model (4.1c) the problem is to find the time evolution of a product state with arbitrary lead indices, momenta, and spins:

\[
|\Psi_{\gamma NkN\sigma N,a_0} \rangle \equiv c_{\gamma NkN\sigma N}^\dagger |a_0 \rangle, \quad |\Psi_{\gamma NkN\sigma N,a_0}(t) \rangle \equiv e^{-iHt}|\Psi_{\gamma NkN\sigma N,a_0} \rangle.
\]

(4.11)
The time-evolving odd and even operators are:

\[
\begin{align*}
\hat{c}_{oka}^+(t) &= e^{-ikt} \hat{c}_{oa}^+ \\
\hat{c}_{eka}^+(t) &= \begin{cases} 
    e^{-ikt} \hat{c}_{eka} & J = 0 \text{ basis} \\
    e^{-ikt} \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{-ik(t-x)} \ [-2\Theta(0 < x < t)] \psi_{e\alpha}(x) & |J| = \infty \text{ basis}
\end{cases}
\end{align*}
\]  

As shown in Sec. 2.5, we can use the same crossing states of the one lead model [with each \(\hat{\psi}_{a}^+(x)\) replaced by \(\hat{\psi}_{e\alpha}(x)\)] to find the wavefunction of the two lead model:

\[
|\Psi_{\gamma_{N\kappa_{\alpha_{N_0}}}^{N\kappa_{\alpha_{N_0}}}}(t)\rangle = \sum_{n=0}^{N} 2^{-n/2} \sum_{m \in I_n(N)} (\delta_{n_1 m_1} \cdots \delta_{n_m m_m}) c_{\gamma_{N_{(N+m)}}}^{\dagger} c_{\alpha_{N_{(N+m)}}}^{\dagger} (t) |\Phi_{\kappa_{\alpha_{N_0}}}^{m_1 m_2 \cdots m_m}(t)\rangle. 
\]

Thus, the core difficulty of the problem is the construction of the unsymmetrized crossing states \(|\chi(t)\rangle\) of the one lead model. From Eqs. (2.42a)-(2.42c), we see these states are determined by:

\[
\begin{align*}
\left( H - i \frac{d}{dt} \right) |\chi_{k_{1 \cdots k_{n_0}}}^{(t)}\rangle &= -A_{k_{1} a_{1}}^{(t)} |\chi_{k_{1} a_{1} \cdots k_{n-1} a_{n-1} a_{0}}^{(t)}\rangle, \\
|\chi_{k_{1} a_{1} \cdots k_{n_0}}^{(t = 0)}\rangle &= 0, \\
|\chi_{a_{0}}^{(t)}\rangle &= |a_{0}^{(t)}\rangle,
\end{align*}
\]

where \(n \geq 1\) and the momenta are arbitrary. Our next task is to construct these states explicitly. We do this in each basis.

### 4.1.1 Solution in the \(J = 0\) basis

We define the time-dependent momentum operators via Eq. (4.6). A short calculation yields the \(A(t)\) and \(B(t)\) operators in this basis:

\[
\begin{align*}
A_{k_{1} a_{1}}^{(t)} &= [H, c_{k_{1} a_{1}}^{\dagger} (t)] - i \frac{\partial}{\partial t} c_{k_{1} a_{1}}^{\dagger} (t) = \frac{1}{\sqrt{L}} e^{-ik_{1}^{t} J_{s_{1} a_{1}}} \cdot S_{k_{1} a_{1}}^{\dagger} (0), \\
B_{k_{1} a_{1} k_{2} a_{2}}^{(t)} &= \{A_{k_{2} a_{2}}^{(t)}, c_{k_{1} a_{1}}^{\dagger} (t)\} = 0.
\end{align*}
\]
Crossing states for $n = 1$.

The problem is to find a time-evolving state $|\chi_{k_1a_1,a_0}(t)\rangle$ that vanishes at $t = 0$ and satisfies:

$$\left(H - i \frac{d}{dt}\right) |\chi_{k_1a_1,a_0}(t)\rangle = -A_{k_1a_1}(t)|a_0(t)\rangle$$

$$= -e^{-ik_1t} J_{b_1a_1} \cdot S_{b_0a_0} e^{ia_{0}B_{t}\psi_{b_{1}}^{\dagger}(0)|b_{0}\rangle}$$

$$= -[\Theta(-t) + \Theta(t)] e^{-ik_1t} J_{b_1a_1} \cdot S_{b_0a_0} e^{ia_{0}B_{t}\psi_{b_{1}}^{\dagger}(0)|b_{0}\rangle}.$$  

As in the non-interacting models of Chapter 3, we have written $1 = \Theta(-t) + \Theta(t)$, and the question of how the Heaviside functions add up to unity at $t = 0$ does not need to be answered [since we will organize the calculation so that the terms multiplying $\Theta(-t)$ and the terms multiplying $\Theta(t)$ each sum to zero separately].

We make the following ansatz:

$$|\chi_{k_1a_1,a_0}(t)\rangle = \frac{1}{\sqrt{L}} \int dx_1 \left[ F_{k_1a_1,a_0}^{b_1b_0} (t - x_1) \Theta(0 < x_1 < t) + G_{k_1a_1,a_0}^{b_1b_0} (t - x_1) \Theta(t < x_1 < 0) \right] e^{iBt\psi_{b_1}^{\dagger}(x_1)|b_0\rangle},$$

where $F$ and $G$ are functions to be determined. Ultimately, this ansatz is justified by the fact that it works; however, we can give some motivation. The quench occurs at $t = 0, x = 0$ and the effect should travel to the right at unit speed (that is, at the Fermi velocity). This accounts for the Heaviside function $\Theta(0 < x_1 < t)$. The other Heaviside function encodes the time evolution backwards in time to negative $t$. Negative times are unnecessary for quench problems, but it will be useful to have the solution there in order to resolve any possible doubt that the differential equations hold at $t = 0$. Also, the negative time part of the solution can be used to generate scattering “out” states (just as the positive time part generates “in” states). Finally, we note that $F$ and $G$ have been taken to be functions only of the difference $t - x_1$, not of $t$ and $x_1$ separately; the point of this will become clear shortly.
We split up the action of \( H - i \frac{d}{dt} \) on the ansatz state into two parts: the action of \( H^{(0)} - i \frac{d}{dt} \) and the action of \( H^{(1)} \). In the former, the kinetic term will act like \(-i \frac{d}{dx_1}\), so we can drop any function of the difference \( t - x_1 \). Note also that \( H^{(0)} - i \frac{d}{dt} \) yields zero on \( e^{ib_0Bt}|b_0\rangle \). We therefore obtain:

\[
\left( H^{(0)} - i \frac{d}{dt} \right) |\chi_{k_1a_1,a_0}(t)\rangle = -i \frac{1}{\sqrt{L}} \int dx_1 \left[ F^{b_1b_0}_{k_1a_1,a_0}(t-x_1)\delta(x_1)\Theta(0 < t) \right. \\
- \left. G^{b_1b_0}_{k_1a_1,a_0}(t-x_1)\Theta(t < 0)\delta(x_1) \right] e^{ib_0Bt}\psi_{b_1}^\dagger(x_1)|b_0\rangle
\]

\[\text{(4.18a)}\]

Notice that this result is a linear combination of terms of the form \( \psi_{b_1}^\dagger(0)|b_0\rangle \) – i.e., the same type of linear combination as \( A(t)|a_0(t)\rangle \), the quantity we are trying to cancel. Had we chosen the functions \( F \) and \( G \) to depend on \( t, x_1 \) in a general way (rather than just on the difference \( t - x_1 \)), we would have obtained an additional contribution of an incorrect form: an integral over \( \psi_{b_1}^\dagger(x_1)|b_0\rangle \).

The action of \( H^{(1)} \) on the ansatz state is:

\[
H^{(1)}|\chi_{k_1a_1,a_0}(t)\rangle = J\sigma_{b_1c_1} \cdot S_{b_0c_0} \frac{1}{\sqrt{L}} \int dx_1 \left[ F^{c_1c_0}_{k_1a_1,a_0}(t-x_1)\frac{1}{2}\delta(x_1)\Theta(0 < t) \right. \\
+ \left. G^{c_1c_0}_{k_1a_1,a_0}(t-x_1)\frac{1}{2}\Theta(t < 0)\delta(x_1) \right] e^{ic_0Bt}\psi_{c_1}^\dagger(x_1)|b_0\rangle
\]

\[\text{(4.19a)}\]

\[
= \frac{1}{\sqrt{L}} J\sigma_{b_1c_1} \cdot S_{b_0c_0} \frac{1}{2} \left[ F^{c_1c_0}_{k_1a_1,a_0}(t)\Theta(0 < t) + G^{c_1c_0}_{k_1a_1,a_0}(t)\Theta(t < 0) \right] \\
\times e^{ic_0Bt}\psi_{c_1}^\dagger(0)|b_0\rangle.
\]

\[\text{(4.19b)}\]

Here, we used the “averaging prescription” – the identification \( \delta(x)\Theta(0 < x < t) = \delta(x)\Theta(t - x) = \frac{1}{2}\delta(x)\Theta(0 < t) \) – discussed in more detail in Sec. 3.4. Separately collecting terms that multiply \( \Theta(t) \) and \( \Theta(-t) \), we see that the desired equation (4.16c)
Note that the equation for $G$ holds provided that $I$ is the spin flip operator. Then it is straightforward to verify that the matrix inverse of a $3 \times 3$ matrix in matrix form:

$$\left[ I + \frac{i}{4} J \sigma^j \otimes \sigma^j \right]_{c_1c_0}^{b_1b_0} F_{k_1a_1,a_0}^{c_1,c_0} (t) e^{i c_0 B t} = - \frac{1}{2} e^{-i k_{11}^t J} \left[ \sigma^j \otimes \sigma^j \right]_{a_1a_0}^{b_1b_0} e^{i \frac{1}{2} a_0 B t}, \quad (4.21)$$

where summation over $j = 1, 2, 3$ is implied, $I_{a_1a_0}^{b_1b_0} = \delta_{a_1}^{b_1} \delta_{a_0}^{b_0}$, and where we have noted that $S = \frac{1}{2} \sigma$. We then solve for $F$ by matrix inversion:

$$F_{k_1a_1,a_0}^{b_1,b_0} (t) = M_{a_1a_0}^{b_1b_0} e^{-i [k_1 + (a_0 - b_0) B] t}, \quad (4.22)$$

where we have defined a matrix $M$ that appears frequently in the solution and in subsequent calculations:

$$M_{a_1a_0}^{b_1b_0} = - \frac{1}{2} J \left[ I + \frac{i}{4} J \sigma^j \otimes \sigma^j \right]_{c_1c_0}^{b_1b_0} \left[ \sigma^j \otimes \sigma^j \right]_{a_1a_0}^{c_1c_0}. \quad (4.23)$$

A more explicit form for $M$ (as well as confirmation that the inverse matrix above always exists) follows from the same steps as in the determination of the single particle $S$-matrix in the Bethe Ansatz approach [41]. We use the identity $\sigma^j \otimes \sigma^j = I - 2P$, where $P_{a_1a_0}^{b_1b_0} = \delta_{a_1}^{b_1} \delta_{a_0}^{b_0}$ is the spin flip operator. Then it is straightforward to verify that the matrix inverse of a linear combination of $I$ and $P$ is given by $[\alpha_1 I + \alpha_2 P]^{-1} = (\alpha_1 I - \alpha_2 P) (\alpha_1^2 - \alpha_2^2)^{-1}$. We thus obtain:

$$M = \frac{i \frac{1}{4} J}{1 - i \frac{1}{2} J + \frac{3}{16} J^2} \left[ \left( 1 + i \frac{3}{4} J \right) I - 2 P \right] = 2 \left( -I + \frac{1}{1 + i \frac{3}{4} J} P_+ + \frac{1}{1 - i \frac{3}{4} J} P_- \right), \quad (4.24)$$
where $P_{\pm} \equiv \frac{1}{2}(I \pm P)$. The matrix $\mathcal{M}$ is related to the single particle $S$-matrix and $T$-matrix of the model via:

$$\mathcal{M} = -iT, \quad S = I - iT. \quad (4.25)$$

Reassuringly, the leading order expression for the $T$-matrix is $J\sigma \cdot S$, in agreement with the Born approximation. Comparison to the Bethe Ansatz provides a more stringent test, and indeed we find the same bare $S$-matrix (see Sec. A.1 in the Appendix).

As in the Bethe Ansatz, the interacting nature of the problem appears in the non-commutative nature of the $S$-matrix; in particular, the fact that $S$ has a spin flip component [41]. For $J = 0$, the $S$-matrix simplifies to the identity, and the problem is trivial. It is of interest, then, that in the opposite limit of $|J| \to \infty$, the $S$-matrix simplifies to a multiple of the identity:

$$\lim_{|J| \to \infty} S = -I. \quad (4.26)$$

This is exactly what would be obtained in a potential scattering model with $|J'| \to \infty$ [see Eq. (3.7)]. This motivates the definition of the second basis, given above in Eq. (4.7b). We return to this second basis later, but first complete the solution in the $J = 0$ basis.

**Crossing states for general $n$.**

Generalizing the $n = 1$ ansatz, we write:

$$|\chi_{k_1a_1...k_na_n,a_0}(t)\rangle =$$

$$L^{-n/2} \int dx_1...dx_n \, T^c_{a_0c_n} \left[ \left( \prod_{j=1}^{n} F^{b_j,c_j}_{k_ja_j,c_j-1}(t-x_j) \right) \Theta(0 < x_n < \cdots < x_1 < t) \right.$$

$$+ \left( \prod_{j=1}^{n} C^{b_j,c_j}_{k_ja_j,c_j-1}(t-x_j) \right) \Theta(t < x_1 < \cdots < x_n < 0) \right] \psi^\dagger_{b_n}(x_n) \cdots \psi^\dagger_{b_1}(x_1) e^{ib_0Bt} |b_0\rangle. \quad (4.27)$$

Since the core difficulty of the quench problem is finding these unsymmetrized crossing states, showing that this ansatz works is one of the main results of this thesis. Note that
the ansatz vanishes at \( t = 0 \) by construction, thus satisfying Eq. (4.14b). The main task, then, is to verify Eq. (4.14a), the differential equation that relates the \( n \)th unsymmetrized crossing state to the \((n-1)\)th.

Since we are interested in the time evolution following a quench, we take \( t \geq 0 \) from now on. (As always, we also require that the quench never reaches the boundaries: \( t < L/2 \).) This means that we need only consider the first term in Eq. (4.27), with the product of \( F \) functions. However, the calculation below carries through straightforwardly for the negative time part of the solution (the product of \( G \) functions) using same relabelling as in the single particle case.

By a similar calculation as in the \( n = 1 \) case, we find:

\[
(H - i \frac{d}{dt}) |\chi_{k_1 a_1 \ldots k_n a_n, a_0}(t)\rangle = \int dx_1 \ldots dx_{n-1} \left( \prod_{j=1}^{n-1} F_{k_j a_j, c_j}(t - x_j) \right) 
\times \left[ -i F_{k_n a_n, c_n-1}^{d_o d_0}(t) \frac{1}{2} F_{k_n a_n, c_n-1}^{d_o d_0}(t) e^{i \delta_{d_0} B t} \right] \times \Theta(0 < x_{n-1} < \ldots < x_1 < t) \psi^\dagger_{b_n}(0) \psi^\dagger_{b_{n-1}}(x_{n-1}) \ldots \psi^\dagger_{b_1}(x_1) |b_0\rangle,
\]

and:

\[
A_{k_n a_n}(t) |\chi_{k_1 a_1 \ldots k_n a_n, a_0}(t)\rangle = L^{-n/2} \int dx_1 \ldots dx_{n-1} \left( \prod_{j=1}^{n-1} F_{k_j a_j, c_j}(t - x_j) \right) 
\times \frac{1}{2} F_{k_n a_n, c_n-1}^{d_o d_0} e^{i \delta_{d_0} B t} \Theta(0 < x_{n-1} < \ldots < x_1 < t) 
\times \psi^\dagger_{b_n}(0) \psi^\dagger_{b_{n-1}}(x_{n-1}) \ldots \psi^\dagger_{b_1}(x_1) |b_0\rangle,
\]

where we have again used the averaging prescription, now in the form \( \delta(x_n) \Theta(0 < x_n < \ldots < x_1 < t) = \frac{1}{2} \Theta(0 < x_{n-1} < \ldots < x_1 < t) \).

Thus, the requirement (4.14a) holds provided that \( F \) satisfies:

\[
-i F_{k_n a_n, c_n-1}^{d_o d_0}(t) \frac{1}{2} F_{k_n a_n, c_n-1}^{d_o d_0}(t) e^{i \delta_{d_0} B t} = -e^{-i k_n t} J \sigma_{b_n a_n} \cdot S_{b_0 d_0} F_{k_n a_n, c_n-1}^{d_o d_0} e^{i \delta_{d_0} B t}.
\]

\(^1\)For \( t = 0 \), the wavefunction position space can only be non-vanishing on a set of measure zero (determined by the constraint \( x_n = 0 \)). This has no effect on the state vector -- that is, its overlap with any “reasonable” state is zero, since one obtains an integral over a function that vanishes except on a set of measure zero.
That is,
\[-iF_{k_n a_n, c_{n-1}}^{b_n b_0} (t)e^{ib_0 Bt} + \frac{1}{2} J\sigma_{b_n d_n} \cdot S_{b_0 d_0} F_{k_n a_n, c_{n-1}}^{d_n d_0} (t)e^{id_0 Bt} =
\]
\[-e^{-ik_n t} J\sigma_{b_n a_n} \cdot S_{b_0 c_{n-1}} e^{ic_{n-1} Bt}. \quad (4.31)\]

This is the same equation as in $n = 1$ case, just with different indices. Hence, we have shown that the ansatz works for general $n$.

This calculation reveals the motivation for writing the ansatz (4.27) with a Heaviside function putting the position variables in order. Roughly speaking, the idea is that the Hamiltonian ends up acting non-trivially only the last variable (i.e. the one closest to zero), reducing the problem back to the $n = 1$ case. The story is similar in some other models, except that the reduction is back to the $n = 2$ case, instead (see Chapters 5 and 6).

### 4.1.2 Solution in the $|J| = \infty$ basis

We define the time-dependent momentum operators via (4.7b). A short calculation yields the $A(t)$ and $B(t)$ operators in this basis:

\[A_{ka}(t) \equiv [H, c^\dagger_{ka}(t)] - i \frac{\partial}{\partial t} c^\dagger_{ka}(t) = \frac{1}{\sqrt{L}} 2ie^{-ikt}\psi_{a}^\dagger(0), \quad (4.32a)\]

\[B_{k_1 a_1 k_2 a_2}(t) \equiv \{A_{k_2 a_2}(t), c^\dagger_{k_1 a_1}(t)\} = 0. \quad (4.32b)\]

(Again we confirm that the model is of type A.) Note that the $A(t)$ operators do not depend on the coupling constant. According to our averaging prescription, the contribution of $H^{(1)}$ is essentially the average of the wavefunction to the left and right of the origin; these average to zero for any non-zero $t$.

**Crossing states for $n = 1$.**

The solution follows along similar lines as in the case of the $J = 0$ basis. The right-hand side of the crossing state condition (4.16c) is found now using the $A(t)$ operators of the
\(|J| = \infty\) basis:

\[
\left( H - i \frac{d}{dt} \right) \chi_{k_1a_1,a_0}(t) = -\frac{1}{\sqrt{L}} 2ie^{-ik_1t} f_{a_1a_0}^{b_1b_0} e^{ia_0 Bt} \psi_{b_1}^+(0) |b_0\rangle. \tag{4.33}
\]

We make the same ansatz (4.17) for the crossing states as in the case of the \(J = 0\) basis; the only change will be in the function \(F\) (and in \(G\), which is again related to \(F\) in a simple way). Following the same steps, we find that Eq. (4.20a) is replaced by:

\[
- iF_{k_1a_1,a_0}^{b_1b_0}(t) e^{ib_0 Bt} + \frac{1}{2} J \sigma_{b_1c_1} \cdot S_{b_0c_0} F_{k_1a_1,a_0}^{c_1c_0}(t) e^{ic_0 Bt} = -2ie^{-ik_1t} f_{a_1a_0}^{b_1b_0} e^{ia_0 Bt}. \tag{4.34}
\]

We again isolate \(F\) by matrix inversion, finding:

\[
F_{k_1a_1,a_0}^{b_1b_0}(t) = M_{a_1a_0}^{b_1b_0} e^{-i(k_1+(a_0-b_0)B)t}, \tag{4.35}
\]

where:

\[
M_{a_1a_0}^{b_1b_0} = -i \frac{8}{3J} \left(1 + \frac{4i}{3J}\right) I + \frac{2P}{1 - i \frac{4}{3J} + \frac{16}{J^2}}. \tag{4.36}
\]

As in the case of the \(J = 0\) basis, we can give this matrix a scattering theory interpretation. It is related to the \(T\)-matrix and \(S\) matrix for the \(|J| = \infty\) free particles created by the \((|J| = \infty) c_{k1}^\dagger(t)\) operators via:

\[
M = iT, \quad S = I - iT. \tag{4.37}
\]

The extra minus sign here (compared to Eq. (4.25) in the \(J = 0\) basis) can be understood by considering the long time limit of the time evolution of a single electron. Roughly speaking, the \(|J| = \infty\) plane wave is \(-e^{ikx}\) to the right of the origin and the crossing state is \(Me^{ikx}\), so the overall wavefunction is \((-1 + M)e^{ikx}\) on the right, which is \(1 - M\) times what the free wavefunction would be (rather than \(1 + M\), as would be obtained by doing the same exercise in the \(J = 0\) basis). It is easily verified that \(S = 1 - M\) is unitary, while the naive \(1 + M\) is not unitary.
Crossing states for general $n$. 

We make the same ansatz (4.27). We find:

$$A_{k,n}(t)\chi_{k_1a_1...k_{n-1}a_{n-1},a_0}(t) = L^{-n/2} \int dx_1...dx_{n-1} \left( \prod_{j=1}^{n-1} F^{b_j,c_j}_{k_ja_j,c_{j-1}}(t-x_j) \right)$$

$$\times 2ie^{-ik_n t} I_{a_n d_0}^{c_0 a_0} e^{i\hbar a_0 B} \Theta(0 < x_{n-1} < ... < x_1 < t)$$

$$\times \psi_{b_n}^\dagger (0) \psi_{b_{n-1}}^\dagger (x_{n-1}) ... \psi_{b_1}^\dagger (x_1) |b_0\rangle. \quad (4.38)$$

The crossing state condition (4.14a) is then satisfied if:

$$-iF^{b_n,c_n}_{k_n a_n,c_{n-1}}(t) I_{a_0 d_0}^{c_0 a_0} e^{i\hbar a_0 B} + \frac{1}{2} J_{b_0 d_0} \cdot S_{b_0 d_0} F^{d_n,c_n}_{k_n a_n,c_{n-1}}(t) I_{a_0 d_0}^{c_0 a_0} e^{i\hbar a_0 B} =$$

$$-2ie^{-ik_n t} I_{a_n d_0}^{b_n b_0} I_{a_0 c_0}^{c_0 a_0} e^{i\hbar a_0 B}, \quad (4.39)$$

which again holds due to the $n = 1$ condition [Eq. (4.34)].

4.1.3 Combined solution and summary

While the wavefunction may be written differently depending on whether we work in the $J = 0$ basis or the $|J| = \infty$ basis, it is the same state in the Hilbert space either way. In particular, any observable quantities we calculate must be independent of the choice of basis, despite possibly appearing to be basis-dependent in intermediate steps of the calculation. Verifying this basis-independence is a useful check of the formalism. To this end, we introduce a notation that permits us to do one calculation covering both bases at once.

We introduce a sign factor $\xi = \pm 1$ that keeps track of which basis we are using:

$$\left\{ \begin{array}{ll}
\xi = 1 & J = 0 \text{ basis}, \\
\xi = -1 & |J| = \infty \text{ basis}.
\end{array} \right. \quad (4.40)$$

Then we can write the time evolution of the even sector operators as a single formula:

$$c_{ekn}^\dagger(t) = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \ e^{-ik(t-x)} [1 + (\xi - 1) \Theta(0 < x < t)] \psi_{c}^\dagger(x). \quad (4.41)$$
The $A(t)$ operator in the even sector is then:

$$A_{ek_1a_1}(t) = \frac{1}{\sqrt{L}} e^{-i k_1 t} \left[ \frac{1 + \xi}{2} J \sigma_{b_1a_1} \cdot S + \frac{1 - \xi}{2} 2i \delta_{b_1a_1} \right] \psi^\dagger_{b_1}(0).$$  \hspace{1cm} (4.42)$$

The calculation of the crossing states proceeds as before (or we can just read off the previous answers); in particular, the bare $S$-matrix can be written as:

$$S \equiv \xi (Z_I I + Z_P P) \equiv I + \xi M,$$  \hspace{1cm} (4.43a)

where: $$Z_I = \frac{1 - \frac{3}{16} J^2}{1 - \frac{1}{2} J + \frac{3}{16} J^2},$$  \hspace{1cm} (4.43b)

and: $$Z_P = \frac{-i J}{1 - \frac{1}{2} J + \frac{3}{16} J^2}. \hspace{1cm} (4.43c)$$

The full wavefunction (in either basis) for the two lead model can thus be written as:

$$e^{-i H t} c_N^\dagger a_N |a_0\rangle = \sum_{n=0}^{N} 2^{-n/2} \sum_{m \in \mathcal{L}_{n} (N)} \langle \text{sgn}\,m \rangle c_m^\dagger |\Phi_{ek_m a_m a_0}(t)\rangle |\Phi_{ek_m a_m a_0}(t)\rangle, \hspace{1cm} (4.44)$$

where the crossing states are given by [labelling the quantum numbers by $n = (1, \ldots, n)$]:

$$|\Phi_{ek_n a_n a_0}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} \langle \text{sgn}\,\sigma \rangle |\chi_{ek_n a_n a_0\sigma}(t)\rangle,$$  \hspace{1cm} (4.45a)

$$|\chi_{ek_n a_n a_0}(t)\rangle = L^{-n/2} \int d x_n \int_{-\pi}^{\pi} \mathcal{I}_{a_0 a_0} \prod_{j=1}^{n} \mathcal{F}_{k_j a_j, c_{j-1}} (t - x_j)$$

$$\times \Theta (0 < x_n < \cdots < x_1 < t) \psi^{\dagger}_{b_n}(x_n)e^{ib_0 B t}|b_0\rangle,$$  \hspace{1cm} (4.45b)

$$\mathcal{F}_{k_1 a_1, a_0}(t) = \mathcal{M}^{b_1 b_0} e^{-i[k_1 + (a_0 - b_0) B]t}. \hspace{1cm} (4.45c)$$

It is important to keep track of which quantities are basis-independent. The matrix $\mathcal{M}$ (which we recall is essentially the single particle $T$-matrix, $\mathcal{M} = \xi i T$) is given in the $J = 0$ basis by Eq. (4.24) and in the $|J| = \infty$ basis by Eq. (4.36). The complex coefficients $Z_I$ and $Z_P$ depend only on the coupling constant $J$, and are therefore basis-independent; it follows that $\xi S$ is also basis-independent (since $\xi^2 = 1$).

### 4.1.4 Non-equilibrium steady state

The preceding calculations can all be repeated in the time-independent version of formalism (see Sec. 2.6), in which the goal is to solve the time-independent Schrodinger equation with
the boundary condition of incoming plane waves that have a given set of quantum numbers \( \gamma_N k_N a_N \) and \( a_0 \). Equivalently, the eigenstate we are looking for solves the many-body Lippmann-Schwinger equation for an “in” state:

\[
|\Psi_{\gamma_N k_N a_N, a_0, \text{in}}\rangle = |\Psi_{\gamma_N k_N a_N, a_0}^0\rangle + \frac{1}{E - H(0) + i\eta} H^{(1)} |\Psi_{\gamma_N k_N a_N, a_0, \text{in}}\rangle.
\] (4.46)

By setting the quantum numbers \( \gamma_N k_N a_N \) to describe two Fermi seas separated by a chemical potential, we obtain the nonequilibrium steady state of the Kondo impurity under bias voltage. Conceptually, the important point is that we can solve for this state directly, without needing to calculate how it develops over time. In the Kondo model, time-dependent and time-independent wavefunctions are very similar, but in other cases (including the infinite-\( U \) Anderson model, considered in Chapter 6) the full time dependence seems too complicated, and it is thus useful to calculate the time-independent wavefunction directly.

Essentially the same calculation as we have shown above yields the nonequilibrium steady state (in either basis; see previous section):

\[
|\Psi_{\gamma_N k_N a_N, a_0, \text{in}}\rangle = \sum_{n=0}^{N} 2^{-n/2} \sum_{m \in \mathbb{Z}_n(N)} (\text{sgn } m) c_{\gamma N/m k N/m a N/m}^\dagger \Phi_{ek_m a_m, a_0, \text{in}},
\] (4.47)

where the free creation operators are now Dirac normalized \( [c_{\gamma k a}^\dagger = \int dx \, e^{ikx} \psi_{\gamma a}(x)] \) and where the time-independent crossing states are given by:

\[
|\Phi_{ek_n a_n, a_0, \text{in}}\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) |\chi_{ek_\sigma a_\sigma a_\sigma, a_0, \text{in}}\rangle,
\] (4.48a)

\[
|\chi_{ek_n a_n, a_0, \text{in}}\rangle = \int dx_n \, F_{a_0 c_n}^{\text{qb}_n} \left( \prod_{j=1}^{n} F_{k_j a_j, c_{j-1}}^{b_{j-1} c_j}(-x_j) \right)
\times \Theta(0 < x_n < \cdots < x_1) \psi_{\text{fb}_n}^\dagger(x_n) |b_0\rangle.
\] (4.48b)

Let us verify that the time-evolving wavefunction (4.44) becomes (4.47) in the long time limit [not uniformly for all \( x \), but in the pointwise sense that we explained earlier in the potential scattering case, Eq. (3.17)]. The prescription for taking this pointwise limit of an \( N \)-body wavefunction is the following (schematically):

\[
|\Psi_{\text{in}}\rangle = \int dx_N \lim_{t \to \infty} \lim_{L \to \infty} L^N |x_N\rangle \langle x_N| e^{-iHt} e^{iH(0)t |\Psi\rangle},
\] (4.49)
where $|\Psi\rangle$ represents the initial state prior to the quench, and where $|x_N\rangle = \psi^\dagger(x_N)|0\rangle$ (for the moment we ignore the lead and spin indices, and the impurity degrees of freedom; these can be restored easily). The free evolution factor gets rid of an overall phase and the $L^N$ converts from Kronecker normalization to Dirac normalization.

It is straightforward to show that the factors of $L$ and time-dependent phase factors in (4.44) can be collected into a single prefactor $\frac{1}{L^N} e^{-iEt}$, where $E = \sum_{j=1}^{N} k_j - Ba_0$ is the energy of the initial state prior to the quench. The phase factor cancels, seeing as $H^{(0)}|\Psi\rangle = E|\Psi\rangle$. The only remaining time dependence is in the upper limit of the Heaviside functions in the time-dependent crossing states; sending this upper limit to infinity then recovers the time-independent solution (4.47).

4.2 The current for $N$ electrons

Our next task is to evaluate the average (in the quantum mechanical sense) of the electric current in the time-evolving wavefunction of the two lead Kondo model.

4.2.1 Setup and reduction to odd/even basis

The definition of the current follows along the same lines as in the potential scattering model (Sec. 3.2.2). The most direct definition of the average charge current from lead 1 to lead 2 is:

$$I(t) \equiv -\frac{d}{dt}\langle \Psi_{\gamma NkN\sigma N,a_0}(t)|\hat{N}_1|\Psi_{\gamma NkN\sigma N,a_0}(t)\rangle,$$

(4.50)

where $\hat{N}_1 = \int_{-L/2}^{L/2} dx \psi_{1a}^\dagger(x) \psi_{1a}(x)$ is the number operator for the electrons in lead 1. Below, we derive an exact formula for $I(t)$ in terms of the arbitrary $N$ quantum numbers of the initial state.

As a check on the calculation, we also calculate the current in several other equivalent forms. There is a standard way to bring $I(t)$ to the form of an expectation value of a local
operator. The Heisenberg equation of motion yields:

\[ I(t) = \langle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) | \hat{I} | \Psi_{\gamma NkN\alpha N,\alpha_0} \rangle + \text{(boundary contribution)}, \]  

(4.51a)

where: \( \hat{I} = \frac{1}{2} J \psi_{1a}^\dagger(0) \sigma_{aa'} \psi_{2a'}(0) \cdot \mathbf{S} + \text{ h.c.}, \)  

(4.51b)

and: (boundary contribution) = \[
\langle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) | \int_{-L/2}^{L/2} dx \frac{d}{dx} \left[ \psi_{1a}\dagger(x) \psi_{1a}(x) \right] \rangle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) \rangle. \]  

(4.51c)

The boundary contribution evaluates to a sum over the discontinuities of the wavefunction; these discontinuities are only at \( x = 0 \) and \( x = t \), so we obtain:

(boundary contribution) = \[
\langle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) | \left[ \psi_{1a}\dagger(0^+) \psi_{1a}(0^+) - \psi_{1a}\dagger(0^-) \psi_{1a}(0^-) \right] \rangle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) \rangle + \langle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) | \left[ \psi_{1a}\dagger(t^+) \psi_{1a}(t^+) - \psi_{1a}\dagger(t^-) \psi_{1a}(t^-) \right] \rangle \Psi_{\gamma NkN\alpha N,\alpha_0}(t) \rangle. \]  

(4.52)

The boundary terms in fact sum to zero (see next paragraph), implying that \( I(t) = \langle \hat{I} \rangle \) (where the expectation value is taken in the time-evolving state). Furthermore, taking just the \( x = 0^\pm \) boundary contributions is another equivalent form of the current: that is, we have \( I(t) = \langle \psi_{1a}\dagger(0^-) \psi_{1a}(0^-) - \psi_{1a}\dagger(0^+) \psi_{1a}(0^+) \rangle \). This form of the current is derived by other means in Ref. [30] and is intuitively clear from the idea that density, current density, and current density are all the same in a one-dimensional system with linear spectrum.

From the above considerations, we see that there are number of equivalent ways of calculating the current. Below, we present the calculation of \( I(t) \) using the basic definition (4.50) and also using the local operator \( \hat{I} \), employing the derivative formula [see Sec. 2.3.2] in the latter case to reduce the calculation to the evaluation of an overlap. In Sec. A.2 in the Appendix, we calculate the expectation value of the local operator \( \hat{I} \) directly (without using the derivative formula) and also calculate \( \langle \psi_{1a}\dagger(0^-) \psi_{1a}(0^-) - \psi_{1a}\dagger(0^+) \psi_{1a}(0^+) \rangle \); both coincide with the answer in the main text. Each of these calculations is done both in the \( J = 0 \) basis and in the \( |J| = \infty \). The fact that all of these distinct calculations yield exactly the same answer for the current in the \( N \)-electron system is a powerful consistency check.
The approach we take to calculate the current in similar for each of the various forms, and can serve as a road map for the evaluation of other observables. The first task is to reduce the current to a sum of (normal ordered) overlaps involving only the even sector of the model, with all dependence on lead indices appearing in coefficients of the sum. This calculation relies heavily on the machinery of Chapter 2. We do the calculation in such a way that the equations can be read as referring to either the $J = 0$ basis or the $|J| = \infty$ basis; the difference is entirely accounted for by the sign factor $\xi = \pm 1$ [see Eq. (4.40)] and the different forms of the matrix $\mathcal{M}$ in either basis. Also, the formula (4.41) for $c_{e,k,a}^\dagger(t)$ will be used without comment. Recall from Sec. 2.3.3 that we define normal ordering to move every creation operator to the left of every annihilation operator (with the appropriate fermionic sign factor), with the exception that crossing states are completely unaffected (though they can be written in terms of creation and annihilation operators).

**Original form.**

It proves convenient to write the current in the odd/even basis. Note that the lead 1 number operator can be written as:

$$\hat{N}_1 = \frac{1}{2} \hat{N} + \frac{1}{2} \left( \int_{-L/2}^{L/2} dx \, \psi_{e,a}^\dagger(x) \psi_{e,a}(x) + \text{h.c.} \right),$$

(4.53)

Then, since $N$ is conserved, the original definition (4.50) yields:

$$I(t) = -\text{Re} \left[ \frac{d}{dt} \int_{-L/2}^{L/2} dx \, \langle \Psi_{e_NN_{\alpha N_{\alpha 0}}(t)} | \psi_{e,x}(x) | \Psi_{e_NN_{\alpha N_{\alpha 0}}(t)} \rangle \right].$$

(4.54)
Thus, we can examine the bilinear $\psi_{oa}^\dagger(x)\psi_{ea}(x)$ instead of $\psi_{1a}^\dagger(x)\psi_{2a}(x)$. This allows us to use Eq. (2.167), yielding:

$$\langle \Psi_{\gamma\alpha\beta,\gamma\alpha\beta}(t) | \psi_{oa}^\dagger(x)\psi_{ea}(x) | \Psi_{\gamma\alpha\beta,\gamma\alpha\beta}(t) \rangle =$$

$$\frac{1}{2} \sum_{m=1}^{N} (-1)^{\gamma_m-1} \{ c_{okm\gamma} \{ \psi_{oa}^\dagger(x), c_{ekm\alpha}^\dagger(t) \} \}$$

$$+ \sum_{n=1}^{N} \frac{1}{2^n(n-1)!} \sum_{m_1,...,m_n=1}^{N} (-1)^{\gamma_{m_n}-1} \{ c_{okm_n \alpha \gamma_m} \{ \psi_{oa}^\dagger(x) \} \}$$

$$\times : \langle \Psi_{ekm/m_n a_{m/m_n} \alpha \gamma_m}(t) | \psi_{ea}(x) | \Psi_{ekm/m_n a_{m/m_n} \alpha \gamma_m}(t) \rangle :$$

(4.55a)

$$\equiv (i) + (ii).$$

(4.55b)

Term (i) and its contribution to the current are easily evaluated:

$$(i) = \frac{1}{2} \sum_{m=1}^{N} (-1)^{\gamma_m-1} \left[ e^{ikm(t-x)} \delta_{am} \frac{1}{\sqrt{L}} \left[ 1 + (\xi - 1)\Theta(0 < x < t) \right] \delta_{am} \right]$$

(4.56a)

$$= \frac{1}{2} \left[ 1 - (1 - \xi)\Theta(0 < x < t) \right] \frac{1}{L} \sum_{m=1}^{N} (-1)^{\gamma_m-1},$$

(4.56b)

thus:

$$-\text{Re} \left[ \frac{d}{dt} \int_{-L/2}^{L/2} dx \right] (i) = \frac{1 - \xi}{2} \frac{1}{L} \sum_{m=1}^{N} (-1)^{\gamma_m-1}.$$ 

(4.56c)

We proceed to term (ii), which is more difficult. The main trick we use is the fact that inside the normal ordering symbol, all position variables lie in the forward lightcone: $0 < x < t$. The reason for this is that the crossing states (expressed in the position basis) vanish if any $x$ variable is outside the forward light cone. The time-dependent field operators extend everywhere, but normal ordering forces them to contract only with crossing states and not with each other. Thus, we have:

$$c_{ea}^\dagger(t) = \frac{1}{\sqrt{L}} \int_0^t dx \xi e^{-ik(t-x)} \psi_{ea}^\dagger(x) + \ldots,$$

(4.57)

where the omitted terms vanish inside the normal ordering symbol.

Since $c(t)$ and $\psi(x)$ operators both behave the same way under normal ordering, we can bring the integral inside the normal ordering symbol; thus, we find that the contribution of
(ii) to the current can be written as:

\[
-Re \left[ \frac{d}{dt} \int_{-L/2}^{L/2} dx \ (ii) \right] = Re \left[ \sum_{n=1}^{N} \frac{1}{2^n (n-1)!} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{\gamma_{m_n} - 1} \times \left( -\xi \frac{d}{dt} : \langle \Psi_{ek_{m/m_n} a_{m_n}, a_0}(t) | e_{km_{n} a_{m_n}}(t) \rangle \Psi_{ek_{m_n} a_{m_n}, a_0}(t) : \right) \right].
\] (4.58)

Before proceeding with further evaluation, we first arrive at the same answer in another way: by evaluating \( \langle \vec{T} \rangle \) using the derivative formula discussed in Sec. 2.3.2.

Local form, derivative calculation.

The setup of this calculation is very similar to the corresponding calculation in the potential scattering model. We generalize the Hamiltonian to a one-parameter family of Hamiltonians:

\[
\overline{H} = -i \int_{-L/2}^{L/2} dx \ \psi_{1a}^\dagger(x) \frac{d}{dx} \psi_{1a}(x) - i \int_{-L/2}^{L/2} dx \ \psi_{2a}^\dagger(x) \frac{d}{dx} \psi_{2a}(x)
\]

\[
+ \frac{1}{2} J \left( \psi_{1a}^\dagger(0) \psi_{2a}^\dagger(0) \right) \sigma_{ab} \left( \begin{array}{cc} 1 & e^{i\phi} \\ e^{-i\phi} & 1 \end{array} \right) \left( \begin{array}{c} \psi_{1b}(0) \\ \psi_{2b}(0) \end{array} \right) \cdot S. \ 
\] (4.59)

Removing the bar sets \( \vec{\phi} \to \phi \equiv 0 \), recovering the original Hamiltonian \( H \). Indeed, we have:

\[
\overline{H} = H + f_1(\vec{\phi}) O_1 + f_2(\vec{\phi}) O_2, \ 
\] (4.60a)

where: \( f_1(\vec{\phi}) = e^{i\phi} - 1, f_2(\vec{\phi}) = e^{-i\phi} - 1, \)

\( O_1 = \frac{1}{2} J \psi_{1a}^\dagger(0) \sigma_{aa'} \psi_{2a'}(0) \cdot S, \ 
O_2 = \frac{1}{2} J \psi_{2a}^\dagger(0) \sigma_{aa'} \psi_{1a'}(0) \cdot S. \) (4.60b)

Then the derivative formula (2.68) yields:

\[
\langle \Psi_{\gamma N k_{N a_N}, a_0}(t) | \overline{T} | \Psi_{\gamma N k_{N a_N}, a_0}(t) \rangle = i \frac{\partial}{\partial t} \frac{\partial}{\partial \phi} \bigg|_{\phi=0} \langle \Psi_{\gamma N k_{N a_N}, a_0}(t) | \overline{\Psi}_{\gamma N k_{N a_N}, a_0}(t) \rangle. \] (4.61)
For further simplification, we note that $\bar{H}$, like $H$, decouples into a non-interacting and an interacting part. We bring the Hamiltonian $\bar{H}$ to an odd/even basis basis with a $\bar{\phi}$-dependent unitary matrix $\bar{U}$:

$$
\begin{pmatrix}
\bar{\psi}_{oa}(x) \\
\bar{\psi}_{ea}(x)
\end{pmatrix} = \bar{U}
\begin{pmatrix}
\psi_{1a}(x) \\
\psi_{2a}(x)
\end{pmatrix}, \text{ where } \bar{U} = \frac{1}{\sqrt{2}}
\begin{pmatrix}
e^{-i\frac{1}{2}\bar{\phi}} & -e^{i\frac{1}{2}\bar{\phi}} \\
e^{-i\frac{1}{2}\bar{\phi}} & e^{i\frac{1}{2}\bar{\phi}}
\end{pmatrix}.
$$

(4.62)

The Hamiltonian separates into two (commuting) parts:

$$
\bar{H}_o = -i \int_{-L/2}^{L/2} dx \bar{\psi}_{oa}^\dagger(x) \frac{d}{dx} \bar{\psi}_{oa}(x),
$$

(4.63a)

$$
\bar{H}_e = -i \int_{-L/2}^{L/2} dx \bar{\psi}_{ea}^\dagger(x) \frac{d}{dx} \bar{\psi}_{ea}(x) + J \bar{\psi}_{ea}(0) \sigma_{ab} \bar{\psi}_{eb}(0) \cdot \mathbf{S},
$$

(4.63b)

$$
\bar{H} = \bar{H}_o + \bar{H}_e.
$$

(4.63c)

We define:

$$
\begin{pmatrix}
\bar{\psi}_{1a}(x) \\
\bar{\psi}_{2a}(x)
\end{pmatrix} = \bar{U}^\dagger
\begin{pmatrix}
\bar{\psi}_{oa}(x) \\
\bar{\psi}_{ea}(x)
\end{pmatrix} = \frac{1}{\sqrt{2}}
\begin{pmatrix}
1 & 1 \\
-1 & 1
\end{pmatrix}
\begin{pmatrix}
\bar{\psi}_{oa}(x) \\
\bar{\psi}_{ea}(x)
\end{pmatrix},
$$

(4.64)

and take our (barred) initial state in the derivative formula to be:

$$
|\Psi_{\gamma N k N a N, a_0}\rangle = \bar{c}_{\gamma N k N a N}^\dagger |a_0\rangle.
$$

(4.65)

As explained in more detail in the potential scattering calculation, the point of making this choice is that the problem of finding $e^{-i\bar{H}t}|\Psi_{\gamma N k N a N, a_0}\rangle$ is then identical (after relabelling unbarred fields as barred) to the problem of finding $e^{-iHt}|\Psi_{\gamma N k N a N, a_0}\rangle$, which we have already solved earlier in this chapter.

We proceed to express the current in terms of quantities in the odd/even sector. Eq.
(2.179) yields:

\[
\left. i \frac{\partial}{\partial t} \frac{\partial}{\partial \phi} \right|_{\phi=0} \langle \Psi_{\gamma N a_{N,0}}(t) | \Psi_{\gamma N a_{N,0}}(t) \rangle = \\
\text{Re} \left[ \left. i \frac{\partial}{\partial t} \frac{\partial}{\partial \phi} \right|_{\phi=0} \left( \sum_{m=1}^{N} (-1)^{m-1} \{ c_{k_{m} a_{m}}(t), \overline{c}^{\dagger}_{k_{m} a_{m}}(t) \} \right) \right] + \sum_{n=1}^{N} \frac{2^{-(n-1)}}{(n-1)!} \sum_{m_{1},\ldots,m_{n}=1}^{N} (-1)^{\gamma_{m_{n}-1}} \langle \Psi_{\psi_{k_{m_{n}} a_{m_{n}},0}}(t) | c_{k_{m_{n}} a_{m_{n}}}(t) | \Psi_{\psi_{k_{m_{n}} a_{m_{n}},0}}(t) \rangle : \\
\text{and} \left. i \frac{\partial}{\partial \phi} \right|_{\phi=0} \left( \sum_{m=1}^{N} (-1)^{m-1} \{ c_{k_{m} a_{m}}(t), \overline{c}^{\dagger}_{k_{m} a_{m}}(t) \} \right) \right] .
\]

(4.66)

Our task is to show that this is the same answer as was obtained from the original definition of \( I(t) \). Let us start with the simpler first term (the single sum). We have:

\[
\{ c_{oka'}(t), \overline{c}^{\dagger}_{eka}(t) \} = i \sin \left( \frac{1}{2} \phi \right) \left[ 1 + (\xi - 1) \frac{t}{L} \right] \delta_{aa'},
\]

thus:

\[
\left. i \frac{\partial}{\partial t} \frac{\partial}{\partial \phi} \right|_{\phi=0} \left( \begin{array}{c}
\{ c_{oka'}(t), \overline{c}^{\dagger}_{eka}(t) \} \\
\end{array} \right) = \frac{1}{2} \frac{1}{L} \delta_{aa'}.
\]

(4.67a)

(4.67b)

It follows that the contribution to the current of the first term is \( \frac{1}{2} \frac{1}{L} \sum_{m=1}^{N} (-1)^{m-1} \), which agrees exactly with the contribution of term (i) in the previous calculation [see Eq. (4.56c)].

We proceed to the second term. Due to the normal ordering, the odd operator must contract with some \( \overline{\psi}_{ka}(x) \) operator in the crossing state (or else it hits \( |a_{0}(t)\rangle \), yielding zero). Thus, the only \( \phi \) dependence from an anticommutator, which we can easily evaluate:

\[
\{ c_{oka'}(t), \overline{\psi}^{\dagger}_{eka}(x) \} = i \sin \left( \frac{1}{2} \phi \right) \frac{1}{\sqrt{L}} e^{ik_{x}(t-x)} \delta_{aa'},
\]

thus:

\[
\left. i \frac{\partial}{\partial \phi} \right|_{\phi=0} \left( \begin{array}{c}
\{ c_{oka'}(t), \overline{\psi}^{\dagger}_{eka}(x) \} \\
\end{array} \right) = -\frac{1}{2} \frac{1}{\sqrt{L}} e^{ik_{x}(t-x)} \delta_{aa'} = -\frac{1}{2} \xi \{ c_{eka}(t), \overline{\psi}^{\dagger}_{eka}(x) \},
\]

(4.68a)

(4.68b)

where we have taken \( x \) to be inside the light cone (which it will be, due the normal ordering).

What we have shown is that the \( \phi \) derivative essentially turns the odd field operator into even; in other words:

\[
\left. i \frac{\partial}{\partial \phi} \right|_{\phi=0} \langle \Psi_{\psi_{k_{m_{1}} a_{m_{1}},m_{2}} a_{m_{2}},0}(t) | c_{k_{m_{1}} a_{m_{1}}}(t) | \Psi_{\psi_{k_{m_{1}} a_{m_{1}},m_{2}} a_{m_{2}},0}(t) \rangle : = -\frac{1}{2} \xi \langle \Psi_{\psi_{k_{m_{1}} a_{m_{1}},m_{2}} a_{m_{2}},0}(t) | c_{k_{m_{1}} a_{m_{1}}}(t) | \psi_{k_{m_{1}} a_{m_{1}},0}(t) \rangle :.
\]

(4.69)
Substituting into the second term of Eq. (4.66), we find exactly the contribution of term (ii) to the current in the previous calculation [Eq. (4.58)]. We have thus shown that the current in its local form, \( \langle \tilde{I} \rangle \), agrees exactly with the original definition, \(-\frac{d}{dt} \langle N_1 \rangle\).

Summary.

We have brought the time-evolving current to the following form:

\[
I(t) = \frac{1 - \xi}{2} \frac{1}{L} \sum_{m=1}^{N} (-1)^{\gamma_m-1} \text{Re} \left[ \sum_{n=1}^{N} \frac{\xi 2^{-n}}{(n-1)!} \frac{1}{L^n} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{\gamma_m-1} \frac{\partial}{\partial t} \Omega_{n,a_0}(t; k_m a_m) \right],
\]

where we have defined:

\[
\Omega_{n,a_0}(t; k_m a_m) = L^n : \langle \Psi_{e^{k_m/n_a_m/a_m/a_0}(t)} | e^{-k_m a_m/a_0}(t) | \Psi_{e^{k_m/a_m/a_0}(t)} \rangle :.
\]

(4.70)

We have inserted the factors of \( L \) for the convenience of later taking the thermodynamic limit. The point is that \( \Omega_{n,a_0} \), which we evaluate explicitly in the next section, only depends on \( L \) through its dependence on the momenta (which, we recall, are integer multiples of \( 2\pi/L \)). To see this, note that the normal ordered overlap in \( \Omega_{n,a_0} \) has a prefactor of \( 1/L^n \) (seeing as each quantum number on each side is associated with a factor of \( 1/\sqrt{L} \), whether it is put in a field operator or a crossing state); this cancels with the explicit factor of \( L^n \) in \( \Omega \). The overlap itself can be written in position space as an \( n \)-dimensional integral \( \int dx_n \), which in principle is over the full space \([-L/2, L/2]\); however, due to normal ordering, the bounds of integration can be replaced by \((0, t)\). Thus, the only \( L \)-dependence is in the momenta.

Before taking the thermodynamic limit, we make some further simplifications using symmetries of \( \Omega_{n,a_0} \). It turns out to be useful to consider the “off-diagonal” case, defined as follows:

\[
\Omega_{n,a_0}^{(off-diag)}(t; k'_n a'_n; k_n a_n) = L^n : \langle \Psi_{e^{k'_n/a'_n/a_0}(t)} | e^{-k'_n a'_n}(t) | \Psi_{e^{k_n/a_n/a_0}(t)} \rangle :.
\]

(4.72)

Since fermionic symmetries of the wavefunction are valid inside the normal ordering symbol...
[see Sec. 2.3.4], \( \Omega_{n,a_0}^{\text{(off-diag)}} \) has the following symmetries:

\[
\Omega_{n,a_0}^{\text{(off-diag)}}(t; k'_{\sigma'\sigma}, a'_{\sigma'\sigma}; k_{\sigma\sigma} a_{\sigma\sigma}) = (\text{sgn } \sigma)(\text{sgn } \sigma') \Omega_{n,a_0}^{\text{(off-diag)}}(t; k'_{n,a_n}, k_{n,a_n})
\]

\[
[\sigma, \sigma' \in \text{Sym}(n), \sigma'_n = n]. \quad (4.73)
\]

It follows that it must be possible to write \( \Omega_{n,a_0}^{\text{(off-diag)}} \) as an antisymmetrization of a “reduced” function \( \Omega_{n,a_0}^{\text{(red)}}(t; k'_{n,a_n}, k_{n,a_n}) \), i.e.:

\[
\Omega_{n,a_0}^{\text{(off-diag)}}(t; k'_{n,a_n}; k_{n,a_n}) = \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn } \sigma)(\text{sgn } \sigma') \Omega_{n,a_0}^{\text{(red)}}(t; k'_{\sigma'\sigma}, a'_{\sigma'\sigma}; k_{\sigma\sigma} a_{\sigma\sigma}). \quad (4.74)
\]

(The explicit evaluation in the next section confirms this.) With some relabelling of indices, we obtain:

\[
\sum_{m_1,\ldots,m_n=1}^{N} \Omega_{n,a_0}^{\text{(off-diag)}}(t; k_{m,a_m}; k_{m,a_m}) = \sum_{m_1,\ldots,m_n=1}^{N} (n-1)! \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma)
\]

\[
\times \Omega_{n,a_0}^{\text{(red)}}(t; k_{m,a_m}; k_{m,a_m} a_{m,a_m}). \quad (4.75)
\]

Then, noting that \( \Omega_{n,a_0}^{\text{(off-diag)}}(t; k_{n,a_n}; k_{n,a_n}) = \Omega_{n,a_0}(t; k_{n,a_n}) \), we see that Eq. (4.70) becomes:

\[
I(t) = \frac{1 - \xi}{2} \frac{1}{L} \sum_{m=1}^{N} (-1)^{m-1} - \xi \text{Re} \left[ \sum_{n=1}^{N} \frac{1}{2^n} \frac{1}{L^n} \sum_{m_1,\ldots,m_n=1}^{N} (-1)^{\gamma_{m,n}} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma)
\]

\[
\times \frac{\partial}{\partial t} \Omega_{n,a_0}^{\text{(red)}}(t; k_{m,a_m}; k_{m,a_m} a_{m,a_m}) \right]. \quad (4.76)
\]

The next section calculates \( \Omega_{n,a_0}^{\text{(off-diag)}} \) – from which we can extract a convenient form for \( \Omega_{n,a_0}^{\text{(red)}} \) – while also providing the necessary technology for evaluating other normal ordered overlaps in the even sector of the model. The explicit calculations verify the symmetry properties that we have used, which were shown by general arguments in Sec. 2.3.4.

### 4.2.2 Evaluation of normal ordered overlaps

In this section, we calculate \( \Omega_{n,a_0}^{\text{(off-diag)}} \). This allows to extract a useful form for \( \Omega_{n,a_0}^{\text{(red)}} \), which we can then use to proceed with the evaluation of the current. Along the way, we develop a method for calculating normal ordered overlaps in the even sector. We present this method
first in a diagrammatic form that is useful for efficient calculation, then in a fully symbolic form that provides the formal proof for results we get with the diagrams.

The essential point in the calculation is that normal ordering forces the free operators \([c(t) \text{ and } c(t)]\) to contract only with crossing states and never with each other; hence, since crossing states vanish outside the light cone, we are free to set the wavefunction to zero outside the light cone. (Recall that \(0 < t < L/2\) has been assumed all along.) Our strategy will be to bring both halves of the overlap into a form in which the \(x\) variables are all in a canonical order. Schematically, we want \(|\Psi_{ek_n a_n, a_0}(t)\rangle = \int_0^t dx_n (\ldots) \Theta(x_1 < \cdots < x_n) \psi^\dagger_{eb_n}(x_n) |b_0\rangle\) and \( \langle \Psi_{ek_n a'_n a_0'}(t) | c_{k'_n a'_n} \rangle = \int_0^t dx'_1 \ldots dx'_n (\ldots) \Theta(x'_1 < \cdots < x'_n) |b'_0\rangle \psi_{eb'_n}(x'_n)\), so that the \(\psi\) and \(\psi^\dagger\) operators can only contract in the simplest way [each \(\psi^\dagger_{eb_j}(x_j)\) with \(\psi_{eb'_j}(x'_j)\)] and we obtain an integral of the form \(\int_0^t dx_n (\ldots) \Theta(x_1 < \cdots < x_n)\).

Here, the \((\ldots)\) terms stand for functions of the position variables and spins. The momentum dependence of the overlap will thus appear in the following integral:

\[ Q_n(t; q_n) \equiv \int_0^t dx_n e^{-iq_n(t-x_n)} \Theta(x_n < \cdots < x_1) \equiv \int_0^t dx_1 \ldots dx_n e^{-iq_1(t-x_1)} \ldots e^{-iq_n(t-x_n)} \Theta(x_n < \cdots < x_1), \tag{4.77} \]

which we find convenient to leave unevaluated for now.

We set the magnetic field to zero throughout \((B = 0)\). We frequently use the following simple identity to simplify the spin part of the overlap:

\[ \xi I \otimes \mathcal{M} + \xi \mathcal{M}^* \otimes I + \mathcal{M}^* \otimes \mathcal{M} = S^* \otimes S - I \otimes I, \tag{4.78} \]

which follows from \(S = I + \xi \mathcal{M}\) (and \(\xi^2 = 1\)). The simplifications using this identity are not possible if \(B \neq 0\), although a messier answer can still be obtained.
Diagram approach.

An example term in the $n = 2$ ket wavefunction that appears in the overlap is:

$$
c^\dagger_{ek_{2a_2}}(t)|\chi_{ek_{1a_1},a_0}(t)\rangle = \frac{1}{L} \int_{-L/2}^{L/2} dx_1 dx_2 \ e^{-ik_2(x_2)} \ [1 + (\xi - 1) \ \Theta(0 < x_2 < t)] \ \delta_{a_2}^{b_2} \ \psi^\dagger_{eb_2}(x_2) $$

$$
\times e^{-ik_1(t-x_1)} M_{a_1a_0}^{b_1b_0} \ \Theta(0 < x_1 < t) \psi^\dagger_{eb_1}(x_1)|b_0\rangle. \ \ (4.79)
$$

The $x_2$ variable is associated with the free creation operator and can be anywhere $(-L/2$ to $L/2)$. Since we are interested in normal ordered overlaps, we are free to restrict $x_2$ to be between 0 and $t$; then we can sum over both possible orderings ($x_1 < x_2$ and $x_2 < x_1$) and relabel variables to arrive at the desired canonical form:

$$
c^\dagger_{ek_{2a_2}}(t)|\chi_{ek_{1a_1},a_0}(t)\rangle = \frac{1}{L} \int_0^t dx_1 dx_2 \ e^{-ik_1(t-x_1)} e^{-ik_2(t-x_2)} \xi M_{a_1a_0}^{b_1b_0} \ \delta_{a_2}^{b_2} $$

$$
\times [\Theta(x_2 < x_1) + \Theta(x_1 < x_2)] \ \psi^\dagger_{eb_2}(x_2) \psi^\dagger_{eb_1}(x_1)|b_0\rangle + \ldots $$

$$
= \int_{a_0c_0}^{a_0c_0} 1 \ \int_0^t dx_1 dx_2 \ \left( e^{-ik_1(t-x_1)} e^{-ik_2(t-x_2)} \ M_{a_1c_1}^{b_1c_1} \xi I_{a_2c_2}^{b_2c_2} \\
- e^{-ik_2(t-x_1)} e^{-ik_1(t-x_2)} \xi I_{a_2c_2}^{b_1c_1} \ M_{a_1c_1}^{b_2c_2} \right) \ \Theta(x_2 < x_1) \ \psi^\dagger_{eb_2}(x_2) \psi^\dagger_{eb_1}(x_1)|b_0\rangle + \ldots \ \ (4.80)
$$

where the omitted terms lie outside the light cone.

We write $c^\dagger_{ek_{2a_2}}(t)|\chi_{ek_{1a_1},a_0}(t)\rangle$ as the sum of the two diagrams shown in Fig. 4.1a. The rules for interpreting a diagram are as follows. Suppose the $j$th line (counting from the top) is assigned the quantum numbers ($k_{q_j},a_{q_j}$). If the right endpoint of the line is open, we assign a factor of $\xi I_{a_{q_j}c_{j-1}}^{b_{j-1}c_{j}}$; if instead the line ends with a closed dot, then the factor is $M_{a_{q_j}c_{j-1}}^{b_{j-1}c_{j}}$. The product of these $n$ factors is then multiplied by:

$$
(\text{sgn } \sigma) \int_{a_0c_0}^{a_0c_0} 1 \ \int_0^t dx_1 \ \ e^{-ik_0(x_1)} \ \Theta(0 < x_1 < \ldots < x_1) \ \psi^\dagger_{eb}(x_1)|b_0\rangle, \ \ (4.81)
$$

with all $b$ and $c$ spin indices summed. Had we included a magnetic field on the dot, we would have had to assign $e^{-i(k_{q_j}+(c_{j-1}-c_j)B)(t-x_j)} M_{a_{q_j}c_{j-1}}^{b_{j-1}c_{j}}$ to closed dots and $e^{-ik_0(t-x_j)} I_{a_{q_j}c_{j-1}}^{b_{j-1}c_{j-1}}$ to open dots; we continue to set $B = 0$, however. As another example, the diagram in Fig. 4.1b represents the following term in the $n = 3$ wavefunction:
Figure 4.1: Diagrams for states and overlaps. (a) The first diagram represents the term $\int_{a_0}^{b_0} \frac{1}{T} \sum_{x_1} e^{-ik_1(t-x_1)} e^{-ik_2(t-x_2)} \mathcal{M}_{a_1 c_0}^{b_1 c_1} T_{a_2 c_2}^{b_2 c_2}$, and the second term represents the same with an overall minus sign and $(k_1 \leftrightarrow k_2, a_1 \leftrightarrow a_2)$. (b) One of three diagrams that sum together to produce the ket $| \psi_k a_1 \rangle (t)$ (see main text for more detail). (c) A bra and ket diagram are joined to produce an overlap. Open lines (i.e. neither side ends on a dot) are not allowed in a normal ordered overlap, since the normal ordering means that the time-dependent field operators have to contract with crossing states and not with each other. (d) When we sum over all normal ordered overlap diagrams, we find that any given line in the diagram appears in three possible configurations, since a closed dot (crossing state contribution) must occur on one side or on both sides of the line. It is convenient to sum these terms using the identity (4.78), and represent the result, $S_{a_0}^{b_0} c_j^c_j c_{j-1}^c_j S_{a_0 c_j}^{b_0 c_j} c_{j-1}^c_j a_{j-1}$, by a single thick line.
\[
I_{a_0c_3}^{\text{cob}_0} \frac{1}{L^{3/2}} \int_0^t dx_1 dx_2 dx_3 \ e^{-ik_3(t-x_1)} e^{-ik_1(t-x_2)} e^{-ik_2(t-x_3)} \mathcal{M}^{b_1c_1}_{a_3c_0} \xi^{b_2c_2}_{a_1c_1} \mathcal{M}^{b_3c_3}_{a_2c_2} \\
\times \Theta(x_3 < x_2 < x_1) \psi_{eb_1}^\dagger(x_3) \psi_{eb_2}^\dagger(x_2) \psi_{eb_3}^\dagger(x_1) |b_0\rangle, \quad (4.82)
\]

which is one of three terms\(^2\) contained in \(c_{ek_{\alpha}}^\dagger(t)|\psi_{ek_{a_n}a_0}(t)\rangle\).

The full ket wavefunction \(|\psi_{ek_{a_n}a_0}(t)\rangle\) is the sum of all such diagrams (plus terms that can be dropped when the ket is inside the normal ordering symbol). Before calculating \(\Omega_{n,a_0}^{(\text{red})}\) using these diagrams, let us do a simpler calculation first. We showed earlier by formal arguments \([\text{normal ordered formula 1, (2.75)}]\) that the normal ordered overlap of two time-evolving states is zero unless they are both fixed impurity states; in the one lead Kondo model, this statement translates to:

\[
: \langle \psi_{ek_{a_n}a_0'}(t) | \psi_{ek_{a_n}a_0}(t) \rangle : = 0 \quad (n \geq 1). \quad (4.83)
\]

Let us verify this explicitly. We can use essentially the same diagrams to represent the bra wavefunction \(\langle \psi_{ek_{a_n}a_0'}(t) | \psi_{ek_{a_n}a_0}(t) \rangle\) – we just put the closed dots on the left instead of on the right, to indicate taking the adjoint. The overlap of any two diagrams is represented by joining each line to the one opposite, as in Fig. 4.1c. It makes sense to join each line only with the line opposite, since the \(x\)-variables in each wavefunction are in the canonical order \(x_n < \cdots < x_1\). Integration over \(x\)-variables yields a factor of \(Q_n(t; k_{\alpha n} - k_{\alpha' n})\) \([\text{recall Eq. (4.77)}]\). The impurity spin indices are contracted by inserting a factor of \(\langle b_0' | b_0\rangle = \delta_{b_0' b_0}\); more generally, this contribution is \(\langle b_0' | O_{\text{imp}} | b_0\rangle\) if an impurity operator is inserted between the two states.

The example diagram shown in Fig. 4.1c thus represents the following term:

\[
\frac{1}{L^3} Q_n(t; k_3-k_1', k_1-k_2', k_2-k_3') I_{a_0c_3}^{\text{cob}_0} \delta_{b_0' b_0} \mathcal{I}_{a_0c_3}^{b_0'c_0} \mathcal{M}_{a_3c_0}^{b_1c_1} \mathcal{M}_{a_2c_2}^{b_3c_3} \xi_{a_1c_1}^{b_2c_2} \xi_{a_2c_2}^{b_3c_3} \mathcal{M}_{a_2c_2}^{b_3c_3} \mathcal{M}_{a_2c_2}^{b_3c_3}. \quad (4.84)
\]

\(^2\)The three terms correspond to the three possible orderings \(x_1 < x_3 < x_2, x_3 < x_2 < x_1, \text{ and } x_3 < x_2 < x_1\). The \(x_1\) variable is associated with the \(c_{ek_{\alpha}}^\dagger(t)\) operator (and hence can be anywhere), and the \(x_2, x_3\) variables are in the crossing state (and hence are in the order \(x_2 < x_3\)). The \(x\) variables in all three terms are relabelled so that they all yield the canonical ordering \(x_3 < x_2 < x_1\).
The normal ordered inner product of the two states is the sum of all diagrams in which every line ends on at least one closed dot. A line that is open at both ends corresponds to the contraction of a $c(t)$ operator with a $c^\dagger(t)$ operator, which is forbidden by the normal ordering.

In the normal ordered inner product that we are considering, every line will thus be summed over three possibilities – closed on both sides, or open on either the left or right (but not both). The spin factors in these three possibilities take the form of the left-hand side of the identity (4.78). We therefore introduce a new diagrammatic rule for normal ordered overlaps: a thick line with quantum numbers $(k_{\sigma_j}, a_{\sigma_j})$ on the right and $(k'_{\sigma_j'}, a'_{\sigma_j'})$ on the left is associated with the spin factor $S_{a_{\sigma_j}c_{\sigma_j}; a'_{\sigma_j'}c'_{\sigma_j'}}^b_{b_jc_j} S_{a\sigma_jc_{\sigma_j-1}}^b_{b_jc_j} - I_{a'_{\sigma_j'}c'_{\sigma_j'}j_{\sigma_j-1}}^{b_{\sigma_j}c_{\sigma_j}} I_{a_{\sigma_j}c_{\sigma_j-1}}^{b_{\sigma_j}c_{\sigma_j}}$ (see Fig. 4.1d).

The normal ordered inner product (4.83) is the sum of all diagrams of the form shown in Fig. 4.2a, resulting in:

$$
\langle \Psi_{ek_n a'_n, a'_0} | \Psi_{ek_n a_n, a_0} \rangle = \frac{1}{I^n} \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn } \sigma)(\text{sgn } \sigma') Q_n(t; k_{\sigma n} - k'_{\sigma' n}) \times I_{a'_{\sigma' j_0}c'_{\sigma' j_0}}^{b_{\sigma' j_0}b_{\sigma' j_0}} I_{a_{\sigma}c_{\sigma}}^{b_{\sigma}b_{\sigma}} \prod_{j=1}^{n} \left( S_{a'_{\sigma_j}c'_{\sigma_j}j_{\sigma_j-1}}^{b_{\sigma_j}c_{\sigma_j}} S_{a\sigma_jc_{\sigma_j-1}}^{b_{\sigma_j}c_{\sigma_j}} - I_{a'_{\sigma_j'}c'_{\sigma_j'}j_{\sigma_j-1}}^{b_{\sigma_j}c_{\sigma_j}} I_{a_{\sigma_j}c_{\sigma_j-1}}^{b_{\sigma_j}c_{\sigma_j}} \right). \quad (4.85)
$$
For $n \geq 1$, the identity matrices turn the $j = n$ term of the product into a matrix multiplication that vanishes due to the unitarity of the bare $S$-matrix: $S^{\alpha_{k_n} b_0}_{\alpha_{n-1} a_{n-1}} S^{b_0 a_0}_{\alpha_{n} c_{n-1}} = I^{\alpha_{n} c_{n-1}}_{\alpha_{n-1} a_{n-1}}$. Thus, we have confirmed Eq. (4.83) using the diagram approach.

We proceed to evaluate $\Omega^{(\text{off-diag})}_{n,a_0}$ using diagrams. We have seen above how to represent the wavefunction $\Psi_{e k_n a_n, a_0}(t)$, which is one part of the overlap we need. The trick is to note that the other part, $\langle \Psi_{e k_n a_n, a_0}(t)|c_{k_n'} a_n'(t)\rangle$, has almost exactly the same diagram representation as the full wavefunction $\langle \Psi_{e k_n a_n, a_0}(t)|c_{k_n'} a_n'(t)\rangle$; the only difference is that the line associated with $(k_n', a_n')$ cannot end on a closed dot. For this line only, we cannot do the sum given in Eq. (4.78), and we instead just have a closed dot on the right ($\text{a factor of } M$). An example diagram is shown in Fig. 4.2b.

Summing all such diagrams, the end result is [temporarily writing $(\sigma')^{-1}(n)$ as $r$]:

$$
: \langle \Psi_{e k_n a_n, a_0}(t)|c_{k_n'} a_n'(t)\rangle \Psi_{e k_n a_n, a_0}(t) : = \frac{1}{L^n} \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn } \sigma)(\text{sgn } \sigma') Q_n(t; k_{\sigma \text{on}} - k_{\sigma' \text{on}}) I^{c_{k_n'}}_{a_0 c_n} \delta^{k_0 b_0}_{a_0 c_0} \prod_{j=1}^{n} \left( S^{s_{j} c_{j}}_{a_{j} c_{j}} S^{b_{j} c_{j}}_{a_{j+1} c_{j+1}} - I^{b_{j} c_{j}}_{a_{j} c_{j}} I^{b_{j} c_{j}}_{a_{j+1} c_{j+1}} \right) \xi I^{b_{r} c_{r}}_{a_{r} c_{r}} M^{b_{r} c_{r}}_{a_{r} c_{r}}. \quad (4.86)
$$

If $r \neq n$ (that is, if $\sigma'(n) \neq n$), then we get zero due to the unitarity of the bare $S$-matrix. Thus, we are left with:

$$
: \langle \Psi_{e k_n a_n, a_0}(t)|c_{k_n'} a_n'(t)\rangle \Psi_{e k_n a_n, a_0}(t) : = \frac{1}{L^n} \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn } \sigma)(\text{sgn } \sigma') \prod_{j=1}^{n-1} \left( S^{s_{j} c_{j}}_{a_{j} c_{j}} S^{b_{j} c_{j}}_{a_{j+1} c_{j+1}} - I^{b_{j} c_{j}}_{a_{j} c_{j}} I^{b_{j} c_{j}}_{a_{j+1} c_{j+1}} \right) \xi M^{a_{n} c_{n}}_{a_{n-1} c_{n-1}}. \quad (4.87)
$$

This confirms that $\Omega^{(\text{off-diag})}_{n,a_0}$ has the symmetry properties that allow us to write Eq. (4.74) (which, we recall, was also established by a general argument). We can now read off a formula for $\Omega^{(\text{red})}_{n,a_0}$; but first, we repeat the above calculations in a more formal way.
Formal calculation.

The main tool we need in order to repeat the above calculations is the following:

**Overlap resummation identity.** Given \(1 \leq j \leq n\) and any functions \(X\) and \(Y\), we have:

\[
\sum_{m \in I_j(n)} (\text{sgn } m) \sum_{\sigma \in \text{Sym}(j)} (\text{sgn } \sigma) \int_0^t dx_n X_{\text{Sym}(m)}^b(t, x_m) \Theta(x_{mj} < \cdots < x_{m_1}) \psi_{b_m}^\dagger(x_m)
\]

\[
\times \sum_{w \in \text{Sym}(n-j)} (\text{sgn } w) Y_{\text{Sym}(n/m)\circ w(m/m)\circ w}^b(t, x_{n/m}) \Theta(x_{(n/m)w-j} < \cdots < x_{(n/m)w}) \psi_{b_{n/m}}^\dagger(x_{n/m})
\]

\[
= \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{m \in I_j(n)} \int_0^t dx_n X_{\text{Sym}(m)}^b(t, x_m) Y_{\text{Sym}(n/m)\circ w(m/m)\circ w}^b(t, x_{n/m})
\]

\[
\times \Theta(x_n < \cdots < x_1) \psi_{b_n}^\dagger(x_n), \quad (4.88)
\]

To prove this identity (which is ultimately a trivial piece of bookkeeping), we note that the product of two Heaviside functions can be written as a sum over Heaviside functions, with the summation including all orderings consistent with the two original Heaviside functions. For instance, \(\Theta(x_1 < x_2) \Theta(x_3 < x_4) = \Theta(x_1 < x_2 < x_3 < x_4) + \Theta(x_3 < x_1 < x_4 < x_2) + \) (four more terms) – that is, all the orderings of the four variables such that \(x_1 < x_2\) and \(x_3 < x_4\). As usual, we ignore sets of measure zero, which make no difference in the end; this amounts to assuming that no two of the \(x\) variables are ever equal (so that orderings are always unambiguous). To generalize this example, consider two lists \(m\) and \(\ell\) of equal length chosen from \(n = (1, \ldots, n)\). We declare that the permutation \(\iota[m, \ell] \in \text{Sym}(n)\) puts \(m\) at spots \(\ell\) and leaves \(n/m\) in the original order; that is, we define \(\iota[m, \ell]\) via:

\[
\iota[m, \ell] \circ \text{perm}[m] = \text{perm}[\ell], \quad (4.89)
\]

\[3\] Example: \(n = 5, m = (2, 4), \ell = (1, 5), \iota[m, \ell] = \begin{pmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 3 \\ 4 & 5 \\ 5 & 4 \end{pmatrix}\), \(\text{perm}[m] = \begin{pmatrix} 1 & 1 \\ 2 & 3 \\ 3 & 5 \\ 4 & 2 \\ 5 & 4 \end{pmatrix}\), and \(\text{perm}[\ell] = \begin{pmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \\ 4 & 1 \\ 5 & 5 \end{pmatrix}\).
We can then combine two Heaviside functions as follows:

\[
\Theta(x_{m_j} \cdots < x_{m_1}) \Theta(x_{(n/m)_{n-j}} \cdots < x_{(n/m)_1}) = \sum_{\ell \in I_j(n)} \Theta(x_{[m,\ell](n)} \cdots < x_{[m,\ell](1)}),
\]

(4.90)

Making the change of variables \( x_p \to x_{[m,\ell]^{-1}(p)} \) and \( b_p \to b_{[m,\ell]^{-1}(p)} \), we find that the left-hand side of Eq. (4.88) is equal to:

\[
\sum_{\ell, m \in I_j(n)} (\text{sgn } m) \sum_{\sigma \in \text{Sym}(j), w \in \text{Sym}(n-j)} (\text{sgn } \sigma)(\text{sgn } w) \int_0^t dx_n \ X^{b_{k_{(n/\ell)\circ w}}(t, x_{\ell})} Y^{b_{n/\ell}}_{k_{(n/\ell)\circ w}}(t, x_{n/\ell}) \Theta(x_n \cdots < x_{1})\psi^\dagger_{b_{\ell}}(x_{\ell})\psi^\dagger_{b_{n/\ell}}(x_{n/\ell}).
\]

(4.91)

We rearrange the creation operators \(-\psi^\dagger_{b_{\ell}}(x_{\ell})\psi^\dagger_{b_{n/\ell}}(x_{n/\ell}) = (\text{sgn } \ell) \psi^\dagger_{b_{n}}(x_{n}) - \) and note (recall that \( \text{sgn } m = \text{sgn } \text{perm}[m] \) by definition):

\[
(\text{sgn } m)(\text{sgn } \ell) = \text{sgn } \iota[m, \ell].
\]

(4.92)

To complete the proof, we relabel several of the summations as a single sum over permutations \( \sigma' \):

\[
\sum_{m \in I_j(n)} \sum_{\sigma \in \text{Sym}(j), w \in \text{Sym}(n-j)} (\text{sgn } \iota[m, \ell]) (\text{sgn } \sigma)(\text{sgn } w) \leftrightarrow \sum_{\sigma' \in \text{Sym}(n)} (\text{sgn } \sigma'),
\]

(4.93)

where the permutation \( \sigma' \in \text{Sym}(n) \) is defined via \( \sigma' \circ \ell = m \circ \sigma \) and \( \sigma' \circ (n/\ell) = (n/m) \circ w \).

The right-hand side of (4.88) is then obtained once we relabel \( \sigma' \) as \( \sigma \) and \( \ell \) as \( m \).

Let us use this identity to repeat the calculation of the normal ordered inner product of two states. We write:

\[
|\Psi_{e_{km_{a_0}}, a_0}(t)\rangle = \sum_{j=0}^n \sum_{m \in I_j(n)} (\text{sgn } m) c^\dagger_{e_{km_{a_0}}}(t)|\Phi_{e_{km/m_{a_{n/m_{a_0}}}a_0}}(t)\rangle.
\]

(4.94)

Note that we have changed the labelling so that we are summing over which subsets of the original quantum numbers are put into \( c^\dagger(t) \) operators (rather than crossing states); the point of this is that we want to keep track of the \( c^\dagger(t) \) operators in order to impose the requirement of normal ordering later.
The crossing states have their $x$ variables in order by construction:

$$
| \Phi_{ek_{\mathbf{n}/m}a_{\mathbf{n}/m},a_{0}}(t) \rangle = \sum_{w \in \text{Sym}(n-j)} (\text{sgn } w) | \chi_{k_{\mathbf{n}/m} \circ w, a_{\mathbf{n}/m} \circ w, a_{0}}(t) \rangle \tag{4.95a}
$$

$$
= \frac{1}{L^{(n-j)/2}} \sum_{w \in \text{Sym}(n-j)} (\text{sgn } w) e^{-ik_{\mathbf{n}/m} \circ w(t-x_{\mathbf{n}/m})} M_{b_{\mathbf{n}/m},b_{0}}^{a_{\mathbf{n}/m},a_{0}}
\times \Theta( x_{\mathbf{n}/m}(n-j) < \cdots < x_{\mathbf{n}/m}(1)) \psi_{eb_{\mathbf{n}/m}}^{\dagger}( x_{\mathbf{n}/m}|b_{0}) , \tag{4.95b}
$$

where we have introduced a compact notation for products of $M$ matrices:

$$
M_{a_{n},b_{0}}^{b_{n},b_{0}} = \mathcal{I}_{a_{0}b_{0}}^{c_{0}b_{0}} \prod_{j=1}^{n} M_{a_{j},c_{j}}^{b_{j},c_{j-1}}. \tag{4.96}
$$

With a bit more effort, we can also write the product of $c^{\dagger}(t)$ operators with the $x$ variables in order. We begin with:

$$
c_{ek_{\mathbf{m}a_{\mathbf{m}m}},a_{0}}^{\dagger}(t) = \frac{1}{L^{j/2}} \int_{0}^{t} dx_{\mathbf{m}} \xi_{j} \ e^{-ik_{\mathbf{m}a_{\mathbf{m}m}}(t-x_{\mathbf{m}})} f_{a_{m}}^{b_{m}} \sum_{\sigma \in \text{Sym}(j)} \Theta( x_{m(\sigma_{j})} < \cdots < x_{m(\sigma_{1})})
\times \psi_{eb_{\mathbf{m}}}^{\dagger}( x_{\mathbf{m}}) + \cdots , \tag{4.97}
$$

where the sum over Heaviside functions is just an insertion of 1, and where the omitted terms are outside the light cone and hence can be dropped. Relabeling $x_{m(\sigma_{p})} \rightarrow x_{m_{p}}$ and $b_{m(\sigma_{p})} \rightarrow b_{m_{p}}$ yields:

$$
c_{ek_{\mathbf{m}a_{\mathbf{m}m}},a_{0}}^{\dagger}(t) = \frac{1}{L^{j/2}} \sum_{\sigma \in \text{Sym}(j)} (\text{sgn } \sigma) \int_{0}^{t} dx_{\mathbf{m}} \xi_{j} \ e^{-ik_{\mathbf{m}a_{\mathbf{m}m}}(t-x_{\mathbf{m}})} f_{a_{m_{\sigma_{j}}}^{b_{m_{\sigma_{j}}}}} \Theta( x_{m_{j}} < \cdots < x_{m_{1}})
\times \psi_{eb_{\mathbf{m}}}^{\dagger}( x_{\mathbf{m}}) + \cdots \tag{4.98}
$$

We can now deploy the identity (4.88) to obtain:

$$
| \Psi_{ek_{\mathbf{n}/m}a_{\mathbf{n}/m},a_{0}}(t) \rangle = L^{-n/2} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{j=0}^{n} \sum_{m \in \mathcal{I}_{j}(n)} \int_{0}^{t} dx_{n} \ e^{-ik_{\mathbf{n}a_{\mathbf{n}/m}}(t-x_{n})} \xi_{j} f_{a_{n+1}^{b_{m}}}^{b_{m+1}} \times M_{a_{n}/m}^{b_{n}/m,b_{0}} \Theta( x_{n} < \cdots < x_{1}) \psi_{eb_{\mathbf{n}}}( x_{\mathbf{n}}|b_{0}) + \cdots , \tag{4.99}
$$

where $\mathbf{m}$ are the indices that were assigned to $c^{\dagger}(t)$ operators. All that remains in order to reach the same answer as the diagrams is to relabel some spin indices in convenient way.
Let us consider \( \sigma = \text{identity for the moment}; \) we have:

\[
I_{b_{a_0}b_0}^{b_{n/m}b_{0}} \equiv I_{a_0c_n}^{b_{0}} \left( \prod_{p=1}^{j} I_{b_{m/p}c_{mp}}^{b_{0}} \right) \left( \prod_{p'=1}^{n-j} \mathcal{M}_{i_d^{(n/m)}(p')c^{(n/m)}(p')}^{b_{(n/m)}(p')} \right) \tag{4.100a}
\]

\[
= I_{a_0c_n}^{b_{0}} \prod_{p=1}^{n} [s_p \xi I + (1 - s_p) \mathcal{M}_{i_d^{(n/m)}c_{p-1}}^{b_{p}c_{p}}] \quad (s_p = 1 \text{ if } p \in m, \text{ 0 if } p \in n/m). \tag{4.100b}
\]

The sum \( \sum_{j=0}^{n} \sum_{m \in I_j(n)} \) is equivalent to \( \prod_{p=1}^{n} s_p = 0,1 \). Thus, we have arrived at the symbolic form of the statement that the ket wavefunction is the sum of diagrams:

\[
|\Psi_{e_k a_n a_0}(t)\rangle = L^{-n/2} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn} \sigma) I_{a_0c_n}^{b_{0}} \sum_{s_1, \ldots, s_n = 0,1} \prod_{p=1}^{n} [s_p \xi I + (1 - s_p) \mathcal{M}_{i_d^{(n/m)}c_{p-1}}^{b_{p}c_{p}}] \int_{0}^{t} dx_{n} e^{-ik_{\sigma \alpha n}(t-x_n)} \Theta(x_n < \cdots < x_1) \psi_{e_k a_n}^{\dagger}(x_n)|b_{0}\rangle + \ldots, \tag{4.101}
\]

where each \( s_p = 1 \) corresponds to an open line.

Putting a prime on all variables and taking the adjoint yields the other half of the desired inner product in Eq. (4.83). In the inner product, the Heavside functions force the field operators to contract in the simplest way. We impose normal ordering by eliminating all terms in which there is any \( p \) for which \( s_p = s'_p = 1 \). Thus, we find:

\[
: \langle \Psi_{e_k a'_n a'_0}(t)|\Psi_{e_k a_n a_0}(t)\rangle :=
\]

\[
= \frac{1}{\mathcal{L}} \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn} \sigma)(\text{sgn} \sigma') Q_{n}(t; k_{\sigma \alpha n} - k'_{\sigma' \alpha n}) I_{a_0c_n}^{b_{0}} \delta_{b_{0}b_{0}} I_{a_0c_n}^{b_{0}} \prod_{p=1}^{n} [s_p \xi I + (1 - s_p) \mathcal{M}_{i_d^{(n/m)}c_{p-1}}^{b_{p}c_{p}}] \cdot
\]

\[
\times \sum_{s_1, \ldots, s_n = 0,1} (1 - \delta_{s_p}^{1} \delta_{s_p}'^{1}) \prod_{p=1}^{n} [s_p \xi I + (1 - s_p) \mathcal{M}_{i_d^{(n/m)}c_{p-1}}^{b_{p}c_{p}}] \cdot
\]

\[
(4.102)
\]

The final step is to use the unitarity relation (4.78) to rewrite the spin terms in terms of

---

\(^4\)This identity is nothing more than the generalization of, e.g.,

\[
I_{a_1a_2a_3a_4a_5}^{b_1b_2b_3b_4b_5} = I_{a_1a_2a_3}^{b_1b_2b_3} M_{a_2a_3}^{b_2b_3} + I_{a_1a_2a_3}^{b_1b_2b_3} M_{a_2a_3}^{b_2b_3} + I_{a_1a_2a_3}^{b_1b_2b_3} M_{a_2a_3}^{b_2b_3} + I_{a_1a_2a_3}^{b_1b_2b_3} M_{a_2a_3}^{b_2b_3} + I_{a_1a_2a_3}^{b_1b_2b_3} M_{a_2a_3}^{b_2b_3} \quad (\text{where } n = 5 \text{ and } m = (1,3,5) \text{ in this case}).
\]
the bare $S$-matrix. To do this, we interchange the sums with the product:

$$
\sum_{s_1, \ldots, s_n=0,1} (1 - \delta_{s_p}^1 \delta_{s_p}^1) \prod_{p=1}^n \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right] \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right] =
$$

$$
\prod_{p=1}^n \sum_{s_p=0,1} (1 - \delta_{s_p}^1 \delta_{s_p}^1) \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right] \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right] =
$$

$$
\prod_{p=1}^n \left[ S_{a_{s_p}^{\prime}(p)} c_p^{s_p} - I_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right]. \tag{4.103}
$$

Thus, we have confirmed the result (4.85) that we reached earlier using diagrams.

We proceed to the formal calculation of Eq. (4.87). We start by noting:

$$
e^{-i} \frac{1}{n!} \left( \sum_{j=1}^{n} \sum_{m \in \mathcal{M}_n} \left( \text{sgn} \, m \right) e^{-i m_{\alpha n}^{\dagger}} \right) \Psi_{e_k n / m_{\alpha n}^{\prime}}(t) = \sum_{j=1}^{n} \sum_{m \in \mathcal{M}_n} \left( \text{sgn} \, m \right) e^{-i m_{\alpha n}^{\dagger}} \Psi_{e_k n / m_{\alpha n}^{\prime}}(t). \tag{4.104}
$$

[Note the similarity to the full wavefunction given by Eq. (4.94)]. The same manipulations that we used to arrive at Eq. (4.101) can be repeated with the extra requirement $n \in \mathcal{M}_n$, yielding:

$$
e^{-i} \frac{1}{n!} \left( \sum_{j=1}^{n} \sum_{m \in \mathcal{M}_n} \left( \text{sgn} \, m \right) e^{-i m_{\alpha n}^{\dagger}} \right) \Psi_{e_k n / m_{\alpha n}^{\prime}}(t) = L^{-n/2} \sum_{\sigma \in \text{Sym}(n)} \left( \text{sgn} \, \sigma \right) R_{a_0 c_0} \sum_{s_1, \ldots, s_n=0,1} \delta_{s_p}^{s_p - 1(n)} \prod_{p=1}^n \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right] \int_0^t dx_n \, e^{-i \sigma_{\text{on}}(t-x_n)} \Theta(x_n < \cdots < x_1) \psi_{e_k n}(x_n) |b_0\rangle + \cdots, \tag{4.105}
$$

where, as before, the omitted terms are outside the light cone. Note that the Kronecker delta forces the spin tensor associated with $a_n$ to be $\xi I$ and not $\mathcal{M}$. Taking the adjoint of this state (with a prime over all variables) and forming the normal ordered inner product with (4.101), we find:

$$
\langle \Psi_{e_k n / m_{\alpha n}^{\prime}}(t)| e_{k_0 n_{\prime}}^{\dagger}(t) \Psi_{e_k n / m_{\alpha n}^{\prime}}(t) \rangle = \frac{1}{L_n} \sum_{\sigma, \sigma' \in \text{Sym}(n)} \left( \text{sgn} \, \sigma \right) \left( \text{sgn} \, \sigma' \right) \times Q_n(t; k_{\sigma_{\text{on}} - k_{\sigma'_{\text{on}}}}) \sum_{s_1, \ldots, s_n=0,1} \sum_{s_1', \ldots, s_n'=0,1} \prod_{p=1}^n \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right] \left[ s_p \xi I + (1 - s_p) \mathcal{M}^{-1}_{a_{s_p}^{\prime}(p)} c_p^{s_p} \right]. \tag{4.106}
$$
Temporarily, we write \((\sigma')^{-1}(n)\) as \(r\). For the \(p = r\) term of the product, we obtain \(\xi I^{b_jc_j}_{a_jc_j-1} M^{b_rc_r}_{a_rc_r-1}\), seeing as \(s_r = s'_r = 1\). The product over \(p \neq r\) can be brought outside the sum over the remaining \(s_p\) and \(s'_p\) variables, yielding the same product as in (4.103) with the restriction \(p \neq r\). Thus, we reach the same result (4.86) as we found earlier using diagrams.

**Summary.**

Let us summarize the results of these calculations using a notation that will be very useful hereafter. We define the following tensor:

\[
\Xi_n[a'_n; a_n]^{b'_0c_0}_{a'_0a_0} = I^{b'_0c_0}_{a'_0a_0} \prod_{j=1}^{n} \left( S_{a'_j, c'_j} S_{a_j, c_j} - I_{a'_j, c'_j} I_{a_j, c_j} \right). \tag{4.107}
\]

If \(n = 0\), i.e. \(n\) is the empty list, then \(\Xi_0[a'_0; a'_0]^{b'_0c_0}_{a'_0a_0} = I^{b'_0c_0}_{a'_0a_0}\). Let us note two properties of this tensor for later reference. (1) For \(n \geq 1\), the unitarity of the bare \(S\)-matrix implies that \(\Xi_n\) vanishes if its upper two indices are contracted with each other: \(\Xi_n[a'_n; a_n]^{b'_0b_0}_{a'_0a_0} = 0\). (2) The tensor \(\Xi\) is basis-independent. To see this, note that the \(S\)-matrix only appears in the combination \(S^*S = (\xi S)^* \xi S\), and recall from Eq. (4.43a) and the discussion below that \(\xi S\) is basis-independent.

Using this tensor, we rewrite Eq. (4.85) as:

\[
: \langle \Psi_{ek_n a'_n,a'_0}(t) | \Psi_{ek_n a_n,a_0}(t) \rangle : = \frac{1}{N^n} \sum_{\sigma,\sigma' \in \text{Sym}(n)} (\text{sgn} \sigma)(\text{sgn} \sigma') Q_n(t; k \sigma \sigma \sigma \sigma \sigma - k'_n) \times \Xi_n[a'_n; a_n]^{b'_n b_0}_{a'_n a_0}, \tag{4.108}
\]

which is zero (for \(n \geq 1\)) because the upper two indices of \(\Xi\) are contracted. The index \(b_0\) ultimately comes from the \(|b_0\rangle\) and \langle b_0| on either side of the inner product. As an aside, we note that we can read o the normal ordered expectation value of the impurity spin \(S\) by
replacing the factor of $\langle b'_0|b_0 \rangle = \delta_{b'_0b_0}$ in Eq. (4.85) by $\langle b'_0|S|b_0 \rangle = S_{b'_0b_0}$, yielding:

$$\langle \Psi_{ek'_n a'_n a'_0(t)}|S|\Psi_{ek_n a_n a_0(t)} \rangle = \frac{1}{L^n} \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn } \sigma)(\text{sgn } \sigma') Q_n(t; k_{\sigma\sigma'} - k'_{\sigma'\sigma\sigma'})$$

$$\times \Xi_n[a'_\sigma a_{\sigma\sigma'}b'_0b_0]_{a'_0a_0} S_{b'_0b_0}. \quad (4.109)$$

Our result (4.87) becomes:

$$\langle \Psi_{ek'_n a'_n a'_0(t)}|e_{ek'_n a'_n(t)}|\Psi_{ek_n a_n a_0(t)} \rangle = \frac{1}{L^n} \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn } \sigma)(\text{sgn } \sigma')$$

$$\times Q_n(t; k_{\sigma\sigma'} - k'_{\sigma'\sigma\sigma'}) \Xi_{n-1}[a'_\sigma a_{\sigma\sigma'}(n/n); a'_\sigma a_{\sigma\sigma'}(n/n)]_{a'_0a_0} \xi M_{a'_n b'_0} a_{\sigma a_n b_0}^{a_n b'_0} \quad (4.110)$$

With practice, Eqs. (4.108), (4.109), (4.110), and variations thereof can all be written down essentially by inspection.

From Eq. (4.110), we read off the reduced (or unsymmetrized) form [see (4.74)]:

$$Q^{(\text{red})}_{n,a_0}(t; k'_n a'_n; k_n a_n) = Q_n(t; k_n - k'_n) \Xi_{n-1}[a'_n(n/n); a_n(n/n)]_{a'_0a_0} \xi M_{a_n b_0}^{a_n b'_0} \quad (4.111a)$$

$$= Q_n(t; k_n - k'_n) \Xi_{n-1}[a'_n(n/n); a_n(n/n)]_{a'_0a_0} \left(S_{a_n b_0}^{a_n b'_0} - \delta_{n,1} I_{a_n b_0}^{a_n b'_0} \right), \quad (4.111b)$$

where the second line follows from Eq. (4.43a) and from noting that the identity term can be dropped for $n \geq 1$ (since it contracts the upper two indices of the $\Xi$ tensor, yielding zero). Returning to the expression we derived for $I(t)$ in terms of $Q^{(\text{red})}_{n,a_0}$ [Eq. (4.76)], we obtain:

$$I(t) = \frac{1 - \xi}{2} \frac{1}{L} \sum_{m=1}^{N} (-1)^{\gamma_m-1} - \text{Re} \left[ \sum_{n=1}^{N} \frac{1}{2^n} \frac{1}{L^n} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{\gamma_{m_n}-1} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \right]$$

$$\times \frac{\partial}{\partial t} Q_n(t; k_{m_{\sigma\sigma'}} - k_m) \Xi_{n-1}[a_{m/m_0}; a_{(m/m_0)\sigma}]_{a_0a_0} \left(\xi S_{a_{m_0} b_0}^{a_{m_0} b'_0} - \delta_{n,1} I_{a_{m_0} b_0}^{a_{m_0} b'_0} \right). \quad (4.112)$$

To complete the N-particle calculation, we note that the first term (single sum over $m$) can be combined with the $n = 1$ sum, cancelling off the dependence on the sign factor $\xi$. To see this, note that $\frac{\partial}{\partial t} Q_1(t; 0) = \frac{\partial}{\partial t} I = 1$, and also that (recalling that $a_j$ and $a_0$ indices are fixed and not summed):

$$\Xi_0[; b'_0b_0]_{a_0a_0} \left( -\xi \delta_{1,1} I_{a_{m_1} b_0}^{a_{m_1} b'_0} \right) = -\xi I_{a_0a_0}^{a_{m_1} b'_0} a_{m_1} b'_0 = -\xi. \quad (4.113)$$
Thus, we can combine terms to obtain a manifestly basis-independent answer (recall that $\xi S$ is basis-independent):

$$I(t) = -\text{Re} \left[ \sum_{n=1}^{N} \frac{1}{2^n L^n} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{\gamma m_n} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn} \sigma) \right. $$

$$\times \left. \frac{\partial}{\partial t} Q_n(t; k_m \omega - k_m) \Xi_{n-1} [a_m / m_n; a(m / m_n) \omega] a_0 \left( \xi S a_m n^{b_0} - \delta a_m n^{b_0} \right) \right] .$$

(4.114)

This is the exact answer for the average current in the time-evolving state $|\Psi_{\gamma k_N a_N a_0}(t)\rangle$.

The system size $L$, evolution time $t$, coupling constant $J$, and all initial quantum numbers are arbitrary. The coupling constant appears in $\Xi$ and $\xi S$ [which are explicit sums and products of rational functions of $J$ – see Eqs. (4.43a)-(4.43c) and (4.107)]. The quantity $Q_n$ is defined in Eq. (4.77) as an integral; it can be done in a closed form involving only exponentials and rational functions of the momenta.

Although we have here the exact answer for $N$ electrons, it is not easy find the numerical value of the answer in the physically-interesting case of a large number $N$. The difficulty is that the number of terms in the sum grows very rapidly with $N$. The starting point for this calculation is a linearized Hamiltonian, so the answer we obtain for a small number $N$ of electrons does not have physical meaning.

We therefore adopt the strategy of taking $N \to \infty$ – the thermodynamic limit – term-by-term in the sum over $n$. As we will see, this amounts to doing a series expansion either in powers of $J$ (with small $J$) or in powers of $1/J$ (with large $|J|$). Though this approach does not allow us to access the full parameter space of the model, it has some advantages, including making contact with conventional perturbation theory in $J$ and showing that $I(t)$ reaches a limit as $t \to \infty$ (order-by-order in $J$ or $1/J$, with $t \ll L$ since we take the thermodynamic limit before the steady state limit).
4.3 The current in the thermodynamic limit

4.3.1 Setup and series form for the current

We are interested in the current following a quench performed on an initial density matrix in which the two leads are at temperatures $T_1, T_2$ and chemical potentials $\mu_1, \mu_2$:

$$ I(T_1, \mu_1; T_2, \mu_2; t) = -\frac{d}{dt} \text{Tr} \left( \rho \ e^{iHt} \hat{N}_1 e^{-iHt} \right) / \text{Tr} \rho, $$

where $\rho$ is a Boltzmann distribution in each lead with the modes cutoff by the bandwidth $D$:

$$ \rho = \exp \left[ -\frac{1}{T_1} \sum_{|k|<D} (k - \mu_1) c^\dagger_{1ka} c_{1ka} \right] \otimes \exp \left[ -\frac{1}{T_2} \sum_{|k|<D} (k - \mu_2) c^\dagger_{2ka} c_{2ka} \right] \otimes |a_0\rangle \langle a_0|.$$

We have assumed a given initial impurity spin $a_0$, though later we will average over $a_0$ (the same answer is obtained for either spin). Our approach will be to set up the calculation with $T_1 = T_2 = 0$ – permitting us to use a state rather a density matrix – and then generalize to the case of arbitrary $T_1, T_2$. As discussed in section 2.4, this procedure yields exactly the same answer as would be obtained by starting with a density matrix with arbitrary temperatures.

Thus, we are to consider the zero temperature limit of $\rho$. The corresponding ground state (of the non-interacting Hamiltonian with chemical potentials and cutoff by $D$) is:

$$ |\Psi_{\gamma_NkN\alpha_N,a_0}\rangle \equiv |\Psi\rangle = \left( \prod_{j=1}^{N_1} c^\dagger_{2kj\uparrow} c^\dagger_{2kj\downarrow} \right) \left( \prod_{j=1}^{N_1} c^\dagger_{1kj\uparrow} c^\dagger_{1kj\downarrow} \right) |a_0\rangle,$$

where the quantum numbers $\gamma_Nk_N\alpha_N$ describe two Fermi seas that start from $-D$ and fill up to chemical potentials $\mu_1$ and $\mu_2$. (The other ground state is identical with the impurity spin $a_0$ flipped). At zero temperature, we have:

$$ \rho = |\Psi_{\gamma_NkN\alpha_N,a_0}\rangle \langle \Psi_{\gamma_NkN\alpha_N,a_0}|,$$

$$ I(t) = -\frac{d}{dt} \langle \Psi_{\gamma_NkN\alpha_N,a_0}(t) | \hat{N}_1 | \Psi_{\gamma_NkN\alpha_N,a_0}(t) \rangle. $$
We proceed to specialize the general $N$-particle answer, Eq. (4.114), to the case of two filled Fermi seas. Writing $\mathcal{K}_\gamma$ for the set of allowed momenta in lead $\gamma$ (i.e. filling up from $-D$ to $\mu_\gamma$), we obtain:

\[
I(t) = -\text{Re} \left[ \sum_{n=1}^{N} \frac{1}{2^n} \frac{1}{L^n} \sum_{\gamma_1,\ldots,\gamma_n=1,2} \left( \prod_{j=1}^{n} \sum_{k_j \in \mathcal{K}_{\gamma_j}} \right) \sum_{a_1 \ldots a_n} (-1)^{n-1} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn} \sigma) \right. \\
\times \left. \frac{\partial}{\partial t} Q_n(t; k_{n\sigma} - k_n) \Xi_n - 1[a_{n/n}; a_{\sigma(n/n)}]_{a_0 a_0}^{b'_0 b_0} \left( \xi \xi_{a_0 b_0}^{a'_0 b'_0} - \delta_{n,1} I_{a_0 b_0}^{a'_0 b'_0} \right) \right].
\] (4.119)

To include temperature, we only need to insert Fermi functions [i.e. $\prod_{j=1}^{n} f_{\gamma_j}(k_j)$] and let the momentum sums range over $[-D, D]$ (see Sec. 2.4). It is convenient to collect various factors and summations into a single spin sum term defined as follows:

\[
W_n^{(\sigma)}(J) = -\frac{1}{2^{n+1}} \left( \sum_{a_0, a_1, \ldots, a_n}^{\Xi_n - 1[a_{n/n}; a_{\sigma(n/n)}]_{a_0 a_0}^{b'_0 b_0}} \left( \xi \xi_{a_0 b_0}^{a'_0 b'_0} - \delta_{n,1} I_{a_0 b_0}^{a'_0 b'_0} \right) \right). \] (4.120)

Here, we have written all the spin summations explicitly, and also averaged over the initial impurity spin $a_0$. It is straightforward to verify that both impurity spins lead to the same answer, so this averaging is only for notational convenience.

We carry out the sum over lead indices by interchanging the product and sums, then take the thermodynamic limit (generalizing to include temperature). Schematically, leaving out the function of momenta that is first summed and then integrated, this amounts to:

\[
\sum_{\gamma_1,\ldots,\gamma_n=1,2} \left( \prod_{j=1}^{n} \sum_{k_j \in \mathcal{K}_{\gamma_j}} \right) (-1)^{n-1} = \left( \prod_{j=1}^{n-1} \sum_{\gamma_j=1,2} \sum_{k_j \in \mathcal{K}_{\gamma_j}} \right) \left( \sum_{k_n \in \mathcal{K}_1} - \sum_{k_n \in \mathcal{K}_2} \right)
\] (4.121a)

therm. limit, including temperature
\[
\int_{-D}^{D} \frac{dk_n}{(2\pi)^n} \left[ \prod_{j=1}^{n-1} f_1(k_j) + f_2(k_j) \right] \left[ f_1(k_n) - f_2(k_n) \right],
\] (4.121b)

where $f_\gamma(k) = \left[ e^{(k-\mu_\gamma)/T} + 1 \right]^{-1}$ is the Fermi function for lead $\gamma$. Thus, Eq. (4.119) becomes
the following series in the thermodynamic limit:

\[
I(T_1, \mu_1; T_2, \mu_2; t) = \text{Re} \left\{ \sum_{n=1}^{\infty} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) W_n^{(\sigma)}(J) \times \right. \\
\left. \int_{-D}^{D} \frac{dk_n}{(2\pi)^n} \prod_{j=1}^{n-1} \left( f_1(k_j) + f_2(k_j) \right) \left[ f_1(k_n) - f_2(k_n) \right] \frac{\partial}{\partial t} Q_n(t; k_n - k_{\sigma_0^n}) \right\}. \tag{4.122}
\]

**Discussion of the current series.**

We have arrived at a series expression for the time-evolving current in terms of spin sums \([W_n^{(\sigma)}(J)]\) and integrals [the integration of \(Q_n\), which is itself defined as an integration over position variables in Eq. (4.77)]. This series will be the focus of the remaining calculations in this chapter.

There are several points to make about this series. First, the limit \(t \to 0^+\) does not yield zero. To see this, note that \(\frac{\partial}{\partial t} Q_n|_{t=0} = 0\) for \(n \geq 2\); thus, the entire sum from \(n = 2\) onward vanishes at \(t = 0\), leaving only the single integral term (which, we find, does not vanish). This is surprising, seeing as we would expect the current to start from zero at the time of the quench. We can explain this, at least for weak coupling, by doing a tree level Keldysh calculation with a cutoff \(D_H\) on the modes in the Hamiltonian (in addition to the cutoff \(D\) on the modes in the initial density matrix). At leading order, we find that that the current starts at zero and reaches its steady state value on a timescale of order \(1/D_H\).

Since our calculation has \(D_H = \infty\) from the beginning, this initial transient regime is not seen. Note that there are transients there remain other time scales in the problem (e.g. \(1/V\)) and other transients which are captured in this series answer.

The next point is that we have actually arrived at two different series expressions: one in powers of \(J\) for small \(J\) and one in powers of \(1/J\) for large \(|J|\). We prove this below by studying the spin sums \(W_n^{(\sigma)}(J)\). First, let us see some examples; in Table 4.1, we list all spin sums up to \(n = 4\), leaving out seven of the permutations at \(n = 4\) that start at order \(O(J^6)\) or \(O(1/J^6)\). The product structure of the tensor (4.107) permits fairly quick evaluation of these sums; an ordinary computer can produce Table 4.1 from the definition.
Table 4.1: First several non-vanishing spin sums.

<table>
<thead>
<tr>
<th>$\sigma \equiv (\sigma_1, \ldots, \sigma_n)$</th>
<th>$W_n^{(\sigma)}(J)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>$1 - Z_I - \frac{1}{2} Z_P$</td>
</tr>
<tr>
<td>(2,1)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(3,1,2)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(2,3,1)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(3,2,1)</td>
<td>$-\frac{3}{4}</td>
</tr>
<tr>
<td>(2,3,4,1)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(2,4,1,3) and (3,1,4,2)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(3,4,1,2)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(4,1,2,3)</td>
<td>$\frac{3}{4}</td>
</tr>
<tr>
<td>(4,3,2,1)</td>
<td>$\frac{3}{4}</td>
</tr>
</tbody>
</table>

(4.120) in a matter of seconds.

We prove below that for $n \geq 2$, $W_n^{(\sigma)}(j)$ has at least $n + 1$ powers of $Z_P$ (where $Z_P$ and $Z_P^*$ are treated as equivalent for power counting purposes). From Eq. (4.43c), we can see that $Z_P$ goes as $J$ for small $J$, and that $Z_I$ goes to ±1; hence, we have a series either in $J$ or $1/J$. Before presenting the proof, we give a simple argument based on the fact that we have found the wavefunction in two different bases.

In the $J = 0$ basis, the $J$ series is manifest and the $1/J$ series is a surprise; in the $|J| = \infty$ basis, the situation is reversed. Let us consider the weak coupling basis first. What we are really doing is expanding Eq. (4.114) (the current for a fixed number of electrons) to a fixed order in powers of $J$ and then taking the thermodynamic limit. Taking the expansion order to infinity corresponds to bringing the thermodynamic limit inside the summation sign to yield an infinite, possibly asymptotic, series (see the discussion in Sec. 2.4) in powers of $J$. The existence of such a series is not surprising, seeing as we can equally well expand the wavefunction itself in powers of $J$ before calculating the current. The wavefunction, in this basis, is simple for $J = 0$ and becomes increasingly complicated as we allow higher powers of $J$. Indeed, since $|\Phi_{ek_{a_n,a_0}}(t)| = O(J^n)$, each higher power of $J$ allows more quantum numbers to be put into crossing states. However, the wavefunction in this basis does does have any obvious expansion for large $|J|$; indeed, $|\Phi_{ek_{a_n,a_0}}(t)| = 1 + O(1/J)$, so
all crossing states appear in the limit \(|J| \to \infty\). [There must be cancellations in this limit which produce a simple wavefunction in the end; the point is that this requires more effort than just noting that the nth crossing state has n powers of \(\mathcal{M} = O(J)\)].

If we instead work in the \(|J| = \infty\) basis, the situation is reversed. The wavefunction in this basis is simple for \(|J| ! 1\) and becomes more complicated as we include more powers of \(1/J\) (adding crossings); whereas in the opposite limit, \(J \to 0\), the wavefunction is complicated (or at least, appears to be, since all crossings are there), and we need to do more work to access the regime of small \(J\).

We proceed with the detailed proof. From the definition (4.107), we have the following rule for generating \(\Xi_{n+1}\) from \(\Xi_n\):

\[
\Xi_{n+1}[a'_1, a'_2, \ldots, a'_n, a'_{n+1}; a_n, a_{n+1}]_{a'_{00} a_0}^{c' c} = -|Z_P|^2 \Xi_n[a'_n; a_n]_{a'_{00} a_0}^{c' c} \delta_{a_{n+1}}^{a'_{n+1}} + Z_I Z_P^* \left( \Xi_n[a'_n; a_n]_{a'_{00} a_0}^{a'_{00} c} - \Xi_n[a'_n; a_n]_{a'_{00} a_0}^{c a_{n+1}} \delta_{a_{n+1}}^{c c} \right). \tag{4.123}
\]

The base case, \(n = 1\), can be found by a short calculation:

\[
\Xi_1[a'_1; a_1]_{a'_{00} a_0}^{c' c} = |Z_P|^2 \left( 2I_{a'_{11} c} - I_{a_1 c}^{c'} \right). \tag{4.124}
\]

Consider \(n \geq 2\). From Eq. (4.120), \(S = \xi(Z_I I + Z_P P)\), and the fact that the tensor \(\Xi_n\) vanishes when its upper two indices are contracted, we obtain:

\[
W_n^{(\sigma)}(J) = -\frac{1}{2^{n+1}} (\text{sgn} \sigma) \sum_{a_0, a_1, \ldots, a_n} Z_P \Xi_n[a_{n/n}; a_{(n/n)} c]_{a_0 a_0}^{a_{n/n}}. \tag{4.125}
\]

The base case and the the update rule (4.123) then confirm that \(W_n^{(\sigma)}(J)\) has at least \(n + 1\) powers of \(Z_P\).

**Further simplification of the current series.**

We proceed to bring the current series (4.122) to a form that is more convenient for calculations, and that allows us to show convergence in the steady state limit to all orders (in \(J\) or \(1/J\)), and . We begin by rewriting \(\frac{\partial}{\partial t} \mathcal{Q}_n\) in a form that makes it straightforward to
do the momentum integrals; we then are left with integrations over position that are easier to study than the momentum integrals that would be obtained from first integrating over position. Starting from the definition (4.77) of the function \( Q_n \) and doing some relabeling of integration variables, we obtain:

\[
\frac{\partial}{\partial t} Q_n(t; k_{n\sigma} - k_n) = \frac{\partial}{\partial t} \int_0^t dx_1 \ldots dx_n \left( \prod_{\ell=1}^n e^{i(k_{n\ell} - k_\ell)x_\ell} \right) \Theta(x_n < \cdots < x_1) \tag{4.126a}
\]

\[
= \int_0^t dx_1 \ldots dx_{n-1} \left( \prod_{\ell=1}^n e^{i(k_{n\ell} - k_\ell)x_\ell} \right) \Theta(x_n < \cdots < x_1) \tag{4.126b}
\]

\[
= \int_0^\infty dx_1 \ldots dx_{n-1} \left( \prod_{\ell=1}^n e^{-ik_\ell y_\ell^{(\sigma)}} \right) \Theta(t - x_1 - \cdots - x_{n-1}), \tag{4.126c}
\]

where we have defined certain linear combinations of the \( x \) variables:

\[
y_\ell^{(\sigma)} = \sum_{m=\ell}^{n-1} x_m - \sum_{m=\sigma^{-1}(\ell)}^{n-1} x_m. \tag{4.127}
\]

We can therefore bring the current series (4.122) to the following form:

\[
I(T_1, \mu_1; T_2, \mu_2; t) = \frac{1}{2\pi} \text{Re} \left\{ \sum_{n=1}^{\infty} \frac{1}{(n\pi)^{n-1}} \sum_{\sigma \in \text{Sym}(n)} W_n^{(\sigma)}(J) \varphi_n^{(\sigma)}(T_1, \mu_1; T_2, \mu_2; t) \right\}, \tag{4.128}
\]

where we have defined:

\[
\varphi_n^{(\sigma)}(T_1, \mu_1; T_2, \mu_2; t) = \left( \frac{i}{2} \right)^{n-1} \int dx_{n/\sigma} \Theta(t - x_1 - \cdots - x_{n-1})
\]

\[
\times \int_{-D}^D dk_n \left[ \prod_{j=1}^{n-1} [f_1(k_j) + f_2(k_j)] e^{-i k_\ell y_\ell^{(\sigma)}} \right] [f_1(k_n) - f_2(k_n)] e^{-ik_n y_n^{(\sigma)}}. \tag{4.129}
\]

Thus, we see that doing the momentum integrals first requires us to find the Fourier transform of the Fermi function, with the modes cutoff by the bandwidth \( D \). It is interesting to note here that we can contemplate using a different cutoff scheme (for instance, a smooth decay of the high energy modes rather than a sharp cutoff at \( \pm D \)), with an aim towards having a simple result for the Fourier transform. Here we proceed with the sharp cutoff.

The Fourier transform of the Fermi function \( f(k) \) (with temperature \( T \) and chemical potential \( \mu \)) can be done analytically; for convenience, we use the asymptotic result in the large bandwidth regime:

\[
\int_{-D}^D dk \, f(k) e^{-iky} = \frac{1}{i} \left( \frac{e^{iDy}}{y} - \pi T e^{-iy\mu} \right) + O(e^{-\frac{1}{2}(D-|\mu|)}). \tag{4.130}
\]
Note that despite the $\frac{1}{y}$ term, the right-hand side is perfectly well-behaved at $y = 0$, as can be seen from the expansion of the sinh function. The error term is extremely small, seeing as we are always interested in the universal regime (in which $T, |\mu| \ll D$); thus, it will be dropped. Eq. (4.130) is arrived at from the following exact integral:

$$\int_{-\ln s_1}^{\ln s_2} dv \frac{1}{e^v + 1} e^{-ivu} = e^{-\pi u} \left[ B(-s_2; -iu, 0) - B \left( -\frac{1}{s_1}; -iu, 0 \right) \right], \quad (4.131)$$

where $B$ is the incomplete Beta function, $u$ is real, and $s_1, s_2 \geq 1$. From this we obtain:

$$\int_{-D}^{D} dk \ f(k)e^{-iky} = T e^{-\mu y} e^{-\pi Ty} \left[ B \left( -e^{\frac{1}{2}(D-\mu)}; -iT y, 0 \right) - B \left( -e^{\frac{1}{2}(D+\mu)}; -iT y, 0 \right) \right]. \quad (4.132)$$

Then the stated result (4.130) follows from the following asymptotics:

$$e^{-\pi u} B(-s_2; -iu, 0) = \frac{i\pi}{\sinh(\pi u)} + O \left( \frac{1}{s_2} \right) \quad (u \in \mathbb{R}, s_2 \to \infty), \quad (4.133a)$$

$$e^{-\pi u} B \left( -\frac{1}{s_1}; -iu_1, 0 \right) = i \frac{s_1 u}{u} + O \left( \frac{1}{s_1} \right) \quad (u \in \mathbb{R}, s_1 \to \infty). \quad (4.133b)$$

We insert the asymptotic form (4.130) into Eq. (4.129), then use the identity $\sum_{\ell=1}^{n} \gamma_{\ell}^{(s)} = 0$ (which can be proven by interchanging the order of summations) to multiply both sides by $1 = \exp^\i (\mu_1 + \mu_2)^2 \sum_{\ell=1}^{n} \gamma_{\ell}^{(s)}$. The result is:

$$\varphi_{n}^{(s)}(T_1, \mu_1; T_2, \mu_2; t) = \frac{1}{i} \int dx_1 \ldots dx_{n-1} \Theta(t - x_1 - \cdots - x_{n-1})$$

$$\times \prod_{j=1}^{n-1} \left[ e^{i\tilde{D}y_j^{(s)}} - \frac{\pi T_1 e^{-\frac{1}{2}V y_j^{(s)}}}{2 \sinh(\pi T_1 y_j^{(s)})} - \frac{\pi T_2 e^{i\frac{1}{2}V y_j^{(s)}}}{2 \sinh(\pi T_2 y_j^{(s)})} \right]$$

$$\times \left[ \frac{\pi T_2 e^{i\frac{1}{2}V y_n^{(s)}}}{\sinh(\pi T_2 y_n^{(s)})} - \frac{\pi T_1 e^{-i\frac{1}{2}V y_n^{(s)}}}{\sinh(\pi T_1 y_n^{(s)})} \right], \quad (4.134)$$

where $\tilde{D} \equiv D + (\mu_1 + \mu_2)/2$ and $V \equiv \mu_1 - \mu_2$. The average $(\mu_1 + \mu_2)/2$ of the two Fermi levels represents a choice of the zero of energy, and should not be of any significance as long as we work in the large bandwidth regime. Thus, we expect that we can replace $\tilde{D} \to D$, leaving the current as a function of $D, T_1, T_2, V$, and $t$. We will show this explicitly for the first several terms of the series ($1 \leq n \leq 4$) in the steady state limit.
4.3.2 The steady state limit of the current

For the remainder of the chapter, we focus on the steady state limit \( t \to \infty \) of the current series (4.128). A basic question is, does this limit exist? The calculation we have done does not include any explicit relaxation mechanism (i.e. coupling to an external bath whose degrees of freedom appear in the Hamiltonian); instead, it is expected that sending the system size to infinity provides sufficient relaxation. For further discussion of this point, we refer the reader to Ref. [30].

Existence of the steady state limit.

We show now that each order of the series (4.128), either in powers of \( J \) or \( 1/J \), converges in the limit \( t \to \infty \). More precisely, we prove that it suffices to show that a certain general form of multi-dimensional integral converges in the limit, and argue based on the one-dimensional case that the convergence is intuitively obvious. Detailed evaluation of several of the integrals, in the next section, agrees with these expectations.

The key point is to show that for any permutations \( \sigma \) such that the corresponding spin sum \( W_n^{(\sigma)}(J) \) is non-vanishing, there is a finite limit \( \lim_{t \to \infty} \varphi_n^{(\sigma)}(T_1, \mu_1; T_2, \mu_2; t) \).

The qualification that the spin sum be non-vanishing is an important one, since there are many cases in which the integral \( \varphi_n^{(\sigma)} \) does not converge in time. The simplest example is \( \varphi_2^{(1,2)}(T_1, \mu_1; T_2, \mu_2; t) = e^{DtV} \). This linear divergence is of no consequence for the current because it is multiplied by a vanishing spin sum: \( W_2^{(1,2)}(J) = 0 \).

More generally, divergences for large time are to be expected if one or more of the integration variables \( x_1, \ldots, x_{n-1} \) appears only in the Heaviside function and nowhere else in the integrand. [E.g., for \( \sigma = (1,2) \), we have \( y_1^{(\sigma)} = y_2^{(\sigma)} = 0 \), so \( x_1 \) only appears in the Heaviside function, and \( \varphi_2^{(1,2)} \sim t \).] If instead all \( x_j \) variables appear somewhere in the integrand (aside from in the Heaviside function), then the only possible sources of divergences in time are the oscillating phase terms (since the \( 1/\sinh \) terms are very small at large \( x \)). We expect that there are no divergences in time even from the oscillating
phases, since these are essentially multi-dimensional versions of the one-dimensional integral
\[ \int_1^b du \frac{e^{iu}}{u} \] (which is finite as \( b \to \infty \)).

Our task, then, is to show that for any permutation \( \sigma \in \text{Sym}(n) \) such that one or more of the \( x_j \) variables is absent from \( y_1^{(\sigma)}, \ldots, y_n^{(\sigma)} \), the corresponding spin sum \( W_n^{(\sigma)}(J) \) vanishes. These permutations are exactly the reducible ones – those for which the permutation rearranges the first \( m \) entries independently of the last \( n - m \) (for some \( m < n \)). From Eq. (4.120) and from the product structure (4.107) of the tensor \( \Xi_n \), we see that the spin sums for all reducible permutations vanish provided that the following identity holds:
\[
\sum_{a_0, a_1, \ldots, a_n} \Xi_n[a_n; a_n\sigma_0]_{a_0a_0}^{c,c} = 0 \quad \text{[for any } n \geq 1, \sigma \in \text{Sym}(n)]
\] (4.135)
which we prove in Sec. A.3 in the Appendix. The proof does not rely on the detailed form of the coefficients \( Z_I \) [Eq. (4.43b)] and \( Z_P \) [Eq. (4.43c)], but only on the fact that they lead to a unitary \( S \)-matrix [which amounts to the constraints \( |Z_I|^2 + |Z_P|^2 = 1 \) and \( \text{Re}(Z_I Z_P^*) = 0 \)].

A natural question to ask at this point is, why are we concerned with showing that the time-evolving current converges in the long time limit if we have already shown in Sec. 4.1.4 that the wavefunction reaches a NESS? The steady state current should be the same as the expectation value in the NESS:
\[
\lim_{t \to \infty} I(t) = \langle \Psi_{\text{in}} \mid \hat{I} \mid \Psi_{\text{in}} \rangle.
\] (4.136)
Since we have \( |\Psi_{\text{in}}\rangle \) explicitly, one might think that this proves that the long time limit exists. However, this is not so. Evaluating the right-hand side of Eq. (4.136) with the time-independent version of our formalism, we find that it contains many infrared divergences; introducing an infrared regulator, we find that the problem of showing that these divergences cancel is exactly equivalent to the problem of showing that \( I(t) \) converges for large time, which we have just addressed. Indeed, having a finite \( t \) is itself an example of an infrared regulator. If the limit on the left-hand side of Eq. (4.136) does exist, then our calculations confirm that the equality holds.
Further evaluation of the steady state current.

Having established the existence of the steady state limit, we can write:

\[
I_{\text{steady state}}(T_1, T_2, V) \equiv \lim_{t \to \infty} I(T_1, \mu_1; T_2, \mu_2; t) \bigg|_{\mu_1=0, \mu_2=-V}, \quad (4.137)
\]

where both sides depend implicitly on the cutoff \( \bar{D} \) through \( \bar{D} = D - V/2 \) [see Eq. (4.134) and below]. Setting \( \mu_1 = 0 \) is no real loss of generality, since working with arbitrary \( \mu_1 \) (given fixed voltage difference \( V \)) only means that \( \bar{D} = D + (\mu_1 + \mu_2)/2 \), instead; we will see that this makes no difference in the large bandwidth limit (\( \bar{D} \to D \) either way).

The steady state current, then, depends on the three external parameters \( T_1, T_2, \) and \( V \). Each one has dimensions of energy (in the natural units we have used throughout). It is convenient to work in spherical coordinates with \( V \) as the “Z-axis”:

\[
(T_1/\sqrt{2}, T_2/\sqrt{2}, V) \leftrightarrow (M, \theta, \phi), \quad (4.138)
\]

that is,

\[
V = M \cos \theta; \ T_1 = \sqrt{2}M \sin \theta \cos \phi; \ T_2 = \sqrt{2}M \sin \theta \sin \phi, \quad (4.139a)
\]

\[
M = \sqrt{V^2 + \frac{1}{2}(T_1^2 + T_2^2)}. \quad (4.139b)
\]

The basic integral we need to consider is the steady state limit of (4.134), which is obtained simply by deleting the Heaviside function:

\[
\varphi_n^{(\sigma)}(T_1, T_2, V) \equiv \lim_{t \to \infty} \varphi_n^{(\sigma)}(T_1, \mu_1; T_2, \mu_2; t) \bigg|_{\mu_1=0, \mu_2=-V}, \quad (4.140a)
\]

\[
= \frac{1}{i} \int dx_1 \ldots dx_{n-1} \left[ \prod_{j=1}^{n-1} \left( \frac{e^{iDy_j^{(\sigma)}}}{y_j^{(\sigma)}} - \frac{\pi T_1 e^{-i\frac{1}{2}V y_j^{(\sigma)}}}{2 \sinh(\pi T_1 y_j^{(\sigma)})} - \frac{\pi T_2 e^{i\frac{1}{2}V y_j^{(\sigma)}}}{2 \sinh(\pi T_2 y_j^{(\sigma)})} \right) \right] \times \left[ \frac{\pi T_2 e^{i\frac{1}{2}V y_n^{(\sigma)}}}{\sinh(\pi T_2 y_n^{(\sigma)})} - \frac{\pi T_1 e^{-i\frac{1}{2}V y_n^{(\sigma)}}}{\sinh(\pi T_1 y_n^{(\sigma)})} \right]. \quad (4.140b)
\]

Thus, from Eq. (4.128) we obtain:

\[
I_{\text{steady state}}(T_1, T_2, V) = \frac{1}{2\pi} \operatorname{Re} \left\{ \sum_{n=1}^{\infty} \frac{1}{(i\pi)^{n-1}} \sum_{\sigma \in \text{Sym}(n)} W_n^{(\sigma)}(J) \varphi_n^{(\sigma)}(T_1, \mu_1; T_2, \mu_2) \right\}. \quad (4.141)
\]
We express the integral \( \varphi_n^{(\sigma)} \) in the spherical coordinates, denoting it by the same symbol. Rescaling to dimensionless variables \( u_j \equiv \frac{1}{2} M x_j \) and \( v_j^{(\sigma)} \equiv \frac{1}{2} M y_j^{(\sigma)} \), we obtain:

\[
\varphi_n^{(\sigma)}(M, \theta, \phi) = M \cos \theta \int du_1 \ldots du_{n-1} \left[ \prod_{j=1}^{n-1} \left( e^{i(2D/M - \cos \theta)v_j^{(\sigma)}} - f(\theta, \phi; v_j^{(\sigma)}) \right) / v_j^{(\sigma)} \right] \times h(\theta, \phi; v_n^{(\sigma)}),
\]

where:

\[
f(\theta, \phi; v) = \frac{\sqrt{2} \sin \theta \cos \phi}{\sinh(2\pi \sin \theta \cos \phi)} e^{-i(\cos \theta)v},
\]

\[
h(\theta, \phi; v) = \frac{1}{i} \left( \frac{2 \pi \tan \theta \sin \phi}{\sinh(2\pi \sin \theta \sin \phi)} e^{-i(\cos \theta)v} - \frac{2 \pi \tan \phi}{\sinh(2\pi \cos \theta)} \right).
\]

Note that \( f(\theta, \phi; v = 0) = h(\theta, \phi; v = 0) = 1 \). In writing (4.142), we have assumed \( V > 0 \) (i.e. \( \cos \theta \neq \pi/2 \)), which allowed us to multiply through by \( 1 = \cos \theta \cos \phi \); the case of \( V = 0 \) can be treated separately, leading to different functions \( f \) and \( h \) (with the main difference being that \( h \) vanishes at \( v = 0 \)).

It is convenient to rewrite Eq. (4.142) in a more compact form. We write \( \lambda \equiv 2D/M - \cos \theta \) and suppress the variables \( \theta \) and \( \phi \), as follows:

\[
\varphi_n^{(\sigma)}(M, \theta, \phi) = (M \cos \theta) R^{(\sigma)}(\lambda),
\]

where:

\[
R^{(\sigma)}(\lambda) \equiv \int du_1 \ldots du_{n-1} \left[ \prod_{j=1}^{n-1} \frac{e^{i\lambda v_j^{(\sigma)}} - f(\theta, \phi; v_j^{(\sigma)})}{v_j^{(\sigma)}} \right] h(v_n^{(\sigma)}),
\]

where the \( v_j^{(\sigma)} \) variables are, as defined earlier, the dimensionless versions of the \( y_j^{(\sigma)} \) variables:

\[
v_j^{(\sigma)} = \sum_{m=\ell}^{n-1} u_m - \sum_{m=\sigma^{-1}(\ell)}^{n-1} u_m.
\]

Our task is to determine the asymptotic behavior of \( R^{(\sigma)}(\lambda) \) as \( \lambda \to \infty \). This regime corresponds to the universal or scaling limit, in which the bandwidth is much larger than any other energy scale. We have found this asymptotic expansion for \( 1 \leq n \leq 4 \) for all permutations with non-vanishing spin sums – that, is the permutations in Table 4.1 (see...
Appendix B for details). Since the Kondo model involves the physics of many scales, these asymptotic expansions include powers of \( \ln \lambda \).

While we leave the detailed discussion to the Appendix, we give here a flavor of the evaluation of these integrals. It is helpful to generalize the problem somewhat, using only certain properties of the functions \( f \) and \( h \) – in particular, the location of their poles and their values at zero and infinity – rather than their detailed functional forms. Then the asymptotic expansion is some functional of \( f \) and \( h \). The simplest non-trivial example is \( n = 2 \) with the permutation \( \sigma = (2, 1) \), for which we have \( v_1^{(\sigma)} = -v_2^{(\sigma)} = u_1 \) and the following asymptotic result:

\[
R^{(2, 1)}(\lambda) \equiv \int_0^\infty du_1 \frac{e^{iu_1} - f(u_1)}{u_1} h(-u_1) \xrightarrow{\lambda \to \infty} \frac{-h(0) \ln \lambda - h(0) \left( \gamma - i\frac{\pi}{2} \right) + \int_0^\infty du \ \ln u \ \frac{d}{du} [f(u)h(-u)]}{\lambda},
\]

where \( \gamma \) is the Euler constant [not to be confused with the anomalous dimension \( \gamma(g) \) that we discuss later]. In the steady state current in the regime of small \( J \), the \( \ln \lambda \) divergence here will be appear multiplied by \( J^3 \) – indeed, it is the equivalent of the one loop divergence that appears in a Keldysh calculation (as we verify in more detail, below).

Notice that the constant (\( \lambda \)-independent) term in (4.146) is a more complicated functional of \( f \) and \( h \) than the log term. This is the beginning of a pattern that persists to higher orders. For example, in the case of \( n = 3 \) and \( \sigma = (2, 3, 1) \) that is explicitly written in Appendix B, there is a \( \ln^2 \lambda \) term that depends only on \( h(0) \), a \( \ln \lambda \) term involving both \( h(0) \) and the same single variable integral over \( f \) and \( h \) that appears in (4.146), and then a \( \lambda \)-independent constant that depends on the same quantities already encountered in \( \ln^2 \lambda \) and \( \ln \lambda \) and also on a double integral involving \( f \) and \( h \). These terms then appear in the small \( J \) current multiplied by \( J^4 \) (two loops). This pattern of asymptotic expansion is important in getting the Callan-Symanzik equation that we discuss later.

Using the spins sum in Table 4.1 and the integral asymptotics in Appendix B, we evaluate the steady steady state current series (4.141) up to several orders in \( J \) and in \( 1/J \). For easier
comparison with the literature, we use a rescaled Kondo coupling $g \equiv \rho_{\text{per length}} J = \frac{1}{\pi} J$ from now on, where $\rho_{\text{per length}}$ is the density of states per length and per spin; this $g$ coincides with the dimensionless coupling $\rho J$ in the more typical convention (which relates to ours via $J = J/L$ and $\rho/L = \rho_{\text{per length}}$). We write $I_{\text{steady state}} \equiv I$ and $\frac{\partial I}{\partial V} \equiv G$.

### 4.3.3 Weak coupling regime

We evaluate our current series in the regime of $|g| \ll 1$, with $g$ of either sign. We first review what scaling properties are expected on general grounds (focusing on the interesting case of antiferromagnetic coupling, $g > 0$), then present the results of our calculations.

It is expected that, when all other scales in the problem are much smaller than the bandwidth, the current becomes a universal function $f_{\text{universal}}(T_1/T_K, T_2/T_K, V/T_K)$, where the Kondo temperature $T_K = De^{-\frac{1}{2g} + \frac{1}{4} \ln g}$ is a dynamically generated scale. The “scaling limit” consists of taking $D \to \infty$ and $g \to 0^+$ with $T_K$ fixed; the resulting $f_{\text{universal}}$ is then the same as that which would be obtained from taking the low energy limit of a calculation done with a more realistic Hamiltonian, e.g. with a more complicated band structure than the wide-band limit we have considered.

Universal scaling should manifest itself in a pattern of logarithmic divergences as $D/M$ is sent to infinity. In the regime of small $|g|$ and large $D/M$, the perturbative renormalizability of the Kondo model constrains the steady state current to the form $I(T_1, T_2, V) \to V \sum_{n=2, m<n} a_{nm} g^n \ln^m \frac{2D}{M}$, where the coefficients $a_{nm}$ depend only on the ratios $T_1/V$ and $T_2/V$. This is shown in a very general setting by Delamotte in [5]. Our choice of $V$ for the dimensionful prefactor and $2/M$ for the argument of the log is one of convenience. We have assumed that the current starts at order $g^2$, as is confirmed by calculation.

The current (assuming large bandwidth from now on) should satisfy the Callan-Symanzik equation $\left[ \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g} + \gamma(g) \right] I(T_1, T_2, V) = 0$, which is a differential form of the statement that all UV divergences can be absorbed by using a running coupling constant and rescaling the current operator. The solution to the Callan-Symanzik equation takes the
form $I(T_1, T_2, V) = f_{\text{universal}}(T_1/T_K, T_2/T_K, V/T_K)e^{-\int_0^g dg' \gamma(g')},$ and the anomalous dimension $\gamma(g)$ should start at the same order or higher in $g$ as $\beta(g)$ so that the $g$-dependent scale factor goes to unity in the scaling limit. (Such a scale factor has been seen before in the Kondo problem; see Ref. [59].)

We will write the series in a triangular structure \cite{5} in which the $n$th column contains the $g^{n+1}$ terms, while the $n$th row contains terms of the form $g^{n+j} \ln^{j-1} \frac{2M}{D}$ ($j \geq 1$). The entries in the first row are called the “leading logarithms,” the second row the “sub-leading logarithms,” and so on. For large bandwidth, we find:

$$I(T_1, T_2, V) = \frac{3\pi}{4} V \left\{ g^2 + 4g^3 \ln \frac{2D}{M} + 12g^4 \ln^2 \frac{2D}{M} + 32g^5 \ln^3 \frac{2D}{M} + C_1(\theta, \phi) g^3 + 6C_1(\theta, \phi) g^4 \ln \frac{2D}{M} + [24C_1(\theta, \phi) - 32] g^5 \ln^2 \frac{2D}{M} + C_2(\theta, \phi) g^4 - \left( 16C_1(\theta, \phi) - 8C_2(\theta, \phi) \right) g^5 \ln \frac{2D}{M} + C_3(\theta, \phi) g^5 + O(g^6) \right\}. \quad (4.147)$$

where $C_1$ and $C_2$ are given by:

$$C_1(\theta, \phi) = 4 \text{Re} \left\{ \gamma - \int_0^\infty du \ln u \frac{\partial}{\partial u} \left[ f(\theta, \phi; u) h(\theta, \phi; -u) \right] \right\} \quad (4.148a)$$

$$C_2(\theta, \phi) = \text{Re} \left\{ 6\gamma C_1(\theta, \phi) - 12\gamma^2 + \frac{7}{12} \pi^2 - 4 \int_0^\infty du \ln^2 u \frac{\partial}{\partial u} \left[ f(\theta, \phi; u) h(\theta, \phi; -u) \right] + 8 \int_0^\infty du_1 du_2 \ln u_1 \ln u_2 \frac{\partial}{\partial u_1} \frac{\partial}{\partial u_2} \left[ f(\theta, \phi; u_1) f(\theta, \phi; u_2) h(\theta, \phi; -u_1 - u_2) \right] + 8 \int_0^\infty du_1 du_2 \frac{1}{u_2} \ln \frac{u_1 + u_2}{u_1} \frac{\partial}{\partial u_1} \left[ f(\theta, \phi; u_1 + u_2) f(\theta, \phi; -u_1) h(\theta, \phi; -u_2) \right] \right\}. \quad (4.148b)$$

We omit a very lengthy explicit form of $C_3$ (a sum of integrals over $f$ and $h$, including triple integrals).

As discussed in more detail by Delamotte \cite{5}, this triangular structure makes clear the operation of perturbative renormalizability. [Delamotte does not consider anomalous scaling $\gamma(g)$, but this is a simple modification.] One can see that the leading logs are built from
pure numbers, the sub-leading logs include pure numbers and the constant $C_1$, and so on.

We emphasize that we do not require the answer to take this form; we find it as the result of a detailed calculation.

Eq. (4.147) satisfies the Callan-Symanzik equation:

$$\left(D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g} + \gamma(g)\right) I(T_1, T_2, V) = 0,$$

(4.149a)

with: $\beta(g) = -2g^2 + \beta_3 g^3 + \beta_4 g^4 + O(g^5) \quad (\beta_3 = 16),

\gamma(g) = \gamma_2 g^2 + (64 + 3\pi^2 - 2\beta_4)g^3 + O(g^4) \quad (\gamma_2 = -32),

(4.149b)

(4.149c)

where the constant $\beta_4$ would be determined by the next order of the current ($g^6$, or the equivalent of four loops). As expected on general grounds, $\beta(g)$ and $\gamma(g)$ are found to depend only on the coupling constant $g$; the terms $C_1$ and $C_2$ (which contain all dependence on the angles $\theta$ and $\phi$) drop out of the scaling equation entirely. The third order contribution to the beta function disagrees with the standard result $\beta_3 = 2$; this is probably an artifact of the unconventional cutoff scheme we have used, as we discuss in more detail in Sec. A.5 in the Appendix. In the following calculations, we leave $\beta_3$ unspecified in order to see what effect it has on the final answers.

The calculation that follows uses some standard steps (see Sec. A.4 in the Appendix), and we omit many details. We write the current in a universal form in the scaling limit ($g \to 0^+$ with $T_K$ fixed). The Kondo temperature $T_K$ is determined by $[D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g}] T_K = 0$, and is given by:

$$T_K = \alpha^{-1} D \exp\left[-\frac{1}{2g} + \frac{\beta_3}{4} \ln |g| + O(g)\right],$$

(4.150)

where $\alpha > 0$ is an arbitrary normalization constant. The running coupling at scale $M$, denoted $g_M$, is such that $(D, g)$ and $(M, g_M)$ correspond to the same $T_K$. In the high energy regime ($M \gg T_K$) it is given by:

$$g_M = \frac{1}{2 \ln \frac{M}{T_K}} \left[ 1 + \frac{\beta_3}{4} \ln \ln \frac{M}{T_K} + \left( \frac{\beta_3}{4} \ln 2 + \ln \alpha \right) \frac{1}{\ln \frac{M}{T_K}} + \frac{\beta_2}{16} \frac{\ln^2 \ln \frac{M}{T_K}}{\ln^2 \frac{M}{T_K}} 

+ \frac{\beta_3}{2} \left( \frac{\beta_3}{4} \ln 2 + \ln \alpha - \frac{\beta_3}{8} \right) \frac{\ln \ln \frac{M}{T_K}}{\ln^2 \frac{M}{T_K}} \right] + O \left( \frac{1}{\ln^3 \frac{M}{T_K}} \right).$$

(4.151)
We set the normalization constant $\alpha = 1$ for now. Solving the Callan-Symanzik equation and taking the scaling limit yields:

$$I(T_1, T_2, V) = \frac{3\pi}{4} V g_M^2 \left[ 1 + \left( C_1(\theta, \phi) + 4 \ln 2 - \frac{1}{2} \gamma_2 \right) g_M \right] + O(g_M^3). \quad (4.152)$$

The leading term, which is the sum of the leading log terms of the series, yields:

$$I(T_1, T_2, V) = \frac{3\pi}{16 \ln^2 \frac{M}{T_K}} V + \ldots \quad (M \gg T_K), \quad (4.153a)$$

$$\text{hence: } G(T_1, T_2, V) = \frac{3\pi^2 G_0}{16 \ln^2 \frac{M}{T_K}} + \ldots \quad (M \gg T_K), \quad (4.153b)$$

where we have restored physical dimensions in the differential conductance $G \equiv \partial I/\partial V$ ($G_0 = 2e^2/h = 1/\pi$ is the unitarity limit of conductance). This is a slight generalization of a well-known result, first found in Ref. [28] (in the case of $T_1 = T_2 = 0$ with $V$ as the variable, or $V = 0$ with $T_1 = T_2 \equiv T$ as the variable); see also Ref. [30] for the case of equal temperatures and arbitrary voltage.

At the next approximation beyond leading log, the coefficient $\beta_3$ enters into the current as a term of the form $\beta_3 \ln \ln \frac{M}{T_K}$, and so our result cannot be fully correct.\(^5\) It seems probable, based on a toy calculation (Sec. A.5), that our unusual cutoff scheme has led to some extra “cutoff artifact” terms in the current that changes the coefficient $\beta_3$. For the moment, we can say that since the leading logs are correct in the small $g$ case, the leading logs of the large $|g|$ regime (i.e. the new results presented in next section) should also be correct.

A calculation we can do reliably, at the next order beyond, is the effect of temperature on the current; in particular, the following quantity in the regime $V \gg T_K$:

$$\Delta I(T_1, T_2, V) \equiv I(T_1, T_2, V) - I(T_1 = 0, T_2 = 0, V). \quad (4.154)$$

\(^5\)There is no other term than generates the double logarithm over log cubed, and $\beta_3 = 2$ is very well-established. The fact that $\beta_3$ enters the physical answer is a manifestation of the well-known fact that $\beta_2$ and $\beta_3$ are universal among cutoff schemes in which the coupling constants are analytically related (i.e. the coupling constant in one scheme is a power series in the coupling constant in the other scheme). An exception occurs in the Bethe Ansatz solution of the equilibrium problem, where it appears to be the case that the coupling constant is related non-analytically to the coupling constant of the conventional scheme, and one finds $\beta_3 = 0$ but the universal final answers are still correct [40]; however, there is no sign of non-analytic dependence on $g$ in our calculation, so we do not believe this is the explanation for our unconventional value of $\beta_3$.\)
The idea is that this subtraction eliminates the leading order effect of $\beta_3$. We note the following:

$$g_M = g_V + \frac{1}{2} \ln \frac{V}{T_K} \left[ \frac{\ln(\cos \theta)}{\ln \frac{V}{T_K}} + \frac{\beta_3}{2} \ln(\cos \theta) \ln \frac{V}{T_K} \right] + O \left( \frac{1}{\ln^3 \frac{V}{T_K}} \right), \quad (4.155a)$$

hence:

$$g_M^2 - g_V^2 = \ln(\cos \theta) \frac{1}{2 \ln^3 \frac{V}{T_K}} + O \left( \frac{\ln \ln \frac{V}{T_K}}{\ln^4 \frac{V}{T_K}} \right), \quad (4.155b)$$

and so:

$$\Delta I(T_1, T_2, V) = \frac{3\pi}{32} \ln^3 \frac{V}{T_K} \left[ C_1(\theta, \phi) - C_1(\theta = 0, \phi) + 4 \ln(\cos \theta) \right]$$

$$+ O \left( \frac{\ln \ln \frac{V}{T_K}}{\ln^4 \frac{V}{T_K}} \right), \quad (4.156)$$

where the $\phi$ coordinate in $C_1$ does not matter when $\theta = 0$. What we have calculated corresponds to the leading temperature-dependent term in the summation of the sub-leading logarithms [the second row of (4.147)]; the first contribution is temperature-independent and has been cancelled, and higher contributions again are affected by the coefficient $\beta_3$.

Eq. (4.156) is essentially a one loop result. It agrees with the calculations of Doyon and Andrei in Ref. [30] (hereafter “DA”). Translating their calculation of the current into our notation and calculating the difference $\Delta I$, we find:

$$\Delta I_{\text{DA}}(T, V) = \frac{3\pi}{32} \ln^3 \frac{V}{T_K} \left[ 4(\cot \theta - P(\infty)) + 4 \ln(\cos \theta) \right] + O \left( \frac{\ln \ln \frac{V}{T_K}}{\ln^4 \frac{V}{T_K}} \right), \quad (4.157)$$

where the function $P$ is given in an integral form in DA. Specializing our result (4.156) to equal temperatures sets $\phi = \pi/4$, and we find numerically that our function $C_1(\theta, \phi = \pi/4) = 4P(\cot \theta) + \text{constant}$; thus, $C_1(\theta, \phi = \pi/4) - C_1(\theta = 0, \phi = \pi/4) = 4[P(\cot \theta) - P(\infty)]$, so our result agrees with that of DA.

We can specialize the above calculation to two commonly-considered quantities: the conductance $G$ as a function either of voltage at zero temperature [$G(V)$] or of temperature
at zero voltage \([G(T)]\). Restoring the dimensionful factor \(G_0 = 2e^2/h = 1/\pi\), we find:

\[
G(T) = \frac{3\pi^2 G_0}{4} \left( g^2 + 4g^3 \ln \frac{D}{T} + 12g^4 \ln^2 \frac{D}{T} + 32g^5 \ln^3 \frac{D}{T} \\
- 4\ln \frac{2\pi}{e^{1+\gamma}} g^3 - 24 \ln \frac{2\pi}{e^{1+\gamma}} g^4 \ln \frac{D}{T} - 32 \left( \ln \frac{2\pi}{e^{1+\gamma}} + 1 \right) g^4 \ln^2 \frac{D}{T} \\
- 7.75g^5 - 138.90g^5 \ln \frac{D}{T} \\
+ 9.01g^5 + O(g^6) \right). \tag{4.158a}
\]

\[
G(V) = \frac{3\pi^2 G_0}{4} \left( g^2 + 4g^3 \ln \frac{D}{V} + 12g^4 \ln^2 \frac{D}{V} + 32g^5 \ln^3 \frac{D}{V} \\
- 32g^5 \ln^2 \frac{D}{V} \\
- \frac{7}{4} \pi^2 g^4 - (64 + 17\pi^2) g^5 \ln \frac{D}{V} \\
+ 2 \left( \pi^2 - 32 + 48 \ln 2 - 24\zeta(3) \right) g^5 + O(g^6) \right), \tag{4.158b}
\]

where \(\zeta\) is the Riemann zeta function. Using the Callan-Symazik equation to take the scaling limit, we find the following results in the high energy regime \((T \gg T_K\) or \(V \gg T_K\)):

\[
G(T) = \frac{3\pi^2 G_0}{16 \ln^2 \frac{T}{T_K}} \left[ 1 + 8 \ln \frac{T}{T_K} + \frac{\alpha_1^{(T)}}{\ln \frac{T}{T_K}} + \frac{48 \ln^2 \ln \frac{T}{T_K}}{\ln^2 \frac{T}{T_K}} + \frac{\alpha_2^{(T)} \ln \ln \frac{T}{T_K}}{\ln^2 \frac{T}{T_K}} + O \left( \frac{1}{\ln^2 \frac{T}{T_K}} \right) \right], \tag{4.159a}
\]

\[
G(V) = \frac{3\pi^2 G_0}{16 \ln^2 \frac{V}{T_K}} \left[ 1 + 8 \ln \frac{V}{T_K} + \frac{\alpha_1^{(V)}}{\ln \frac{V}{T_K}} + \frac{48 \ln^2 \ln \frac{V}{T_K}}{\ln^2 \frac{V}{T_K}} + \frac{\alpha_2^{(V)} \ln \ln \frac{V}{T_K}}{\ln^2 \frac{V}{T_K}} + O \left( \frac{1}{\ln^2 \frac{V}{T_K}} \right) \right], \tag{4.159b}
\]

where the \(\alpha_j^{(T)}, \alpha_j^{(V)}\) constants are:

\[
\alpha_1^{(T)} = 8 \left( 1 + \ln 2 \right) - 2 \ln \frac{2\pi}{e^{1+\gamma}}, \tag{4.160a}
\]

\[
\alpha_1^{(V)} = 8 \left( 1 + \ln 2 \right), \tag{4.160b}
\]

\[
\alpha_2^{(T)} = 4 \left( 2 + 3 \ln 2 \right) + 3 \ln \frac{2\pi}{e^{1+\gamma}}, \tag{4.160c}
\]

\[
\alpha_2^{(V)} = 4 \left( 2 + 3 \ln 2 \right). \tag{4.160d}
\]
The individual values of $\alpha_1^{(T)}$ and $\alpha_1^{(V)}$ can be changed by rescaling $T_K$ by an overall constant prefactor, but not their difference. Indeed, one can define $T_K^{(T)}$ as the rescaling that sets $\alpha_1^{(T)}$ to zero, with a similar definition for $T_K^{(V)}$; then the ratio $T_K^{(T)}/T_K^{(V)} = \exp \left[ \frac{\left( \alpha_1^{(T)} - \alpha_1^{(V)} \right)}{2} \right] = \frac{e^{1+i\pi}}{2\pi}$ is independent of rescaling. This ratio agrees with the real-time renormalization group calculation of Pletyukhov and Schoeller [32], and also with the calculation of DA once a minor error there is corrected.\footnote{The function $P(w)$ defined in DA has the small $w$ asymptotic form $P(w) \rightarrow \ln w - \frac{2\pi}{\ln w}$, contrary to Eq. (76) of DA. This can be traced to line (4) of Appendix E in DA, in which the terms $\int_0^1 dp \frac{e^{-\frac{k^2}{T}}}{p} + \int_1^\infty dp \frac{e^{-\frac{k^2}{T}}}{p}$ should instead be $\int_0^1 dp \frac{e^{-\frac{k^2}{T}}}{p} + \int_1^\infty dp \frac{e^{-\frac{k^2}{T}}}{p}$.}

The first terms in Eq. (4.159a) and Eq. (4.159b) that are affected by our unconventional coefficient $\beta_3$ are the double log terms $\frac{\ln \ln T}{\ln^{3/2} T_K}$ and $\frac{\ln \ln V}{\ln^{3/2} T_K}$; with the expected $\beta_3 = 2$, the coefficient 8 would instead be 1. The coefficients of the leading terms, $1/\ln^2(T/T_K)$ and $1/\ln^2(V/T_K)$, are unaffected.

In sum, our approach yields the correct leading behavior in the high energy regime ($T \gg T_K$ or $V \gg T_K$, or more generally, $M \gg T_K$). The leading correction, however, differs by an overall constant from the conventional cutoff scheme. We have confirmed this surprising result by doing the calculation in several equivalent ways. As discussed above, we can subtract off the zero temperature current to remove the cutoff artifacts at leading order, leaving a result (4.156) that agrees with the literature.

Another way to summarize the checks we have just done is that the top row of (4.147) is correct and the first entry in the second row ($\sim C_1(\theta, \phi) g^3$) is correct; furthermore, the coefficients of $C_1$ in each of the next columns in the second row is also correct [otherwise we would find that $\beta(g)$ or $\gamma(g)$ would depend on the external parameters $\theta$ and $\phi$ instead of just on $g$]. However, there should have been additional terms with constant (pure number) coefficients in the second row beyond the first column (i.e. $g^4 \ln \frac{2D}{M}$, $g^5 \ln \frac{2D}{M}$). Such terms are very similar to the “cutoff artifact” we find in a toy calculation, which we can remove by a projection procedure (see Sec. A.5 for details); we suspect, then, that the same projection procedure would recover the expected $\beta_3 = 2$ in the current.
We also find that the thermoelectric current \( I(T_1, T_2, V = 0) \) vanishes up to and including the third loop order term \((g^5)\). This follows from a detailed cancellation of many terms, and we do not know if there is any non-vanishing contribution from higher orders in \( g \), or if this statement is affected by cutoff artifacts.

### 4.3.4 Strong coupling regime

Our approach reveals a new universal regime of the Kondo model: strong ferromagnetic coupling \((g < 0, |g| \gg 1)\). We note that there are several proposed mesoscopic realizations \([60, 61, 62]\) of the ferromagnetic model with weak coupling; according to the lead author of one of these papers, it may be possible to realize strong coupling with ferromagnetic sign by modifying these proposals to use the charge Kondo effect \([63]\). We find that the strong ferromagnetic model generates a Kondo temperature given at leading order by \( T_K = De^{-\frac{3\pi^2}{8}|g|} \). A very similar discussion applies in this case as in the antiferromagnetic regime. (Indeed, the quantity \(-1/g\), which is small and positive, plays much the same role as a small antiferromagnetic coupling, though the parallel is not exact.) The scaling limit in this regime consists of taking \( D \to \infty \) and \( g \to -\infty \) with \( T_K \) fixed; the resulting universal functions are expected to agree with the low energy results from a more realistic Hamiltonian.

We proceed in much the same way as in the antiferromagnetic case. Taking large bandwidth, we again find a series of logarithmic terms:

\[
I(T_1, T_2, V) = \\
\frac{1}{\pi} V \left\{ 1 - \frac{4}{9\pi^2} \left[ \frac{7}{g^2} - \frac{16}{\pi^2 g^3} \ln \frac{2D}{M} + \frac{64}{\pi^4 g^4} \ln^2 \frac{2D}{M} \right] \\
- C_1 \frac{16}{\pi^2 g^3} + C_1 \frac{128}{\pi^4 g^4} \ln \frac{2D}{M} + (4 - 12C_1) \frac{512}{\pi^6 g^5} \ln^2 \frac{2D}{M} \\
+ \left( 3C_2 + 6\pi \tilde{C}_1 - 22\pi^2 \right) \frac{16}{9\pi^4 g^4} + \left( \frac{32 - 8C_2 + 16C_1}{-12\pi \tilde{C}_1 + 11\pi^2} \right) \frac{64}{9\pi^6 g^5} \ln \frac{2D}{M} \\
+ C_4 \frac{1}{g^5} + O \left( \frac{1}{g^6} \right) \right\}
\]

(4.161a)

where \( C_1, C_2, \tilde{C}_1, \) and \( C_4 \) depend on the ratios \( T_1/V \) and \( T_2/V \); the first two have been
defined already in Eq. (4.148a) and Eq. (4.148b), $\tilde{C}_1$ is the imaginary part of the same quantity that appears in $C_1$:

$$\tilde{C}_1(\theta, \phi) = 4 \text{Im} \left\{ \gamma - \int_0^\infty du \ln u \frac{\partial}{\partial u} \left[ f(\theta, \phi; u) h(\theta, \phi; -u) \right] \right\},$$  \hspace{1cm} (4.162)

and $C_4$ is given by a lengthy sum of integrals over $f$ and $h$, which we omit. This expansion is valid for either sign of $g$, though we focus on the ferromagnetic case $g < 0$ for now.

For $T_1 = T_2$, we find that the Callan-Symanzik equation holds with a non-zero anomalous dimension $\gamma(g)$:

$$\beta(g) = -\frac{8}{3\pi^2} \left[ 1 + \frac{32}{9\pi^2} g + \frac{\tilde{\beta}_2}{\pi^4} g^2 + O \left( \frac{1}{g^3} \right) \right],$$  \hspace{1cm} (4.163a)

$$\gamma(g) = \frac{256}{27\pi^4 g^3} \left\{ 1 + \frac{56}{9\pi^2} g \
+ \frac{1}{\pi^4} \left[ \frac{7}{4} \beta_2 - \frac{115}{9\pi^2} + \frac{64}{3\pi^4} \right] \frac{1}{g^2} + O \left( \frac{1}{g^3} \right) \right\},$$  \hspace{1cm} (4.163b)

where the constant $\tilde{\beta}_2$ would be determined by the next order ($1/g^6$). The scaling invariant is the Kondo temperature for this regime:

$$T_K \equiv D e^{\frac{3\pi^2}{2\pi} g - \frac{1}{4} \ln |g|}.$$  \hspace{1cm} (4.164)

Let us emphasize that the non-zero anomalous dimension $\gamma(g)$ for the current operator is necessary in this case to resum even the *leading* logarithms. Concretely, this means that one would *not* obtain the correct beta function by compensating a change in coupling constant in the $1/g^2$ term by a change of bandwidth in the $(1/g^3) \ln(2D/M)$ term; the resulting beta function would not be consistent with the next term, $(1/g^4) \ln^2(2D/M)$. One is forced rescale the whole observable as well, which is equivalent to introducing $\gamma(g)$.

Curiously, the scaling breaks down if the lead temperatures are different ($T_1 \neq T_2$). This occurs due to terms at a fairly high order ($g^5 \ln(2D/M)$, i.e. a sub-sub-leading log) and may be another cutoff artifact.

\footnote{In the Bethe Ansatz solution of the equilibrium problem – with the regularization scheme and notation used in Ref. [40] – the limits $J \to -\infty$ and $J \to 0^+$ both correspond to $c \to 0^+$. We can thus read off (noting that the conventions are related by $J = 2J_{\text{Bethe Ansatz}}$) the same strong ferromagnetic $T_K$ that appears in Eq. (4.164), aside from the $\ln |g|$ term in the exponent. The absence of such log terms in the Bethe Ansatz is well-known in the antiferromagnetic case, as we mentioned in footnote 5.}
As in the antiferromagnetic case, we use RG improvement to find the universal answer in the high energy regime. We write \( \beta(g) = -\frac{8}{3\pi^2} [1 + \beta_1'/g] \) and \( \gamma(g) = \frac{256}{27\pi^2 g^4} (1 + \gamma_4'1/g) \) to make clear the dependence on the coefficients \( \beta_1' \) and \( \gamma_4' \) (which were calculated above, but which may be affected by the same cutoff artifacts as in the antiferromagnetic case).

The leading-log answer is (see also Fig. 4.3):

\[
I(T, V) = \frac{1}{\pi} V \left( 1 - \frac{3\pi^2}{16\ln^2 \frac{M}{T_K}} + \ldots \right), \tag{4.165a}
\]

hence:

\[
G(T, V) = G_0 \left( 1 - \frac{3\pi^2}{16\ln^2 \frac{M}{T_K}} + \ldots \right). \tag{4.165b}
\]

The conductance thus reaches the unitarity limit asymptotically at high energy. This the main novel prediction of our method so far. It still should be checked that this regime exists in the lattice model. To see this predicted rise towards unitarity experimentally, one would need a hierarchy of scales \( T_K \ll V \ll E_{\text{max}} \) or \( T_K \ll T \ll E_{\text{max}} \), where \( E_{\text{max}} \) is the lowest energy scale at which the Kondo model is no longer an accurate description of the system.

Ultimately, the unitary conductance traces back to the fact that the bare \( S \)-matrix of
the model becomes a single particle phase shift of \(\pi/2\) in the limit \(|J| \to \infty\). See Fig. 3.1 from the potential scattering case.

Further corrections to the leading behavior (4.165b) depend on the coefficients \(\beta'_1\) and \(\gamma'_4\). As in the antiferromagnetic case, we can cancel off the leading dependence on these coefficients by computing the current with the zero temperature value subtracted. The result is:

\[
\Delta I(T, V) \equiv I(T, V) - I(T = 0, V) = - \frac{3\pi V}{8\ln^3 \frac{V}{T_K}} [C_1(\theta, \phi) - C_1(\theta = 0, \phi) + \ln(\cos \theta)] + O\left(\frac{V \ln \ln \frac{V}{T_K}}{\ln^4 \frac{V}{T_K}}\right) \quad (V \gg T_K),
\]

(4.166)

and we plot the corresponding \(\Delta G \equiv \frac{\partial}{\partial \theta} (\Delta I)\) in the inset of Fig. 4.3.

For the special cases \(G(T)\) and \(G(V)\), we obtain:

\[
G(T) = G_0 \left\{ 1 - \frac{4}{9\pi^2} \left[ \frac{7}{g^2} - \frac{16}{\pi^2 g^3} \ln \frac{D}{T} + \frac{64}{\pi^4 g^4} \ln^2 \frac{D}{T} - \frac{2048}{9\pi^6 g^6} \ln^3 \frac{D}{T} + \frac{16}{\pi^2 g^3} \ln \frac{2\pi}{e^{1+\gamma}} - \frac{128}{\pi^4 g^4} \ln \frac{2\pi}{e^{1+\gamma}} \ln \frac{D}{T} + \frac{2048}{9\pi^6 g^6} \left( 3 \ln \frac{2\pi}{e^{1+\gamma}} + 1 \right) \ln^2 \frac{D}{T} - 4.39 \frac{1}{g^4} + 1.61 \frac{1}{g^5} \ln \frac{D}{T} - 0.22 \frac{1}{g^6} \right] + O\left(\frac{1}{g^6}\right) \right\},
\]

(4.167a)

\[
G(V) = G_0 \left\{ 1 - \frac{4}{9\pi^2} \left[ \frac{7}{g^2} - \frac{16}{\pi^2 g^3} \ln \frac{D}{V} + \frac{64}{\pi^4 g^4} \ln^2 \frac{D}{V} - \frac{2048}{9\pi^6 g^6} \ln^3 \frac{D}{V} + \frac{2048}{9\pi^6 g^6} \ln^2 \frac{D}{V} - \frac{436}{9\pi^2 g^5} + \frac{64}{9\pi^2} \left( 64 + 25\pi^2 \right) \frac{1}{g^5} \ln \frac{D}{V} + \frac{16}{27\pi^6 g^6} [192 (4 - 6 \ln 2 + 3\zeta(3)) - 24\pi^2] \right] + O\left(\frac{1}{g^6}\right) \right\},
\]

(4.167b)

In the high energy regime (\(T \gg T_K\) or \(V \gg T_K\)), the running coupling constant is large and negative, and we can use the Callan-Symanzik equation to find the following universal
results:

\[
G(T) = G_0 \left\{ 1 - \frac{3\pi^2}{16 \ln^2 \frac{T}{T_K}} \left[ 1 + \frac{8}{3} \ln \ln \frac{T}{T_K} + \frac{\tilde{\alpha}_1^{(T)}}{\ln \frac{T}{T_K}} + \frac{16}{3} \ln^2 \ln \frac{T}{T_K} + \frac{\tilde{\alpha}_2^{(T)}}{\ln^2 \frac{T}{T_K}} \right] + O \left( \frac{1}{\ln^2 \frac{T}{T_K}} \right) \right\}, \tag{4.168a}
\]

\[
G(V) = G_0 \left\{ 1 - \frac{3\pi^2}{16 \ln^2 \frac{V}{V_K}} \left[ 1 + \frac{8}{3} \ln \ln \frac{V}{V_K} + \frac{\tilde{\alpha}_1^{(V)}}{\ln \frac{V}{V_K}} + \frac{16}{3} \ln^2 \ln \frac{V}{V_K} + \frac{\tilde{\alpha}_2^{(V)}}{\ln^2 \frac{V}{V_K}} \right] + O \left( \frac{1}{\ln^2 \frac{V}{V_K}} \right) \right\}, \tag{4.168b}
\]

where the \( \tilde{\alpha}_j^{(T)}, \tilde{\alpha}_j^{(V)} \) constants are:

\[
\tilde{\alpha}_1^{(T)} = \frac{8}{9} - \frac{8}{3} \ln \frac{3\pi^2}{8} - 2 \ln \frac{2\pi}{e^{1+\gamma}}, \tag{4.169a}
\]

\[
\tilde{\alpha}_1^{(V)} = \frac{8}{9} - \frac{8}{3} \ln \frac{3\pi^2}{8}, \tag{4.169b}
\]

\[
\tilde{\alpha}_2^{(T)} = -8 \left( \frac{4}{9} \ln \frac{27\pi^6}{512} + \ln \frac{2\pi}{e^{1+\gamma}} \right), \tag{4.169c}
\]

\[
\tilde{\alpha}_2^{(V)} = -\frac{32}{9} \ln \frac{27\pi^6}{512}. \tag{4.169d}
\]

Defining \( T_K^{(T)} \) and \( T_K^{(V)} \) in the same way as in the antiferromagnetic case (see (4.159b) and below), we find that the universal ratio is the same in this regime: \( T_K^{(T)}/T_K^{(V)} = \frac{e^{1+\gamma}}{2\pi^2} \).

### 4.3.5 RG discussion

Here, we discuss the RG picture of the model in more detail (Fig. 4.4) and also address the meaning of the remaining two regimes that are accessible to our method, but which we did not emphasize in the previous two sections (namely, weak ferromagnetic coupling and strong antiferromagnetic coupling). The standard Kondo effect refers to the case of bare coupling \( g \) that is weak and antiferromagnetic (0 \( \ll \) g \( \ll \) 1). At high energies, the running coupling \( g_R \) is close to the bare coupling, but as the energy is reduced, the running coupling increases. This regime has been much studied; our calculations reproduce the beginning of this flow by obtaining the standard scaling invariant Kondo temperature \( T_K = De^{-1/(2g)} \).

Our calculations have also found a similar flow in a new universal regime: bare coupling
Figure 4.4: Kondo scaling picture. The two universal regimes are weak antiferromagnetic bare coupling \((0 < g \ll 1, T_K = De^{-1/(2g)})\) and strong ferromagnetic bare coupling \((g < 0, |g| \gg 1, T_K = De^{-3\pi^2/8|g|})\). The former has much studied, and the latter is predicted by our calculations. In either case, the running coupling \(g_R\) is close to the bare coupling if the system is probed at a high energy scale (high relative to \(T_K\) but always small compared to the bandwidth), but moves away from the bare coupling as the energy scale is reduced.

that is strong and ferromagnetic \((g < 0, |g| \gg 1)\), with a Kondo temperature given by \(T_K = De^{-3\pi^2/8|g|}\). For high energies, the running coupling is close to the bare coupling, and we can see the beginning of a flow in which the running coupling gets smaller in magnitude (i.e. farther from its bare value) as the energy is reduced.

Loosely speaking, one says (in the standard antiferromagnetic Kondo) that the coupling constant increases as one reduces the measurement scale, reaching infinity at zero energy. It is tempting to suggest, then, that a calculation using the Kondo Hamiltonian with large \(g\) (expanding in powers of \(1/g\)) would reproduce the low energy regime of the model with small \(g\). However, this is not so. We show this now, both by general arguments and by examining our explicit answers in the large \(g\) regime. At most, our calculations allow us to identify the extreme point, in the sense that we find that the conductance reaches the unitarity limit if we send (bare) \(g \to \infty\), which is the known answer as the zero energy limit of the theory with small antiferromagnetic \(g\). We indicate this by the dotted line in Fig. 4.4, and speculate that a parallel statement may be true in the strong ferromagnetic regime (indicated by another dotted line). In other words, we would expect that the universal strong ferromagnetic conductance is zero at zero energy (since zero conductance is obtained if we set the bare \(g\) to zero), and that the series in small \(g\) would not tell us anything about how the conductance approaches zero.
In short, starting from weak coupling and flowing to strong coupling at low energy is not the same as starting the theory at strong coupling (except perhaps at the extreme point). This statement does not contradict the many successes of the effective field theory approach to the low energy regime (of the model with small g), which refers to the leading irrelevant operators around the strong coupling fixed point. Instead, the conclusion is that the effective field theory approach is more sophisticated than the simple idea of taking g to be large in the original Hamiltonian and expanding in 1/g.

To clarify the point, we set up the field theoretic version of the renormalization group. For definiteness, we consider a dimensionless observable \( O(D, g, T) \) with temperature \( T \) as the only external scale. Our analysis is not confined to equilibrium, though, and \( T \) can be replaced by any single energy scale (such as a bias voltage). Suppose the observable is calculated as a power series in \( g \), with the leading term being \( g^2 \); then a series expansion in \( g \) must take the form:

\[
O(D, g, T) = g^2 + \sum_{n=3}^{\infty} g^n F_n (D/T),
\]

where \( F_n (D/T) \) are some functions. As discussed in [5], these functions are constrained by the perturbative renormalizability of the model to take a logarithmic form in the \( T \ll D \) regime:

\[
F_n (D/T) = \sum_{m=0}^{n-1} a_{nm} \ln^m \frac{D}{T} + \ldots,
\]

where the \( a_{nm} \) coefficients are pure numbers that depend on the observable being evaluated. The logarithmic terms define the “scaling form” part of the observable:

\[
O_{\text{scaling form}} (D, g, T) = g^2 + \sum_{n=3}^{\infty} \sum_{m=0}^{n-1} a_{nm} g^n \ln^m \frac{D}{T}.
\]

The scaling form satisfies the RG scaling (or Callan-Symanzik) equation:

\[
\left[ D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g} + \gamma(g) \right] O_{\text{scaling form}} = 0.
\]

Assuming (as we find for the current) that the leading order of the anomalous dimension term \( \gamma(g) \) starts at the same order or higher than the leading order of the beta function,
the solution of the Callan-Symanzik equation then implies that the scaling form can be written as a function of $T/T_K$ only (where $T_K$ is the scaling invariant defined by $[D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g}]T_K = 0$), up to corrections that vanish as $g \to 0^+$:

$$\mathcal{O}_{\text{scaling form}}(D, g, T) = f_{\text{universal}}(T/T_K) [1 + O(g)] .$$

In the Kondo model, the leading order of the beta function has negative sign. This implies that $T_K$ can be held fixed while taking the limit $D \to \infty$ and $g \to 0^+$, which means that the function $f_{\text{universal}}(T/T_K)$ is a universal result for the observable $\mathcal{O}$. In contrast, the scaling invariant cannot be held fixed in the limit $D \to \infty$ and $g \to 0^-$ (the ferromagnetic case), and so the function $f_{\text{universal}}(T/T_K)$ only represents what would happen if the simplified model itself were realized.

Let us focus on the antiferromagnetic case for now ($g > 0$). The procedure for calculating the asymptotic behavior of $f_{\text{universal}}(T/T_K)$ for $T \gg T_K$ using the first few series coefficients $a_{nm}$ is well-known. One finds that the solution of the Callan-Symanzik equation is characterized by a running coupling $(g_R = \frac{1}{2 \ln T/T_K}$ at the leading approximation) which is found to grow as $T$ is reduced. As $T$ approaches $T_K$ from above, one finds that infinitely many series coefficients are needed; however, non-perturbative techniques confirm that the running coupling keeps growing as $T$ is reduced. If one ignores momentarily the distinction between the running coupling and the bare coupling, one can imagine that a series in $1/g$ would provide information about the low temperature behavior of $f_{\text{universal}}(T/T_K)$, much in the same way that a series in $g$ yields the high temperature behavior.

The basic problem with this approach is that if one repeats the same steps with the $1/g$ series – i.e., expand each order of the series for large bandwidth and declare the logarithmic part to be the “scaling form” – one arrives at a scaling form that may not be the same as the one found from the $g$ series. Since the ultimate goal is to take $g \to 0^+$ with $T_K$ fixed, the scaling form of the $g$ series is the correct one. But the parts of this scaling form that describe the small $T/T_K$ behavior of the function $f_{\text{universal}}(T/T_K)$ may appear to be negligible in the $1/g$ series.
A simple example illustrates the point. It is known that the universal conductance curve $G(T)$ reaches unitarity at $T = 0$ with corrections of the form $T^2/T^2_K$. Thus, the scaling form for the conductance must include a contribution of the form $1/T^2$, seeing as this term becomes $T^2/D^2$ in the $g \rightarrow 0^+$ scaling limit (we assume the conventional expression $T_K = De^{-\frac{1}{2g} + \frac{1}{2} \ln g}$ in this discussion). Since this term vanishes for large bandwidth rather than diverging logarithmically, it is exactly the type of term that is dropped in determining the scaling form of the $1/g$ series. The logarithmically diverging terms, on the other hand, can easily be negligible in the $g \rightarrow 0^+$ scaling limit; consider, e.g., the expansion $\frac{1}{g + \ln D/T} = \frac{1}{g} - \frac{1}{g} \ln \frac{D}{T} + \ldots$ in powers of $1/g$. Thus, no finite number of terms of the $1/g$ series will yield the low temperature behavior, since there is no obvious way to identify which contributions are important in the $g \rightarrow 0^+$ scaling limit.

The scaling form of the $1/g$ series describes a different physical problem: one in which the bare coupling constant is large in magnitude. The sign of the beta function then indicates that the strong ferromagnetic regime is universal and the strong antiferromagnetic regime is non-universal. The quantity $-\frac{1}{g}$ behaves much like $g$ does in the antiferromagnetic case; that is, the $g = -\infty$ point behaves like $g = 0^+$, and $g = 0^-$ behaves like $g = \infty$. Let us state this more definitely. A system with large negative bare coupling $g$ has a running coupling that is also large and negative at high energies; an RG-improved power series in $\frac{1}{g}$ produces accurate results. At low energies, a more powerful technique is needed; neither a series in $\frac{1}{g}$ nor a series in the inverse parameter $g$ gives any information about the low energy behavior (unless one has all terms of the series), because in this case the correct scaling form is the one generated by the $1/g$ series (which can differ from the scaling form generated by the $g$ series).
Chapter 5
Interacting resonant level model

A simple way to add interaction to the resonant level model is to add a Coulomb repulsion term. We consider the multi-lead case:

\[ H = H^{(0)} + U \sum_{\gamma=1}^{N_{\text{leads}}} \psi_\gamma^\dagger(0) \psi_\gamma(0) d^\dagger d, \]  

(5.1)

where \( H^{(0)} \) is the multi-lead RLM given in Eq. (3.75). We present the exact time-evolving wavefunction below. In the multi-lead case, we cannot separate the Hamiltonian into free fields and a single interacting field (as we can in the multi-lead Kondo and Anderson models), due to the form of the interaction term; this shows that our method does not rely on this separation.

When the interaction term \( U \) is present, we must re-consider the meaning of the bare parameter \( \epsilon \) (the energy of the dot). While we do the wavefunction calculation in terms of \( \epsilon \), in the evaluation of an observable we will make the following shift of \( \epsilon \) (to first order in \( U \)):

\[ \epsilon = \epsilon_d - U \sum_{\gamma=1}^{N_{\text{leads}}} \frac{D - \mu_\gamma}{2\pi} + U \Delta/2, \]  

(5.2)

where \( \epsilon_d \), we find, is the physical (or renormalized) value of the dot energy. To explain this shift, we note that the interaction term of the IRL is usually presented as:

\[ H^{(1)}_{\text{conventional}} = U \sum_{\gamma=1}^{N_{\text{leads}}} : \psi_\gamma^\dagger(0) \psi_\gamma(0) : \left( d^\dagger d - \frac{1}{2} \right), \]  

(5.3)

where the normal ordering is relative to the non-interacting ground state (filled Fermi sea). This normal ordering, and the extra factor of \( 1/2 \), are put in to ensure that the resonance is at \( \epsilon_d = 0 \), where \( \epsilon_d \) is the coefficient of \( d^\dagger d \) in the Hamiltonian with \( H^{(1)}_{\text{conventional}} \) as the
interaction term. This corresponds to half-filling in the lattice version of the model. Let us see first the effect of the normal ordering in the one lead model:

$$\psi^\dagger(0)\psi(0) - \psi^\dagger(0)\psi(0) = -\frac{1}{L} \sum_q \sum_{-D < q' < 0} \left( c_q^\dagger c_{q'} - c_{q'} c_q^\dagger \right) = \frac{1}{L} \sum_{-D < q < 0} = \frac{1}{2\pi} D,$$  \hspace{1cm} (5.4)$$

where we have noted that the non-interacting ground state is a Fermi sea filled from $-D$ up to $\mu = 0$.\(^1\) We see here that normal ordering is equivalent to a shift $\epsilon \rightarrow \epsilon - UD/(2\pi)$. In the case of multiple leads, with different chemical potentials, we will do the normal ordering with respect to the non-interacting ground state (i.e. initial state prior to the quench) with the chemical potentials included:

$$\sum_{\gamma=1}^{N_{\text{leads}}} \psi^{\dagger}_\gamma(0)\psi_\gamma(0) - \psi^{\dagger}_\gamma(0)\psi_\gamma(0) = - \sum_{\gamma=1}^{N_{\text{leads}}} \frac{1}{L} \sum_q \sum_{-D < q' < \mu_\gamma} \left( c_q^\dagger c_{q'} - c_{q'} c_q^\dagger \right)$$

$$= \sum_{\gamma=1}^{N_{\text{leads}}} \frac{1}{L} \sum_{-D < q' < \mu_\gamma} = \frac{1}{2\pi} \sum_{\gamma=1}^{N_{\text{leads}}} (D - \mu_\gamma), \hspace{1cm} (5.5)$$

which is equivalent to a shift $\epsilon \rightarrow \epsilon - U \sum_{\gamma=1}^{N_{\text{leads}}} (D - \mu_\gamma)/(2\pi)$.

It remains only to explain the $U \Delta/2$ term in Eq. (5.2); this is more ad-hoc. The $1/2$ in $(d^\dagger d - \frac{1}{2})$ changes the Hamiltonian by $-\frac{1}{2} U \sum_{\gamma=1}^{N_{\text{leads}}} \psi^{\dagger}_\gamma(0)\psi_\gamma(0)$ (a potential scattering term) and by an additive constant that we can ignore. Including this potential scattering term in $H^{(0)}$ makes the RLM solution messier, and we have not pursued the construction of the crossing states. However, we find that we can enforce the condition that $\epsilon_d = 0$ is the resonance (at least at the leading order in $U$) by including the $U \Delta/2$ term in the shift, thus arriving at Eq. (5.2).

Thus, the shift (5.2) corresponds to normal ordering the interaction term relative to the initial state prior to the quench and including an ad-hoc correction to keep the resonance at $\epsilon_d = 0$ (which would presumably would not be necessary had we included the potential scattering term). One could imagine doing the normal ordering relative to the ground state limit, then we would normal order relative to the free “in” state that encodes the quantum numbers of the incoming plane waves in the Lippmann-Schwinger equation.

\(^1\)Really, we are using the ground state of $H_{\text{initial}} = \sum_{|k| < D} k c_k^\dagger c_k$ (or of $H_{\text{initial}} = \sum_{\gamma=1}^{N_{\text{leads}}} \sum_{|k| < D} (k - \mu_\gamma) c_{\gamma,k}^\dagger c_{\gamma,k}$ in the multi-lead case), i.e. the initial state prior to the quench. If we work directly in the steady state limit, then we would normal order relative to the free “in” state that encodes the quantum numbers of the incoming plane waves in the Lippmann-Schwinger equation.
state with no potentials at all [i.e. setting all $\mu_i = 0$ in Eq. (5.2)]; this would result in a shift independent of any external parameters, and would change our final results out of equilibrium (though not the universality that we find in and out of equilibrium).

Let us defer any further discussion of the meaning of the bare parameters until we have an observable calculated, and proceed with the solution for the wavefunction. The only “fixed impurity” state $|\beta\rangle$ is the empty state $|0\rangle$, so we drop the index $\beta$. We present the one lead solution first in some detail. We then present the multi-lead solution, which re-uses some of the same ingredients.

5.1 Wavefunction for one lead model

We find that the model is type B with the following operators:

$$A_k(t) \equiv [H, c_k^\dagger(t)] - i \frac{\partial}{\partial t} c_k^\dagger(t) = \frac{1}{\sqrt{\mathcal{L}}} U d^\dagger \psi(0) \left[ -e^{-ikt} d + F_k(t) \left( \frac{i}{\nu} \psi(0) - \frac{1}{2} d \right) \right],$$  \hspace{1cm} (5.6a)

$$B_{k_1 k_2}(t) \equiv \{ A_{k_2}(t), c_{k_1}^\dagger(t) \} = B_{k_1 k_2}^{(\text{red})}(t) - B_{k_2 k_1}^{(\text{red})}(t),$$  \hspace{1cm} (5.6b)

where:

$$B_{k_1 k_2}^{(\text{red})}(t) = -\frac{1}{\mathcal{L}} \frac{iU}{\nu} F_k(t)e^{-ikt} d^\dagger \psi(0).$$  \hspace{1cm} (5.7)

Obtaining $B_{k_1 k_2}(t)$ is made easier by noting that $\{ \frac{i}{\nu} \psi(0) - \frac{1}{2} d, c_k^\dagger(t) \} = \{ \frac{i}{\nu} \psi(0) - \frac{1}{2} d, e^{-ikt} c_k^\dagger \}$, using the averaging prescription for the delta function (see Sec. 3.4). Let us note that we are focusing on initial states with the dot unoccupied; thus, the remaining $A(t)$ and $B(t)$ operators for the model [involving the $d^\dagger(t)$ operator] do not need to be calculated.

The general formalism for type B models (see Sec. 2.2.2) yields the following for the many body wavefunction:

$$|\Psi_{kN}(t)\rangle = \sum_{n=0}^{N} \sum_{m \in \mathcal{I}_n(N)} \langle \text{sgn } m c_{kN/m}^\dagger(t) | \Phi_{km}(t) \rangle,$$  \hspace{1cm} (5.8)

where the crossing states $|\Phi(t)\rangle$ are given as sums over unsymmetrized crossing states:

$$|\Phi_{km}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} \langle \text{sgn } \sigma \rangle \sum_{\mathcal{P} \in \mathcal{P}(m)} |\chi_{kP\sigma}(t)\rangle,$$  \hspace{1cm} (5.9)
which in turn satisfy (given $\mathcal{P} \in \mathbb{P}_q(n)$):

\[
(H - i \frac{d}{dt}) |\chi_{k_{\mathcal{P}}}(t)\rangle = \begin{cases}
-B_{k_{n-1}k_n}^{(\text{red})}(t) |\chi_{k_{\mathcal{P}/(n,n-1)}}(t)\rangle & q = 2 \\
-A_{k_n}(t) |\chi_{k_{\mathcal{P}/n}}(t)\rangle & 3 \leq q \leq n
\end{cases},
\]

\begin{align*}
|\chi_{k_{\mathcal{P}}}(t = 0)\rangle &= 0, \quad (5.10a) \\
|\chi_{k_{\mathcal{P}}}(t)\rangle &= |0\rangle \quad \text{when $\mathcal{P}$ is the empty list.} \quad (5.10b)
\end{align*}

We provide the solution for $|\chi_{k_{\mathcal{P}}}(t)\rangle$ below in Eqs. (5.31), (5.32), and (5.33a). We warm up to the case of general $n$ by first doing $n = 2, 3,$ and $4$ in some detail.

**Solution for $n = 2$.**

The problem is to find a state $|\chi_{k_1k_2}(t)\rangle$ that vanishes at $t = 0$ and satisfies:

\[
(H - i \frac{d}{dt}) |\chi_{k_1k_2}(t)\rangle = -B_{k_1k_2}^{(\text{red})}(t) |0\rangle = \frac{1}{L} \frac{U}{v} T(k_1)e^{-ik_1t} \left( e^{-ik_2t} - e^{-izt} \right) d^4 \psi^\dagger(0)|0\rangle.
\]

\begin{equation}
(5.11)
\end{equation}

We make the following ansatz:

\[
|\chi_{k_1k_2}(t)\rangle = \frac{1}{L} \int dx_1 dx_2 \ F_{k_1k_2}(t, x_1, x_2) \bigg[ \Theta(0 < x_2 < x_1 < t) \psi^\dagger(x_2) \\
+ \frac{i}{v} \delta(x_2) \Theta(0 < x_1 < t) d^4 \psi^\dagger(x_1)|0\rangle,
\]

\begin{equation}
(5.12)
\end{equation}

with $F_{k_1k_2}$ being a function to be determined below. This ansatz is ultimately justified by being correct; however, we can give some motivation. The state should vanish outside the light cone, since the effect of the quench travels at the Fermi velocity (which we have set to unity); it should only be non-zero to the right of the origin, since the model contains only right movers. The ordering $x_2 < x_1$ is a convenience and no loss of generality, seeing as the product electron creation operators will have the effect of antisymmetrizing the wavefunction. The only part remaining that requires explanation is the impurity-electron $(d^4 \psi^\dagger(x_1))$ part of the wavefunction. This term is chosen so that the acting on it with the tunneling term of $H$ produces an exact cancellation with the action of the kinetic term.
minus $i \frac{d}{dt}$ on the Heaviside function in the electron-electron part. That is, we have:

$$\int dx_1 dx_2 \, F_{k_1 k_2}(t, x_1, x_2) \left[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) \Theta(0 < x_2 < x_1 < t) \right] \psi^\dagger(x_2) \psi^\dagger(x_1) |0\rangle \tag{5.13}$$

$$+ v \psi^\dagger(0) d \int dx_1 dx_2 \, F_{k_1 k_2}(t, x_1, x_2) \frac{i}{v} \delta(x_2) \Theta(0 < x_1 < t) d^4 \psi^\dagger(x_1) |0\rangle = 0. \tag{5.13}$$

This is easy to show if we write $\Theta(0 < x_2 < x_1 < t) = \Theta(x_2) \Theta(x_1 - x_2) \Theta(t - x_1)$ and $\Theta(0 < x_1 < t) = \Theta(x_1) \Theta(t - x_1)$. This cancellation is desirable because we want $(H - i \frac{d}{dt}) |\chi_{k_1 k_2}(t)\rangle$ to be of the form $\psi^\dagger(0) d^4 |0\rangle$. Proceeding, we find:

$$\left( H - i \frac{d}{dt} \right) |\chi_{k_1 k_2}(t)\rangle = \frac{1}{L} \left\{ \int dx_1 dx_2 \left[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) F_{k_1 k_2}(t, x_1, x_2) \right] \Theta(0 < x_2 < x_1 < t) \psi^\dagger(x_2) \psi^\dagger(x_1) \right. \tag{5.14}$$

$$+ \frac{i}{v} \int dx_1 \left[ \left( -i \frac{\partial}{\partial t} - i \frac{\partial}{\partial x_1} + z \right) F_{k_1 k_2}(t, x_1, 0) \right] \Theta(0 < x_1 < t) d^4 \psi^\dagger(x_1) \right.$$\left. + \frac{i}{v} \left( -i + \frac{1}{2} U \right) F_{k_1 k_2}(t, 0, 0) d^4 \psi^\dagger(0) \right\} |0\rangle,$$\right.\left. \tag{5.14}$$

where we have used the averaging prescription for the delta function. Comparing to Eq. (5.11), we see that the function $F_{k_1 k_2}$ must satisfy three requirements:

$$\left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) F_{k_1 k_2}(t, x_1, x_2) = 0, \tag{5.15a}$$

$$\left[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} \right) + z \right] F_{k_1 k_2}(t, x_1, 0) = 0, \tag{5.15b}$$

$$\left( 1 + i \frac{1}{2} U \right) F_{k_1 k_2}(t, 0, 0) = U \, \mathcal{T}(k_1) \left( e^{-ik_1 t} - e^{-izt} \right) e^{-ik_2 t}. \tag{5.15c}$$

The first requirement will hold if $F_{k_1 k_2}$ is a function of the coordinate differences only $(t - x_1, t - x_2, x_1 - x_2)$, while the second requirement will hold if $F_{k_1 k_2}(t, x_1, 0)$ is a function of $t - x_1$ times $e^{-izx_1}$. From the third requirement, we can then read off:

$$F_{k_1 k_2}(t, x_1, x_2) = \mathcal{T}_U \mathcal{T}(k_1) \left( e^{-ik_1 (t-x_1)} - e^{-iz(t-x_1)} \right) e^{-ik_2 (t-x_1)} e^{-iz(x_1-x_2)}, \tag{5.16a}$$

where: $\mathcal{T}_U = \frac{U}{1 + i \frac{1}{2} U}. \tag{5.16b}$

The quantity $\mathcal{T}_U$ is exactly the $\mathcal{T}$-matrix of the potential scattering model, with potential $U \psi^\dagger(0) \psi(0)$. We will see that the arbitrary crossing state is built from “$U$-crossings” and “RLM-crossings,” i.e. powers of $\mathcal{T}_U$ and $\mathcal{T}(k)$.
Note also that $|e^{-iz(x_1-x_2)} = e^{-\Delta(x_1-x_2)}$, indicating that the two electrons in the crossing state are bound together on a distance scale $1/\Delta$. (Recall that $x_1 > x_2$ due to the Heaviside function, so this is a decaying exponential. Since the $\psi(x_2)\psi(x_1)$ operators ultimately antisymmetrize the wavefunction in position space, we can think of the decay term as $e^{-\Delta|x_1-x_2|}$.)

Solution for $n = 3$.

The $n = 3$ problem is to find an auxiliary state $|\chi_{k_1k_2k_3}(t)\rangle$ that vanishes at $t = 0$ and satisfies:

$$
\left( H - i \frac{d}{dt} \right) |\chi_{k_1k_2k_3}(t)\rangle = -A_{k_3}(t)|\chi_{k_1k_2}(t)\rangle
= \frac{1}{L^{3/2}} v \int dx_1 F_{k_1k_2}(t, x_1, 0) e^{-ik_3t} \Theta(0 < x_1 < t) d^3 \psi(x_1) \psi^\dagger(x_1)|0\rangle. \tag{5.17a}
$$

We extend our previous ansatz (5.12) to $n = 3$:

$$
|\chi_{k_1k_2k_3}(t)\rangle = \frac{1}{L^{3/2}} \int dx_1 dx_2 dx_3 F_{k_1k_2k_3}(t, x_1, x_2, x_3)
\times \left[ \Theta(0 < x_3 < x_2 < x_1 < t) \psi^\dagger(x_3)
+ \frac{i}{v} \delta(x_3) \Theta(0 < x_2 < x_1 < t) d^3 \psi(x_2) \psi^\dagger(x_1)|0\rangle. \tag{5.18}
$$

We require that $F_{k_1k_2k_3}(t, x_1, x_2, x_3)$ is a function of coordinate differences only and that:

$$
F_{k_1k_2k_3}(t, x_1, x_2, 0) = e^{-izx_1} \times \text{(function of } t - x_1 \text{ and } t - x_2). \tag{5.19}
$$

Then we obtain (see the general $n$ solution below for the full computation):

$$
\left( H - i \frac{d}{dt} \right) |\chi_{k_1k_2k_3}(t)\rangle = \frac{1}{L^{3/2}} v \left( -i + \frac{i}{2} U \right) \int dx_1 F_{k_1k_2k_3}(t, x_1, 0, 0) d^3 \psi^\dagger(0) \psi^\dagger(x_1)|0\rangle. \tag{5.20}
$$

Thus, $F_{k_1k_2k_3}$ must satisfy:

$$
\left( 1 + i \frac{1}{2} U \right) F_{k_1k_2k_3}(t, x_1, 0, 0) = iU F_{k_1k_2}(t, x_1, 0) e^{-ik_3t}. \tag{5.21}
$$
We can build a suitable function using the $n = 2$ solution:

$$F_{k_1k_2k_3}(t, x_1, x_2, x_3) = i \mathcal{T}_U F_{k_1k_2}(t, x_1, x_3)e^{-ik_3(t-x_2)}. \quad (5.22)$$

Roughly speaking, the three electrons in the crossing state are bound together on a distance scale $1/\Delta$, with the decay only depending on the distance between the two farthest electrons ($x_1$ and $x_3$). The middle electron ($x_2$) seems to be a "$U$-crossing" plane wave. (After antisymmetrizing in position space, the exponential decay factor would become $e^{-\Delta|x_{\text{max}}-x_{\text{min}}|}$, where "max" and "min" are the largest and smallest of the three given $x$-coordinates, and the plane wave would be a function of the remaining coordinate in the middle.)

**Solution for $n = 4$.**

There are two possible partitions: a single cell of length four, or two cells of length two. So, we must find auxiliary states $|\chi_{k_1k_2k_3k_4}(t)\rangle$ and $|\chi_{k_1k_2k_3k_4}(t)\rangle$ that vanish at $t = 0$ and satisfy:

$$\left( \mathcal{H} - i \frac{d}{dt} \right) |\chi_{k_1k_2k_3k_4}(t)\rangle = -A_{k_4}(t) |\chi_{k_1k_2k_3}(t)\rangle \quad (5.23a)$$

$$= \frac{1}{L^2} \frac{i}{v} U \int dx_1 dx_2 F_{k_1k_2k_3}(t, x_1, x_2, 0)e^{-ik_4t}$$

$$\Theta(0 < x_2 < x_1 < t)d^4\psi^\dagger(0)\psi^\dagger(x_2)\psi^\dagger(x_1)|0\rangle, \quad (5.23b)$$

and:

$$\left( \mathcal{H} - i \frac{d}{dt} \right) |\chi_{k_1k_2k_3k_4}(t)\rangle = -B_{k_3k_4}^{(\text{red})} |\chi_{k_1k_2}(t)\rangle \quad (5.24a)$$

$$= \frac{1}{L^2} \frac{U}{v} \int dx_1 dx_2 F_{k_1k_2}(t, x_1, x_2)\mathcal{T}(k_3) \left( e^{-ik_3t} - e^{-izt} \right)$$

$$\times e^{-ik_4t}\Theta(0 < x_2 < x_1 < t)d^4\psi^\dagger(0)\psi^\dagger(x_2)\psi^\dagger(x_1)|0\rangle. \quad (5.24b)$$

We make the ansatz:

$$|\chi_{k_4}(t)\rangle = \frac{1}{L^2} \int dx_1 dx_2 dx_3 dx_4 F_{k_2}(t, x_1, x_2, x_3, x_4)\left[ \Theta(0 < x_4 < x_3 < x_2 < x_1 < t)\psi^\dagger(x_4) \right.$$

$$+ \frac{i}{v} \delta(x_4)\Theta(0 < x_3 < x_2 < x_1 < t)d^4\psi^\dagger(x_3)\psi^\dagger(x_2)\psi^\dagger(x_1)|0\rangle, \quad (5.25)$$
where $p = (1, 2, 3, 4)$ or $(1, 2, 3, 4)$. We require that $F_{kp}(t, x_1, x_2, x_3, x_4)$ is a function of coordinate differences only, and that $F_{kp}(t, x_1, x_2, x_3, 0)$ is of the form $e^{-ixp}$ times a function of $t-x_1, t-x_2,$ and $t-x_3$; then (see the general $n$ solution below for the full computation):

$$
\left( H - i \frac{d}{dt} \right) \chi_{kp}(t) = \frac{1}{L^2} \overset{i}{\int} \left(-i + \frac{1}{2} \right) F_{kp}(t, x_1, x_2, 0, 0) \Theta(0 < x_2 < x_1 < t)
\times d^\dagger \psi^\dagger(0) \psi^\dagger(x_2) \psi^\dagger(x_1)|0\rangle.

(5.26)

Thus, the two $F_{kp}$ functions must satisfy:

$$
\left(1 + i \frac{1}{2} U\right) F_{k_1 k_2 k_3 k_4}(t, x_1, x_2, 0, 0) = i U F_{k_1 k_2 k_3}(t, x_1, x_2, 0) e^{-ik_4 t},

(5.27a)

\left(1 + i \frac{1}{2} U\right) F_{k_1 k_2 |k_3 k_4}(t, x_1, x_2, 0, 0) = U F_{k_1 k_2}(t, x_1, x_2) T(k_3) \left(e^{-ik_3 t} - e^{-ikt}\right) e^{-ik_4 t}.

(5.27b)

We then find:

$$
F_{k_1 k_2 k_3 k_4}(t, x_1, x_2, x_3, x_4) = i T_U F_{k_1 k_2 k_3}(t, x_1, x_2, x_4) \left(e^{-ik_4(t-x_3)} - e^{-ix(t-x_3)}\right)
= (i T_U)^2 F_{k_1 k_2}(t, x_1, x_4) e^{-ik_3(t-x_2)} e^{-ik_4(t-x_3)},

(5.28a)

and:

$$
F_{k_1 k_2 |k_3 k_4}(t, x_1, x_2, x_3, x_4) = F_{k_1 k_2}(t, x_1, x_2) F_{k_3 k_4}(t, x_3, x_4).

(5.29)

Solution for general $n$.

From the above calculations, the pattern has emerged: each new cell (of length two, from $B^{(red)}(t)$) leads to a $F_{k_1 k_2}(t, x_1, x_2)$-type term, and any cell can be extended (from $A(t)$) by changing the second $x$-coordinate of the $F_{k_1 k_2}$ function to the last coordinate of the cell and introducing a “$U$-crossing” factor of the form $i T_U e^{-ik_3(t-x_2)}$. For example,

$$
F_{k_1 k_2 k_3 |k_4 k_5 k_6 k_7 k_8}(t, x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8) =
(i T_U)^4 F_{k_1 k_2}(t, x_1, x_3) e^{-ik_3(t-x_2)} F_{k_4 k_5}(t, x_4, x_8) e^{-ik_6(t-x_5)} e^{-ik_7(t-x_6)} e^{-ik_8(t-x_7)}.

(5.30)
We now provide the formal construction and proof. Given a partition \( \mathbf{p} \in \mathcal{P}(\mathbf{n}) \) with \( \mathbf{n} = (1, \ldots, n) \), we generalize the ansatz (5.12) to:

\[
|\chi_{\mathbf{p}}(t)| = \frac{1}{E^{n/2}} \int dx_{\mathbf{n}} \, F_{\mathbf{k}_p}(t, x_{\mathbf{n}}) \left[ \Theta(0 < x_n < \cdots < x_1 < t) \psi^\dagger(x_{\mathbf{n}}) + \frac{i}{v} \delta(x_n) \Theta(0 < x_{n-1} < \cdots < x_1 < t) d^\dagger \right] \psi^\dagger(x_{\mathbf{n}/n}) |0\rangle. \tag{5.31}
\]

Before constructing the function \( F_{\mathbf{k}_p}(t, x_{\mathbf{n}}) \) for an arbitrary partition, we first define it for any single-celled partition (which is the same as defining it for a list of length \( n \geq 2 \)):

\[
F_{\mathbf{k}_n}(t, x_{\mathbf{n}}) = (iT_U)^{n-2} \, F_{k_1k_2}(t, x_1, x_n) \prod_{j=2}^{n} e^{-ik_j(t-x_{j-1})}, \tag{5.32}
\]

where \( F_{k_1k_2}(t, x_1, x_2) \) is given in Eq. (5.16a). A generic partition has some number \( s \) cells and can therefore be written as \( \mathbf{p} = (\mathbf{p}(1)\cdots|\mathbf{p}(s)) \), where each \( \mathbf{p}(j) \) is a list; let \( q \) be the length of the last cell, so that \( \mathbf{p}(s) = (n - q + 1, \ldots, n) \). The solution is a product of single-celled solutions:

\[
F_{\mathbf{k}_p}(t, x_{\mathbf{n}}) = \prod_{j=1}^{s} F_{\mathbf{k}_{\mathbf{p}(j)}}(t, x_{\mathbf{p}(j)}) \tag{5.33a}
\]

\[
= F_{k_{\mathbf{p}(1)} \cdots k_{\mathbf{n-q+1}}}(t, x_1, \ldots, x_{n-q}) F_{k_{n-q+1} \cdots k_{\mathbf{n}}}(t, x_{n-q+1}, \ldots, x_n). \tag{5.33b}
\]

Our task is to show that this solution satisfies the auxiliary state condition Eq. (5.10a). To reduce clutter, we use the notation \( \mathbf{n} - 1 = (1, \ldots, n - 1) \), \( \mathbf{n} - 2 = (1, \ldots, n - 2) \), and \( \mathbf{n} - q = (1, \ldots, n - q) \) (note that the minus sign does not mean removing an element from
the list). We have:

\[
\left( H - \frac{id}{dt} \right) |\chi_{k_\mathbf{p}}(t)\rangle = \frac{1}{L^{n/2}} \left\{ \int dx_n \left[ -i \left( \frac{\partial}{\partial t} + \sum_{j=1}^{n} \frac{\partial}{\partial x_j} \right) F_{k_\mathbf{p}}(t, x_n) \right] \right.
\]

\[
\times \Theta(0 < x_n < \cdots < x_1 < t) \psi^\dagger(x_n)
\]

\[
+ \frac{i}{v} \int dx_{n-1} \left[ \left( -i \frac{\partial}{\partial t} - i \sum_{j=1}^{n-1} \frac{\partial}{\partial x_j} + z \right) F_{k_\mathbf{p}}(t, x_{n-1}, 0) \right]
\]

\[
\times \Theta(0 < x_{n-1} < \cdots < x_1 < t) d^\dagger \psi^\dagger(x_{n-1})
\]

\[
+ \frac{i}{v} \left( -i + \frac{1}{2} U \right) \int dx_{n-2} F_{k_\mathbf{p}}(t, x_{n-2}, 0, 0)
\]

\[
\Theta(0 < x_{n-2} < \cdots < x_1 < t) d^\dagger \psi^\dagger(0) \psi^\dagger(x_{n-2}) \right\} |0\rangle. \quad (5.34)
\]

The first term vanishes because \( F_{k_\mathbf{p}}(t, x_n) \) is a function of coordinate differences only. The second term vanishes because \( F_{k_\mathbf{p}}(t, x_{n-1}, 0) \) is \( e^{-izx_{n-1}} \) times a function of coordinate differences. We are left with:

\[
\left( H - \frac{id}{dt} \right) |\chi_{k_\mathbf{p}}(t)\rangle = \frac{1}{L^{n/2}} \frac{i}{v} \left( -i + \frac{1}{2} U \right) \int dx_{n-2} F_{k_\mathbf{p}/(n-1)}(t, x_{n-2})
\]

\[
\times F_{k_{(n-1)}}(t, x_{n-2}) \Theta(0 < x_{n-2} < \cdots < x_1 < t) d^\dagger \psi^\dagger(0) \psi^\dagger(x_{n-2}) |0\rangle, \quad (5.35)
\]

where we used Eq. (5.33b). Let us compare this to the terms we are trying to cancel. If \( q = 2 \) (i.e., \( \mathbf{p}(s) = (n-1, n) \)), we have:

\[
- B_{k_{n-1}k_n}^{(\text{red})}(t) |\chi_{k_{(n-1), n}}(t)\rangle = \frac{1}{L^{n/2}} \frac{U}{v} \int dx_{n-2} F_{k_{(n-1), n}}(t, x_{n-2})
\]

\[
T(k_{n-1}) \left( e^{-ik_{n-1}t} - e^{-izt} \right) e^{-ik_n t} \Theta(0 < x_{n-2} < \cdots < x_1 < t) d^\dagger \psi^\dagger(0) \psi^\dagger(x_{n-2}) |0\rangle, \quad (5.36)
\]

and so the auxiliary state condition holds if we have:

\[
\left( 1 + \frac{i}{2} U \right) F_{k_{n-1}k_n}(t, 0, 0) = U T(k_{n-1}) \left( e^{-ik_{n-1}t} - e^{-izt} \right) e^{-ik_n t}, \quad (5.37)
\]
which has already been shown in the $n = 2$ calculation (see Eq. (5.15c)). If instead $q \geq 3$, we have [again using Eq. (5.33b)]:

$$
-A_{kn}(t)|\chi_{k_p/n}(t)\rangle = \frac{1}{L_{n/2}\psi} \int dx_{n-1} F_{k_p/n}(t, x_{n-2}, 0)
$$

$$
\times e^{-ik_n t} \Theta(0 < x_{n-2} < \cdots < x_1 < t) d^\dagger \psi^\dagger (0) \psi^\dagger (x_{n-2}) |0\rangle =
$$

$$
\frac{1}{L_{n/2}\psi} \int dx_{n-1} F_{k_p/(p,q)}(t, x_{n-q}) F_{k_{p(n)}}(t, x_{n-q+1}, \ldots, x_{n-2}, 0, 0)
$$

$$
\times e^{-ik_n t} \Theta(0 < x_{n-2} < \cdots < x_1 < t) d^\dagger \psi^\dagger (0) \psi^\dagger (x_{n-2}) |0\rangle, \quad (5.38)
$$

and so the auxiliary state condition holds if we have:

$$
\left(1 + \frac{i}{2} U\right) F_{k_p(p)}(t, x_{n-q+1}, \ldots, x_{n-2}, 0, 0) = iU F_{k_p/(p,q)}(t, x_{n-q+1}, \ldots, x_{n-2}, 0, 0)e^{-ik_n t}.
$$

(5.39)

This holds due to the definition (5.32) of the function $F$ for single-celled partitions. We have thus verified Eq. (5.10a), completing the solution.

### 5.2 Wavefunction of the multi-lead model

We proceed to the case of an arbitrary number of leads $N_{\text{leads}}$. Recall that we have chosen the tunneling to take the simplest form, involving only the “even” linear combination of fields defined via:

$$
\psi^\dagger_{e}(x) = \frac{1}{\sqrt{N_{\text{leads}}}} \sum_{\gamma = 1}^{N_{\text{leads}}} \psi^\dagger_{\gamma}(x).
$$

(5.40)

The multi-lead RLM separates into a copy of the one lead RLM (with the even field) and $N_{\text{leads}} - 1$ free fields. Since the Coulomb interaction term breaks this separation, we cannot read off the multi-lead IRLM wavefunction from the one lead wavefunction in the manner of Sec. 2.5. However, we find that some ingredients from the one lead solution can be re-used in the multi-lead solution.
The $A(t)$ and $B(t)$ operators acquire lead indices:

$$A_{\gamma k}(t) = -\frac{U}{\sqrt{L}} \left[ e^{-ikt} d \psi_{\gamma}(0) d + \frac{1}{N_{\text{leads}}} F_k(t) \sum_{\beta=1}^{N_{\text{leads}}} d^\dagger \psi_{\beta}(0) \left( \frac{1}{2} d - \frac{i}{\sqrt{N_{\text{leads}}} v} \psi_{\beta}(0) \right) \right],$$

(5.41a)

$$B_{\gamma_1 k_1 \gamma_2 k_2}(t) = B_{\gamma_1 k_1 \gamma_2 k_2}^{(\text{red})}(t) - B_{\gamma_2 k_2 \gamma_1 k_1}^{(\text{red})}(t),$$

(5.41b)

where:

$$B_{\gamma_1 k_1 \gamma_2 k_2}^{(\text{red})}(t) = -\frac{i}{\sqrt{N_{\text{leads}}} L v} F_k(t) e^{-ikt} d^\dagger \psi_{\gamma_2}(0).$$

(5.42)

The general formalism for type B models (see Sec. 2.2.2) yields the following for the many body wavefunction:

$$|\Psi_{NkN}(t)\rangle = \sum_{n=0}^{N} \sum_{m \in \mathcal{I}_n(N)} (s^m n) c_m^\dagger \chi_{\gamma N/m N/m}(t) |\Phi_{\gamma m k m}(t)\rangle,$$

(5.43)

where the crossing states $|\Phi(t)\rangle$ are given as sums over unsymmetrized crossing states:

$$|\Phi_{\gamma m k m}(t)\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{p \in \mathbb{P}(m)} |\chi_{\gamma p^n k p^n}(t)\rangle,$$

(5.44)

which vanish at $t = 0$ and satisfy:

$$\left( H - i \frac{d}{dt} \right) |\chi_{\gamma p^n k p}(t)\rangle = \begin{cases} -B_{\gamma_{n-1} k_{n-1} \gamma k_n}^{(\text{red})}(t) |\chi_{\gamma p^n/(n-1) k p/(n-1)}(t)\rangle & q = 2, \\ -A_{\gamma n k_n}(t) |\chi_{\gamma p^n/n k p^n/n}(t)\rangle & 3 \leq q \leq n \end{cases},$$

(5.45a)

$$|\chi_{\gamma p^n k p}(0)\rangle = 0,$$

(5.45b)

$$|\chi_{\gamma p^n k p}(t)\rangle = |0\rangle \quad \text{when } p \text{ is the empty list.}$$

(5.45c)

**Solution for $n = 2$.**

The problem is to find a state $|\chi_{\gamma_1 k_1 \gamma_2 k_2}(t)\rangle$ that vanishes at $t = 0$ and satisfies:

$$\left( H - i \frac{d}{dt} \right) |\chi_{\gamma_1 k_1 \gamma_2 k_2}(t)\rangle = -B_{\gamma_1 k_1 \gamma_2 k_2}^{(\text{red})}(t) |0\rangle$$

$$= \frac{1}{\sqrt{N_{\text{leads}}} L v} \mathcal{T}(k_1) \left( e^{-ikt} - e^{-izt} \right) e^{-ikt} d^\dagger \psi_{\gamma_2}(0) |0\rangle.$$

(5.46b)
Noting the similarity to the \( n = 2 \) problem in the one lead model, we can essentially read off the answer:

\[
|\psi_{1\gamma_{1}1\gamma_{2}k_{2}}(t)\rangle = \frac{1}{\sqrt{N_{\text{leads}}}} \frac{1}{L} \int dx_{1} dx_{2} \, F_{k_{1}k_{2}}(t, x_{1}, x_{2}) \left[ \Theta(0 < x_{2} < x_{1} < t) \psi_{e}^{\dagger}(x_{2}) + \frac{i}{v} \delta(x_{2}) \Theta(0 < x_{1} < t) d^{\dagger} \right] \psi_{\gamma_{2}}^{\dagger}(x_{1})|0\rangle, \tag{5.47}
\]

where \( \psi_{e}^{\dagger}(x) = \frac{1}{\sqrt{N_{\text{leads}}}} \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma}^{\dagger}(x) \) and \( F_{k_{1}k_{2}} \) is the same function as in the one lead case, Eq. (5.16a). Indeed, taking \( F_{k_{1}k_{2}} \) to be arbitrary for the moment, we have:

\[
\left( H - i \frac{d}{dt} \right) |\psi_{1\gamma_{1}1\gamma_{2}k_{2}}(t)\rangle = \frac{1}{\sqrt{N_{\text{leads}}}} \frac{1}{L} \left\{ \int dx_{1} dx_{2} \left[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_{1}} + \frac{\partial}{\partial x_{2}} \right) F_{k_{1}k_{2}}(t, x_{1}, x_{2}) \right] \right.
\]

\[
\times \Theta(0 < x_{2} < x_{1} < t) \psi_{e}^{\dagger}(x_{2}) \psi_{\gamma_{2}}^{\dagger}(x_{1})
\]

\[
+ \frac{i}{v} \int dx_{1} \left[ \left( -i \frac{\partial}{\partial t} - i \frac{\partial}{\partial x_{1}} + z \right) F_{k_{1}k_{2}}(t, x_{1}, 0) \right] \Theta(0 < x_{1} < t) d^{\dagger} \psi_{\gamma_{2}}^{\dagger}(x_{1})
\]

\[
+ \frac{i}{v} \left( -i + \frac{1}{2} U \right) F_{k_{1}k_{2}}(t, 0, 0) d^{\dagger} \psi_{\gamma_{2}}^{\dagger}(0) \right\} |0\rangle. \tag{5.48}
\]

Comparing to Eq. (5.46b), we see that the same requirements Eqs. (5.15a), (5.15b), and (5.15c) are sufficient, which leads to the same solution for \( F_{k_{1}k_{2}} \) as before.

A different notation will be more convenient for the general \( n \) case. We write:

\[
|\psi_{1\gamma_{1}1\gamma_{2}k_{2}}(t)\rangle = \sum_{\beta_{1}, \beta_{2}=1,2} \frac{1}{L} \int dx_{1} dx_{2} \, F_{\gamma_{1}k_{1}\gamma_{2}k_{2}}^{\beta_{1}\beta_{2}}(t, x_{1}, x_{2}) \left[ \Theta(0 < x_{2} < x_{1} < t) \psi_{\beta_{2}}^{\dagger}(x_{2}) + \frac{i}{\sqrt{N_{\text{leads}}}} \delta(x_{2}) \Theta(0 < x_{1} < t) d^{\dagger} \right] \psi_{\beta_{1}}^{\dagger}(x_{1})|0\rangle, \tag{5.49}
\]

where:

\[
F_{\gamma_{1}k_{1}\gamma_{2}k_{2}}^{\beta_{1}\beta_{2}}(t, x_{1}, x_{2}) = \frac{1}{N_{\text{leads}}} \delta_{\gamma_{2}k_{2}}^{\beta_{1}} F_{k_{1}k_{2}}(t, x_{1}, x_{2}). \tag{5.50}
\]

The \( \beta_{2} \)-independence of the right-hand side is just another way of obtaining \( \psi_{e}^{\dagger}(x_{2}) \). Indeed, we have:

\[
\sum_{\beta_{2}=1,2} \left( \Theta(0 < x_{2} < x_{1} < t) \psi_{\beta_{2}}^{\dagger}(x_{2}) + \frac{i}{\sqrt{N_{\text{leads}}}} \delta(x_{2}) \Theta(0 < x_{1} < t) d^{\dagger} \right) = \sqrt{N_{\text{leads}}} \left( \Theta(0 < x_{2} < x_{1} < t) \psi_{e}^{\dagger}(x_{2}) + \frac{i}{v} \delta(x_{2}) \Theta(0 < x_{1} < t) d^{\dagger} \right), \tag{5.51}
\]
which is the convenient combination of terms that we have seen to be useful in building crossing states.

**Solution for \( n = 3 \).**

The \( n = 3 \) problem is to find an auxiliary state \( |\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle \) that vanishes at \( t = 0 \) and satisfies:

\[
\left( H - i \frac{d}{dt} \right) |\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle = -A_{\gamma_3\gamma_4}(t)|\chi_{\gamma_1\gamma_2\gamma_3}(t)\rangle
\]

\[
= \frac{1}{\sqrt{2}} \frac{1}{L^{3/2}} U \int dx_1 \int dx_2 \int dx_3 \, F_{k_1k_2k_3}(x_1, x_2, x_3) e^{-ik_4t} \Theta(0 < x_1 < x_2 < x_1 < t) d^4 \psi^\dagger_{\gamma_3}(x_1) \psi^\dagger_{\gamma_4}(x_3) |0\rangle.
\]  

(5.52a)

Comparing to the \( n = 3 \) solution in the one lead model, we can read off:

\[
|\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle = \frac{1}{\sqrt{N_{\text{leads}}}} \frac{1}{L^{3/2}} \int dx_1 dx_2 dx_3 \, F_{k_1k_2k_3}(t, x_1, x_2, x_3)
\]

\[
\times \left[ \Theta(0 < x_3 < x_2 < x_1 < t) \psi^\dagger_e(x_3) + \frac{i}{v} \delta(x_3) \Theta(0 < x_2 < x_1 < t) d^1 \psi^\dagger_{\gamma_3}(x_2) \psi^\dagger_{\gamma_4}(x_1) |0\rangle \right].
\]

(5.52b)

**Solution for \( n = 4 \).**

The problem is to find auxiliary states \( |\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle \) and \( |\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle \) that vanish at \( t = 0 \) and satisfy:

\[
\left( H - i \frac{d}{dt} \right) |\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle = -A_{\gamma_4\gamma_5}(t)|\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle
\]

\[
= \frac{1}{\sqrt{2}} \frac{1}{L^{3/2}} U \int dx_1 dx_2 \int dx_3 \, F_{k_1k_2k_3}(t, x_1, x_2, x_3) e^{-ik_5t}
\]

\[
\times \Theta(0 < x_2 < x_1 < t) d^1 \psi^\dagger_{\gamma_5}(x_2) \psi^\dagger_{\gamma_6}(x_1) |0\rangle \]

(5.54a)

\[
\left( H - i \frac{d}{dt} \right) |\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle = -B_{\gamma_3\gamma_4\gamma_5\gamma_6}(t)|\chi_{\gamma_1\gamma_2\gamma_3\gamma_4}(t)\rangle
\]

\[
= \frac{1}{2} \frac{1}{L^{3/2}} U \int dx_1 dx_2 \, F_{k_1k_2}(t, x_1, x_2) T(k_3) \left( e^{-ik_5t} - e^{-izt} \right)
\]

\[
\times e^{-ik_4t} \Theta(0 < x_2 < x_1 < t) d^1 \psi^\dagger_{\gamma_4}(x_2) \psi^\dagger_{\gamma_5}(x_1) |0\rangle.
\]

(5.54b)
The solutions are again the same as in the one lead case, with some overall constant factors and insertion of appropriate lead indices. We have:

\[
|\chi_{\gamma_1 k_1 \gamma_2 k_2 \gamma_3 k_3 \gamma_4 k_4}(t)\rangle = \frac{1}{\sqrt{N_{\text{leads}}}} \frac{1}{L^2} \int dx_1 dx_2 dx_3 dx_4 \ F_{k_1 k_2 k_3 k_4}(t, x_1, x_2, x_3, x_4) \\
\times \left[ \Theta(0 < x_4 < x_3 < x_2 < x_1 < t) \psi_{\gamma_4}^\dagger(x_4) + \frac{i}{v} \delta(x_4) \Theta(0 < x_3 < x_2 < x_1 < t) d^t \right] \\
\times \psi_{\gamma_4}^\dagger(x_3) \psi_{\gamma_3}^\dagger(x_2) \psi_{\gamma_2}^\dagger(x_1) |0\rangle, \quad (5.55)
\]

and:

\[
|\chi_{\gamma_1 k_1 \gamma_2 k_2 \gamma_3 k_3 \gamma_4 k_4}(t)\rangle = \frac{1}{N_{\text{leads}}} \frac{1}{L^2} \int dx_1 dx_2 dx_3 dx_4 \ F_{k_1 k_2 k_3 k_4}(t, x_1, x_2, x_3, x_4) \\
\times \left[ \Theta(0 < x_4 < x_3 < x_2 < x_1 < t) \psi_{\gamma_4}^\dagger(x_4) + \frac{i}{v} \delta(x_4) \Theta(0 < x_3 < x_2 < x_1 < t) d^t \right] \\
\times \psi_{\gamma_4}^\dagger(x_3) \psi_{\gamma_3}^\dagger(x_2) \psi_{\gamma_2}^\dagger(x_1) |0\rangle. \quad (5.56)
\]

The pattern is that the last entry of each cell is associated with an even operator.

**Solution for general \( n \).**

The general crossing state is given by:

\[
|\chi_{\gamma_1 k_1 \gamma_2 k_2 |\gamma_3 k_3 \gamma_4 k_4}(t)\rangle = \sum_{\beta_1 .. \beta_n = 1,2} \frac{1}{L^{n/2}} \int dx_n \ F_{\gamma_n k_n}(t, x_n) \left[ \Theta(0 < x_n < \cdots < x_1 < t) \psi_{\beta_n}^\dagger(x_n) \right] \\
+ \frac{i}{\sqrt{N_{\text{leads}}}} \delta(x_n) \Theta(0 < x_{n-1} < \cdots < x_1 < t) d^t \psi_{\beta_{n-1}}^\dagger(x_{n-1}) |0\rangle. \quad (5.57)
\]

To define the function \( F \) with lead indices, we proceed in the same way as in the one lead case by considering a single-celled partition first and then writing the general case as a product of single-celled solutions. Given \( n = (1, \ldots, n) \), we define:

\[
F_{\gamma_n k_n}(t, x_n) = \frac{1}{N_{\text{leads}}} F_{k_n}(t, x_n) \prod_{j=1}^{n-1} \delta_{\gamma_j+1}, \quad (5.58)
\]

where \( F_{k_n}(t, x_n) \) is as in the one lead case, i.e., Eq. (5.32). Notice that the last index, \( \beta_n \), does not appear, indicating that the corresponding \( \psi_{\beta_n}^\dagger(x_n) \) operator will become \( \psi_{\beta_n}^\dagger(x_n) \) (up to a constant factor that is compensated for). A generic partition has some number \( s \).
cells and can therefore be written as $p = (p(1) \ldots | p(s))$, where each $p(j)$ is a list; let $q$ be the length of the last cell, so that $p(s) = (n - q + 1, \ldots, n)$. The function $F$ with lead indices is given by a product of single-celled functions:

$$F_{\gamma k p}^\beta (t, x_n) = \prod_{j=1}^{s} F_{\gamma_j p(j) k_j p(j)}^\beta (t, x_{p(j)})$$

(5.59a)

$$= F_{\gamma_p(p(s)) k_p(p(s))}^\beta (t, x_1, \ldots, x_{n-q}) F_{\gamma_{k-p(q+1)} k_{k-p(q+1)}}^\beta (t, x_{n-q+1}, \ldots, x_n).$$

(5.59b)

The demonstration that this solves the multi-lead problem is very similar to the one lead case above.

### 5.3 Dot occupancy to leading order

We use the multi-lead IRL wavefunction to find the dot occupancy to leading order in the interaction strength $U$. Our task is to evaluate:

$$\langle n_d \rangle = \langle \Psi(t) | d^\dagger d | \Psi(t) \rangle,$$

(5.60)

where $|\Psi(t)\rangle = e^{-iHt}|\Psi\rangle$ and $|\Psi\rangle = c_{\gamma_k N}^\dagger |0\rangle$. The initial quantum numbers are arbitrary for the moment, though we later specialize to the case of a Fermi sea in each lead.

The occupancy is more conveniently evaluated directly rather than by using the derivative formula of Sec. 2.3.2 (at least, at leading order). This is to be expected – since $d^\dagger d$ is a projection operator, evaluating its expectation value is already similar to evaluating an overlap (one just removes the $n_d = 0$ part that is projected out).

We begin by expanding the wavefunction to first order in $U$:

$$|\Psi(t)\rangle = |\Psi^0(t)\rangle + |\Psi^2(t)\rangle + O(U^2),$$

(5.61)

where:

$$|\Psi^0(t)\rangle = c_{\gamma N}^\dagger \gamma N (t) |0\rangle,$$

(5.62a)

$$|\Psi^2(t)\rangle = \sum_{m \in \mathbb{Z}_2(N)} \left( \frac{\delta_{\gamma_m m}}{\gamma N m} \right) c_{\gamma N m}^\dagger \Phi_{\gamma m k m} (t) |\Phi_{\gamma m k m} (t)\rangle,$$

(5.62b)

$$|\Phi_{\gamma_1 k_1 \gamma_2 k_2} (t)\rangle = |\chi_{\gamma_1 k_1 \gamma_2 k_2} (t)\rangle - |\chi_{\gamma_2 k_2 \gamma_1 k_1} (t)\rangle.$$
The occupancy to leading order is thus given by:

\[ \langle n_d \rangle_t = \langle n_d \rangle_t^{(0)} + \langle n_d \rangle_t^{(1)} + O(U^2), \]  

(5.63)

where \( \langle n_d \rangle_t^{(0)} = \langle \Psi(t) | d^d | \Psi(t) \rangle \) and \( \langle n_d \rangle_t^{(1)} = 2 \text{ Re} \left( \langle \Psi(t) | d^d | \Psi^2(t) \rangle \right) \) (where \( | \Psi^2(t) \rangle \) is to be expanded to first order in \( U \); we will see that this expansion is simple).

We have already evaluated the zeroth order (RLM) term \( \langle n_d \rangle_t^{(0)} \) in Sec. 3.3.2; we recall here the steady state limit in particular [Eq. (3.102a)]:

\[ \langle n_{d,s.s.} \rangle_t = \lim_{t \to \infty} \langle n_d \rangle_t^{(0)} = \frac{1}{N_{\text{leads}}} \sum_{\gamma=1}^{N_{\text{leads}}} \int_{-B}^{B} \frac{dk}{2\pi} f_{\gamma}(k) \frac{|T(k)|^2}{2\Delta}, \]  

(5.64)

where \( f_{\mu}(k) = \left[ e^{-\frac{k}{T_{\mu}}(k-\mu_\gamma)} + 1 \right]^{-1} \) is the Fermi function of lead \( \gamma \).

We proceed to the leading correction. While we could apply the general result (2.78), we can just as well do the calculation directly using Wick’s Theorem and the fact that the time-evolving field operators have canonical anticommutation relations:

\( \{ c_k(t), c_k^\dagger(t) \} = \delta_{k\bar{k}} \).

The quantum numbers \( \mathbf{N}/\mathbf{m} \) must contract (we assume there are no repeats in the list of initial quantum numbers), which cancels the factor of \( \frac{\text{sgn}}{L^2} \mathbf{m} \) and leaves:

\[ \langle n_d \rangle_t^{(1)} = 2 \text{Re} \left[ \sum_{1 \leq m_1 < m_2 \leq N} \langle 0 | c_{\gamma m_1 k_{m_1}}(t) c_{\gamma m_2 k_{m_2}}(t) d^d | \Phi_{\gamma m_1 \gamma m_2}(t) \rangle \right]. \]  

(5.65)

It is advantageous to consider the “off-diagonal” case, in which the quantum numbers on either side of the overlap we need are arbitrary. By fermionic antisymmetry, the off-diagonal overlap must be the antisymmetrization of another function \( \Omega(t; \gamma_1 k_1', \gamma_2 k_2'; \gamma_1 k_1, \gamma_2 k_2) \) as follows:

\[ \langle 0 | c_{\gamma_1 k_1'}(t) c_{\gamma_2 k_2'}(t) d^d | \Phi_{\gamma_1 k_1 \gamma_2 k_2}(t) \rangle = \frac{1}{L^2} \sum_{\sigma, \sigma' \in \text{Sym}(2)} (\text{sgn} \sigma) (\text{sgn} \sigma') \times \Omega(t; \gamma_1 k_1'; \gamma_2 k_2'; \gamma_1 k_1, \gamma_2 k_2), \]  

(5.66)

where the factor of \( 1/L^2 \) is inserted for the convenience of taking the thermodynamic limit. The key point is that \( \Omega \) does not depend on \( L \), as we will see shortly. Relabelling summation
variables, we obtain:

\[
\langle n_d \rangle_{t}^{(1)} = \frac{1}{L^2} \sum_{m_1, m_2 = 1}^{N} \sum_{\sigma \in \text{Sym}(2)} (\text{sgn } \sigma) 2 \text{Re} \left[ \Omega(t; \gamma_{m_1} k_{m_1}, \gamma_{m_2} k_{m_2}; \gamma_{m_1} k_{m_1}, \gamma_{m_2} k_{m_2}) \right]
\]  

(5.67a)

\[
\text{therm. limit } \lim_{N_{\text{leads}} \to \infty} \sum_{\gamma_1, \gamma_2 = 1}^{N} \int_{-D}^{D} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} f_{\gamma_1}(k_1) f_{\gamma_2}(k_2) \sum_{\sigma \in \text{Sym}(2)} (\text{sgn } \sigma)
\]

\[
\times 2 \text{Re} \left[ \Omega(t; \gamma_1 k_1, \gamma_2 k_2; \gamma_{\sigma_1} k_{\sigma_1}, \gamma_{\sigma_2} k_{\sigma_2}) \right].
\]  

(5.67b)

From Eq. (5.66) [and the explicit forms (3.94b), (5.47), and (5.16a)], we can read off:

\[
\Omega(t; \gamma'_1 k'_1, \gamma'_2 k'_2; \gamma_1 k_1, \gamma_2 k_2) = \frac{1}{2N_{\text{leads}}} \int dx_1 F_{k_1 k_2}(t, x_1, 0) \left[ \delta_{\gamma'_1}^{\gamma_1} e^{i k'_1 (t-x_1)} + \frac{1}{N_{\text{leads}}} F^*_{k'_2}(t-x_1) F^*_{k'_2}(t) \Theta(0 < x_1 < t) \right]
\]

\[
= \frac{1}{2N_{\text{leads}}} \int_0^t dx_1 \mathcal{T}_U \mathcal{T}(k_1) \left( e^{-i k_1 (t-x_1)} - e^{-i z (t-x_1)} \right) e^{-i k_2 (t-x_1)} e^{-i z x_1}
\]

\[
\times \left[ \delta_{\gamma'_1}^{\gamma_1} e^{i k'_1 (t-x_1)} + \frac{1}{N_{\text{leads}}} i \mathcal{T}(k'_1) \left( e^{i k'_1 (t-x_1)} - e^{i z (t-x_1)} \right) \right] i \mathcal{T}(k'_2) \left( e^{i k'_2 t} - e^{i z t} \right),
\]  

(5.68)

where we can replace \( \mathcal{T}_U \to U \) to get the first order expansion. We can assume \( k'_1 + k'_2 = k_1 + k_2 \), since this is the only case we need for evaluating (5.67b).

Recalling that \( \text{Im } z = -\Delta < 0 \), we see that there are several terms in the integrand that decay as \( e^{-\Delta t} \) for large time; they can all be dropped in the limit. The terms \( e^{-i z (t-x_1)} \) and \( e^{i z (t-x_1)} \), which each which have absolute value \( e^{-\Delta (t-x_1)} \), immediately be neglected, since they are of order one when \( x_1 \sim t \); however, the factor of \( e^{-i z x_1} \) can combine with either one of these terms to yield the absolute value \( e^{-\Delta t} \), which then can be neglected. The remaining time-dependent terms are all phases and cancel by assumption \( e^{-i (k_1 + k_2 - k'_1 - k'_2) t} = 1 \), leaving:

\[
\lim_{t \to \infty} \Omega(t; \gamma'_1 k'_1, \gamma'_2 k'_2; \gamma_1 k_1, \gamma_2 k_2) = \frac{1}{2N_{\text{leads}}} \int_0^\infty dx_1 \mathcal{T}_U \mathcal{T}(k_1) e^{i (k_1 + k_2 - k'_1 - k'_2) x_1}
\]

\[
\times \left[ \delta_{\gamma'_1}^{\gamma_1} + \frac{1}{N_{\text{leads}}} i \mathcal{T}(k'_1) \right] i \mathcal{T}(k'_2)
\]  

(5.69a)

\[
= -\frac{1}{4N_{\text{leads}}} \mathcal{T}_U \mathcal{T}(k_1) |\mathcal{T}(k'_2)|^2 \left[ \delta_{\gamma'_1}^{\gamma_1} + \frac{1}{N_{\text{leads}}} i \mathcal{T}(k'_1) \right].
\]  

(5.69b)
We thus obtain:

\[
\lim_{t \to \infty} \sum_{\sigma \in \text{Sym}(2)} (\text{sgn } \sigma) 2 \text{Re} \left[ \Omega(t; \gamma_1 k_1, \gamma_2 k_2; \gamma_{\sigma_1} k_{\sigma_1}, \gamma_{\sigma_2} k_{\sigma_2}) \right] = \\
- \frac{|T(k_2)|^2}{2N_{\text{leads}} \Delta^2} \text{Re} \left\{ T_U \left[ \left( 1 + \frac{i}{N_{\text{leads}}} T^*(k_1) \right) (T(k_1) - T(k_2) - (1 - \delta_{\gamma_1}) T(k_1)) \right] \right\}. \tag{5.70}
\]

We simplify this further by repeated use of the optical identity (3.80); to leading order in $U$, we obtain:

\[
(5.70) = \frac{U}{2N_{\text{leads}} \Delta^2} \left\{ \left( 1 - \frac{1}{2N_{\text{leads}}} |T(k_1)|^2 \right) |T(k_2)|^2 \text{Re} [T(k_2)] \right. \\
- \text{Re} [T(k_1)] |T(k_2)|^2 \left( \delta_{\gamma_1} - \frac{1}{2N_{\text{leads}}} |T(k_2)|^2 \right) \right\}. \tag{5.71}
\]

Note that we have a term independent of $k_1$; this leads to a linear divergence in bandwidth. In particular, we have $\int_{-D}^D \frac{dk_1}{2\pi} f_\gamma(k_1) = (D - \mu_\gamma)/(2\pi) + O \left( e^{-\frac{1}{2}(D-|\mu_\gamma|)} \right)$ [which is a special case of the earlier integral Eq. (4.130)]; we drop the error term from now on. Then, recalling the expression (5.64) for the non-interacting steady state occupancy $\langle n_{d,s.s.}^{(0)} \rangle$, we obtain:

\[
\langle n_{d,s.s.} \rangle \equiv \lim_{t \to \infty} \left( \langle n_{d}^{(0)} \rangle_t + \langle n_{d}^{(1)} \rangle_t \right) = \langle n_{d}^{(0)} \rangle_t \\
+ \frac{U}{2N_{\text{leads}} \Delta} \left\{ \frac{1}{2\pi \Delta} \sum_{\gamma_1=1}^{N_{\text{leads}}} (D - \mu_{\gamma_1}) - \langle n_{d}^{(0)} \rangle_{s.s.} \sum_{\gamma_1=1}^{N_{\text{leads}}} \int_{-D}^D \frac{dk_2}{2\pi} f_{\gamma_2}(k_2) |T(k_2)|^2 \text{Re} [T(k_2)] \right. \\
- \frac{1}{\Delta} \sum_{\gamma_1, \gamma_2=1}^{N_{\text{leads}}} \int_{-D}^D \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} f_{\gamma_1}(k_1)f_{\gamma_2}(k_2) \text{Re} [T(k_1)] |T(k_2)|^2 \left( \delta_{\gamma_1} - \frac{1}{2N_{\text{leads}}} |T(k_2)|^2 \right) \right\}. \tag{5.72}
\]

As usual in a field theory calculation, this answer diverges as the bandwidth is sent to infinity. In this case, there is both a linear and a logarithmic divergence. In the next section, we perform the necessary steps – re-expressing the answer in terms of physical parameters rather than bare parameters – to get a meaningful answer.

### 5.3.1 Universality in and out of equilibrium

To obtain universal results, we take the scaling limit, in which all energy scales are much smaller than the bandwidth.
First, we replace the bare parameter $\epsilon$ by the physical parameter $\epsilon_d$ according to $\epsilon = \epsilon_d - U \sum_{\gamma_1=1}^{N_{\text{leads}}} (D - \mu_\gamma)/(2\pi) + U \Delta/2$. The first term in the shift accounts for using a normal ordered interaction term [see Eq. (5.2) and the discussion there], and the $\Delta$ shift, we will see, has the effect of putting the equilibrium resonance at $\epsilon_d = 0$. Working to first order in $U$ and using Eq. (5.64) and the identity $\frac{\partial}{\partial \epsilon}|T(k)|^2 = \frac{1}{\Delta}|T(k)|^2 \text{Re} T(k)$ [which follows from $T(k) = 2\Delta(k - \epsilon + i\Delta)^{-1}$], we obtain:

$$
\langle n_d \rangle_{\text{s.s.}} = \langle n_d \rangle_{\text{s.s.}}^{(0)} + \frac{U}{2N_{\text{leads}}\Delta} \left\{ \left( 1 - \frac{1}{2} \langle n_d \rangle_{\text{s.s.}}^{(0)} \right) \sum_{\gamma_2=1}^{N_{\text{leads}}} \int_{-D}^D \frac{dk_2}{2\pi} f_{\gamma_2}(k_2) |T(k_2)|^2 \text{Re} \left[ T(k_2) \right] 

- \frac{1}{\Delta} \sum_{\gamma_1,\gamma_2=1}^{N_{\text{leads}}} \int_{-D}^D \frac{dk_1 dk_2}{2\pi f_{\gamma_1}(k_1) f_{\gamma_2}(k_2) \text{Re} \left[ T(k_1) \right] |T(k_2)|^2 \left( \delta_{\gamma_2}^2 - \frac{1}{2N_{\text{leads}}} |T(k_2)|^2 \right) \right\},
$$

(5.73)

where each $T$-matrix is now evaluated with $\epsilon_d$ instead of the original $\epsilon$ [i.e. $T(k) = 2\Delta(k - \epsilon_d + i\Delta)^{-1}$], including in the free occupancy $\langle n_d \rangle_{\text{s.s.}}^{(0)}$ as given in Eq. (5.64).

Since $T(k) \sim 1/k$ for large $k$, the second line of (5.73) diverges logarithmically for large $D$. This encodes the emergence of a universal scale through the Callan-Symanzik equation:

$$
\left( D \frac{\partial}{\partial D} + \beta \Delta \frac{\partial}{\partial \Delta} \right) \langle n_d \rangle_{\text{s.s.}} = O(1/D),
$$

(5.74a)

where: $\beta \Delta = -\frac{U}{\pi} + O(U^2)$.

(5.74b)

To see that the Callan-Symanzik equation holds, we note:

$$
D \frac{\partial}{\partial D} \langle n_d \rangle_{\text{s.s.}} \xrightarrow{D \to \infty} \frac{U}{2\pi N_{\text{leads}} \Delta} \sum_{\gamma_2=1}^{N_{\text{leads}}} \int_{-\infty}^\infty \frac{dk_2}{2\pi} f_{\gamma_2}(k_2) |T(k_2)|^2 \left( 1 - \frac{1}{2} |T(k_2)|^2 \right),
$$

(5.75)

which follows from $DT(\pm D) \xrightarrow{D \to \infty} \pm 2\Delta$ and simple properties of the Fermi function.

Then we obtain the beta function as in Eq. (5.74b) from Eq. (5.64) and the identity

$$
\Delta \frac{\partial}{\partial \Delta} \left( \frac{1}{\Delta} |T(k)|^2 \right) = \frac{1}{\Delta} |T(k)|^2 \left( 1 - \frac{1}{2} |T(k)|^2 \right).
$$

Now that we are focusing on the large bandwidth regime, we can confirm that $\epsilon_d = 0$ is the location of the equilibrium resonance in Eq. (5.73). Setting all $f_\gamma(k) = f(k)$ and
\( \epsilon_d = 0, \) we have \( \langle n_d \rangle_{\text{s.s.}}^{(0)} = 1/2 + O(1/D) \) and \( \int_{-D}^D dk \, f(k)|\mathcal{T}(k)|^2 (1 - \frac{1}{2}|\mathcal{T}(k)|^2) = O(1/D) \) (shown numerically), so that \( \langle n_d \rangle_{\text{s.s.}} = 1/2. \)

The Callan-Symanzik equation encodes the fact that for large bandwidth, \( \langle n_d \rangle_{\text{s.s.}} \) takes a universal form, depending only on the external parameters (\( \epsilon_d \) and the temperatures and chemical potentials of the leads) and on two scaling invariants. One of these invariants is an emergent energy scale:

\[ T_K = \left( 1 - \frac{U}{\pi} \right) D \left( \frac{\Delta}{D} \right)^{\frac{1}{1+U/\pi}}. \]  

(5.76)

It can be verified that \( (D \frac{\partial}{\partial D} + \beta \Delta \frac{\partial}{\partial \Delta}) T_K = O \) and that \( T_K = \Delta \) for \( U = 0 \). The \( U \)-dependent overall scale of \( T_K \) is arbitrary (as we discuss in more detail below), and we have chosen it so that the equilibrium susceptibility at zero field takes the standard form

\[-\langle n_d \rangle_{\text{s.s.}} = 1/(\pi T_K) \frac{\partial}{\partial \epsilon_d} |\mathcal{T} = \epsilon_d = 0 \) (as in Ref. [64]). The second scaling invariant is the coupling constant \( U \) (or equivalently, \( \alpha \)). Thus, staying always in the large bandwidth regime from now on, we can write:

\[ \langle n_d \rangle_{\text{s.s.}} = f_{\text{universal}} \left( U; \left\{ \frac{T_\gamma}{T_K} \right\}; \left\{ \frac{\mu_\gamma}{T_K} \right\}; \frac{\epsilon_d}{T_K} \right), \]  

(5.77)

where the brackets indicate all the channels: \( \left\{ \frac{T_\gamma}{T_K} \right\} = (T_1/T_K, \ldots, T_{N_{\text{leads}}}/T_K), \left\{ \frac{\mu_\gamma}{T_K} \right\} = (\mu_1/T_K, \ldots, \mu_{N_{\text{leads}}}/T_K) \). Below, we evaluate this universal function to leading order in \( U \) in a few regimes at zero temperature. First, we make some general comments on the RG flow of the model and compare our results with the literature.

5.3.2 RG discussion

The RG flow of the model is the following:

\[ \frac{\partial U}{\partial \ln D} \equiv \beta_U = 0, \]  

(5.78a)

\[ \frac{\partial \ln \Delta}{\partial \ln D} \equiv \beta_\Delta(U) = -\frac{U}{\pi} + O(U^2). \]  

(5.78b)

The \( U \)-parameter, which does not flow, determines the direction of flow of \( \Delta \) through the beta function \( \beta_\Delta(U) \). If \( \beta_\Delta(U) \) is negative, then \( \Delta \) increases as the bandwidth \( D \) is reduced.
While our calculation is only to first order in $U$, it is known to all orders that $\frac{\partial U}{\partial D} = 0$, i.e. $U$ does not flow.

While the RG flow of the IRL has been studied by many methods, the most direct comparison we can make to the literature is to other works that have found the flow from the evaluation of an expectation value to leading order in $U$. In particular, previous work on the charge current in the two lead IRL driven by bias has found linear and logarithmic divergences. In either case, the logarithmic divergences are accounted for by the Callan-Symanzik equation, as we did above, with the same result (5.74b) for the beta function at leading order. In Ref. [65], the linear divergences are removed by a some redefinition of $\epsilon$ (though an equation is not given). In Ref. [43], these linear divergences are removed by shifting via $\epsilon = \epsilon_d - \frac{U}{\pi}$, this would correspond to our shift (5.2) with $N_{\text{leads}} = 2$, with the $U \Delta/2$ term dropped (i.e. no attempt to put the resonance at $\epsilon_d = 0$), and with the chemical potentials set to zero (i.e. normal ordering the interaction term with respect to the non-interacting ground state with all chemical potentials set to zero). We believe that putting the resonance at $\epsilon_d = 0$ is useful for making a comparison with equilibrium results, but are less sure about whether or not normal ordering should take into account the chemical potentials.

For further comparison with the literature, let us rewrite our equation for $T_K$ [Eq. (5.76)] in another form:

$$T_K = \left( 1 - \frac{U}{\pi} \right) D \left( \frac{\Delta}{D} \right) \alpha/2,$$

where: $\alpha = \frac{2}{1 + \frac{U}{\pi}}$. (5.79a)

The exponent $\alpha$ in the RG invariant $T_K$ [Eq. (5.76)] has been much discussed in the literature. Various answers for $\alpha$ as a function of $U$ (or as a function of the single particle phase shift, which is $\delta_U = \arctan(U/2)$ in our case) have been found. Our answer, Eq. (5.79b), agrees with some Bethe Ansatz calculations, but not all, and a different answer has been obtained by bosonization. See Table I in Ref. [64] for a summary of the literature.
While all calculations agree that $\alpha = 2$ for zero coupling (or zero phase shift), there is disagreement already at the first order correction.

For the purpose of calculating universal quantities, the precise dependence of $\alpha$ on the coupling constant is only meaningful within a particular cutoff scheme. This theory has two RG invariants, which we choose as $T_K$ and $U$, and they determine results by values assigned to them. The final outputs of a field theory calculation are functions such as $f_{\text{universal}}$ that have RG invariants as inputs. The numerical values of the RG invariants are not themselves calculable in field theory. Instead, one fixes the value of the RG invariants by fitting universal functions to data. One of the advantages of doing a field theory calculation (on what is ultimately a lattice system) is that one has a great freedom to choose a cutoff scheme that makes the calculation of universal functions more convenient; the price one pays is that only these universal functions can be compared meaningfully with a lattice system.

One technical caveat is that the functional form of $\alpha$ does matter insofar as it determines the possible values $\alpha$ can take. This point does not seem to arise in the IRL, seeing as all of the forms of $\alpha$ in the literature permit $\alpha$ to range from $-\infty$ to $\infty$ given $U$ ranging from $-\infty$ to $\infty$. Note that our calculation in this paper is only consistent for $\alpha$ in a narrow range around $\alpha = 2$, since we took $U$ to be small; however, the Bethe Ansatz result for $\alpha$ is given by the same Eq. (5.79b) with no restriction on $U$.

In Ref. [64], Camacho et. al. use bosonization, and hence have a different functional form of $\alpha$ in terms of $U$. They emphasize, however, that their final answer for $\langle n_d \rangle_{\text{equilibrium}}$ at zero temperature agrees exactly with the Bethe Ansatz answer once both are expressed as functions of $\alpha$ and $\epsilon_d/T_K$. This agrees with our discussion in the previous paragraph. To disprove our claim, it would be necessary to find another universal function whose form differs between the bosonization and Bethe Ansatz calculations, even after the invariants $\alpha$ and $T_k$ are fixed by matching the answers for (e.g.) $\langle n_d \rangle_{\text{equilibrium}}$.

A stronger claim of Camacho in Ref. [66] is that the formula for $\alpha$ in terms of $U$ (or
rather the phase shift) is scheme-independent, contrary to what we find in Eq. (5.79b). Though we have not examined the argument in detail, we wonder if the unconventional cutoff schemes employed in this paper and in the Bethe Ansatz might somehow be outside the range of cutoff schemes considered in the bosonization calculation. (These cutoff schemes are unconventional in that the Hamiltonian formally has all energies.)

Similar comments apply to the $U$-dependent prefactor in $T_K$

### 5.3.3 Evaluation at zero temperature

To make the above discussion more definite, we evaluate the steady state occupancy (5.73) at zero temperature. We then use RG improvement to extract the universal function (5.77) in a few specific regimes.

The standard trick for finding a universal function from a perturbative result is RG improvement: one changes the original parameters $(D, \Delta)$ to new parameters $(D', \Delta')$ with the same value of $T_K$, where $D'$ is chosen so as to eliminate large logarithms in the perturbation series. The net effect is to delete these large logarithms and to replace $\Delta$ by the "running" coupling constant $\Delta'$. Note that this replacement is only valid on the part of the answer that satisfies Callan-Symanzik equation – thus, one must first take $D$ to be large before applying RG improvement.

In the zero temperature limit, the momentum integrals in Eq. (5.73) can all be carried out analytically, with the following results in the large bandwidth limit:

\begin{align}
\frac{1}{\Delta} \int_{-D}^{D} \frac{dk}{2\pi} \text{Re} |T(k)| &= -\frac{1}{\pi} \ln \frac{D}{\sqrt{(\epsilon_d - \mu)^2 + \Delta^2}} + O(1/D), \\
\frac{1}{2\Delta} \int_{-D}^{D} \frac{dk}{2\pi} |T(k)|^2 &= \frac{1}{2} - \frac{1}{\pi} \arctan \frac{\epsilon_d - \mu}{\Delta} + O(1/D), \\
\frac{1}{4\Delta} \int_{-D}^{D} \frac{dk}{2\pi} |T(k)|^4 &= \frac{1}{2} - \frac{1}{\pi} \arctan \frac{\epsilon_d - \mu}{\Delta} - \frac{\epsilon_d - \mu}{4\pi \Delta} |T(\mu)|^2 + O(1/D), \\
\frac{1}{\Delta} \int_{-\infty}^{\mu} \frac{dk}{2\pi} |T(k)|^2 \text{Re} |T(k)| &= -\frac{1}{2\pi} |T(\mu)|^2.
\end{align}
We thus obtain:
\[
\langle n_d \rangle^{(0)}_{\text{s.s.}} = \frac{1}{2} - \frac{1}{N_{\text{leads}} \pi} \sum_{\gamma=1}^{N_{\text{leads}}} \arctan \frac{\epsilon_d - \mu_\gamma}{\Delta},
\]  
(5.81)

and:
\[
\langle n_d \rangle_{\text{s.s.}} = \langle n_d \rangle^{(0)}_{\text{s.s.}} + \frac{U}{N_{\text{leads}} \pi} \left[ -\frac{1}{4} \left( \frac{1}{2} - \langle n_d \rangle^{(0)}_{\text{s.s.}} \right) \sum_{\gamma_2=1}^{N_{\text{leads}}} |T(\mu_{\gamma_2})|^2 
+ \sum_{\gamma_1=1}^{N_{\text{leads}}} \left( \frac{1}{N_{\text{leads}}} \sum_{\gamma_2=1}^{N_{\text{leads}}} \frac{\epsilon_d - \mu_{\gamma_2}}{4\pi \Delta} |T(\mu_{\gamma_2})|^2 + \frac{1}{2} - \frac{1}{\pi} \arctan \frac{\epsilon_d - \mu_\gamma}{\Delta} - \langle n_d \rangle^{(0)}_{\text{s.s.}} \right) \right] \times \ln \frac{D}{\sqrt{(\epsilon_d - \mu_\gamma)^2 + \Delta^2}}. 
\]  
(5.82)

Note that there are large logarithms of many different ratios of scales, so that there is no one choice of \(D'\) that will eliminate all of them in the general case (arbitrary chemical potentials \(\mu_\gamma\)). We therefore specialize to some specific regimes in which there are just one or two different large logs to be eliminated, and in which we can obtain universal functions using RG improvement.

**Equilibrium.**

Setting all chemical potentials to zero, we find:
\[
\langle n_d \rangle_{\text{s.s.}} = \frac{1}{2} - \frac{1}{\pi} \arctan \frac{\epsilon_d}{\Delta} + \frac{U}{\pi^2 \epsilon_d^2 + \Delta^2} \left[ \epsilon_d \ln \frac{D}{\sqrt{\epsilon_d^2 + \Delta^2}} - \Delta \arctan \frac{\epsilon_d}{\Delta} \right].
\]  
(5.83)

The large logarithm is to be eliminated by the self-consistent choice \(D' = \sqrt{\epsilon_d^2 + (\Delta')^2}\), which determines the running coupling:
\[
\Delta' = \left\{ 1 + \frac{U}{\pi} \left[ 1 - \frac{1}{2} \ln \left( 1 + \frac{\epsilon_d^2}{T_K^2} \right) \right] \right\} T_K,
\]  
(5.84)

We thus obtain a universal answer, valid to leading order in \(U\):
\[
\langle n_d \rangle_{\text{s.s.}} = \frac{1}{2} - \frac{1}{\pi} \arctan \frac{\epsilon_d}{T_K} + \frac{U}{2\pi^2 (1 + \epsilon_d^2/T_K^2)} \left[ 2 \left( \frac{\epsilon_d}{T_K} - \arctan \frac{\epsilon_d}{T_K} \right) - \frac{\epsilon_d}{T_K} \ln \left( 1 + \frac{\epsilon_d^2}{T_K^2} \right) \right],
\]  
(5.85)
which agrees with the leading order expansion of the exact equilibrium result from Bethe Ansatz (see Appendix C). This confirms, at least in the zero temperature limit and to this order, that in the long time limit following the quench, the occupancy thermalizes.

We emphasize that the output of our field theory calculation is a two-parameter family of functions of $\epsilon_d$, parameterized by $U$ and $T_K$. Redefinitions of $U$ and $T_K$ can change the details of the parameterization, but not the full family of functions that is obtained by letting $U$ and $T_K$ range over all allowed values. We brought our answer to the form (5.85) as a convenient way of showing that the full family of functions agrees with the Bethe Ansatz result in the parameter range we consider: $U$ small (or equivalently, $\alpha$ close to 2) and $T_K$ arbitrary.

In the $U$ part of the final answer (5.85), only the coefficients of the arctan and ln terms have universal meaning. Varying the number $a$ in the shift $\epsilon_d = \epsilon - N_{\text{leads}}D/(2\pi) + aU\Delta$ controls a term proportional to $1/(1 + \epsilon_d^2/T_K^2)$; we took $a = 1/2$ to eliminate this term, putting the resonance is at $\epsilon_d = 0$. (This choice also puts the resonance at $\epsilon_d = 0$ for arbitrary temperature.) Similarly, we can adjust the coefficient of the $(\epsilon_d/T_K)/(1 + \epsilon_d^2/T_K^2)$ term by varying $b$ in $T_K = [1+bU]D(D/D)^{2\alpha}$; this term controls the susceptibility at $\epsilon_d = 0$, and our choice of $b = -1/\pi$ normalizes $T_K$ according to $T_K^{-1} = -\frac{\partial}{\partial \epsilon_d} \langle n_d \rangle_{s,s} |_{T=\epsilon_d=0}$.

**Out of equilibrium – two leads with $\epsilon_d = 0$.**

Consider the two lead model with the leads separated by a bias voltage $V$ and the dot energy at the Fermi level of lead 1 – that is, $N_{\text{leads}} = 2$, $\mu_1 = 0$, $\mu_2 = -V$, and $\epsilon_d = 0$. (The case of arbitrary $\epsilon_d$ is also possible, but messier.) The occupancy (5.82) contains two large logarithms, $\ln \frac{D}{\Delta}$ and $\ln \frac{D}{\sqrt{\Delta^2 + \epsilon_d^2}}$; we can choose $D'$ to cancel either one, with the same final
Figure 5.1: Left: the steady state occupancy $n_d \equiv \langle n_d \rangle_{s.s.}$ at zero temperature in the two lead IRL, either as a function of the dot energy $\epsilon_d$ or the voltage $V$. The leads are held at chemical potentials $\mu_1 = 0$ and $\mu_2 = -V$. The equilibrium ($V = 0$) curves are given by Eq. (5.85) and in fact are independent of the number of leads; see Appendix C for the Bethe Ansatz answer taken from the literature. The non-equilibrium ($V \neq 0$) curves are given by Eq. (5.86). In both cases, we compare the non-interacting case ($\rho U = 0$) with weak interaction (first order in $\rho U = 0.1$). Right: the weakly interacting case with the non-interacting occupancy subtracted, i.e. $\delta n_d \equiv n_d - n_d|_{U=0}$. In equilibrium, $\delta n_d$ reaches finite limits as $\epsilon_d/T_K \to \pm \infty$. Out of equilibrium, $|\delta n_d|$ grows logarithmically as $V/T_K \to \pm \infty$, indicating that some resummation of the series in $\rho U$ is needed to make sense of the extremely large voltage regime.

result (see Fig. 5.1 as well):

$$\langle n_d \rangle_{s.s.} = \frac{1}{2} - \frac{\arctan \frac{V}{T_K}}{2\pi} + U \frac{V^2}{2\pi T_K^2} \left\{ \frac{\arctan \frac{V}{T_K}}{1 + \frac{V^2}{T_K^2}} \right\} - \left( \arctan \frac{V}{T_K} - \frac{V}{T_K} \right) \left[ 1 - \frac{1}{4} \ln \left( 1 + \frac{V^2}{T_K^2} \right) \right].$$  (5.86)

The particular numbers that appear in this answer become meaningful once the values of $U$ and $T_K$ are fixed by (e.g.) the equilibrium answer (5.85) with data. Note that the contribution of the interaction begins at order $V^2$, beyond linear response.

The leading correction in $U$ in Eq. (5.86) grows logarithmically with voltage as $V/T_K \to \pm \infty$; this is a consequence of the fact that no choice of $D'$ can cancel both of the large logarithms. This implies that some resummation of the series in $U$ is needed to make sense of the regime of very large voltage. We can characterize the scale at which the $U$ series breaks down out of equilibrium as the voltage $V_0$ for which the $U$ correction term ($\delta n_d$ in Fig. 5.1) equals 1/2; the result is $V_0 \sim T_K e^{2/(\rho U)}$, where $\rho = 1/(2\pi)$ is the density of states.
per unit length in our convention. The number 2 in the exponent is not sharply defined, since we had to make an arbitrary choice for what value of the $U$ correction is large enough to say that the series breaks down. Though our calculation sends the bandwidth $D \to \infty$, we suggest that this scale $V_0$ could also be significant in the lattice model if it lies in the universal regime, i.e. if $V_0 \ll D_{\text{lattice}}$.

If we instead define the physical parameter $\epsilon_d$ via normal ordering relative to the ground state with no voltage bias – that is, set all $\mu = 0$ in Eq. (5.2) – then the $U$ correction $\langle n_d \rangle_{\text{s.s.}}^{(1)}$ would grow linearly with voltage rather than logarithmically, and so we would obtain $V_0 \sim UT_K$ (up to some overall constant). We believe that the normal ordering prescription we used is the correct one, but it is not completely clear. This issue only arises out of equilibrium.

**Out of equilibrium – two leads close to the particle-hole symmetric point.**

We again consider the two lead model with the leads separated by a voltage drop $V$, this time with $\epsilon_d$ close to halfway between the two chemical potentials. That is, we set $\mu_1 = \epsilon_d + V/2$ and $\mu_2 = \epsilon_d - V/2 - \delta V$. For $\delta V = 0$, the steady state occupancy is its free value, 1/2. Self-consistently setting $D' = \sqrt{\langle \Delta' \rangle^2 + V^2/4}$, we obtain the following correction for small $\delta V$:

$$\langle n_d \rangle_{\text{s.s.}} - \frac{1}{2} = -\frac{1}{2\pi} \left( \frac{\epsilon_d}{\text{TK}} \right)^{\frac{1}{2}} \left[ 1 + \frac{U}{\pi} \left( \frac{V^2}{4T_K^2} + \frac{1}{2} \left( 1 - \frac{V^2}{4T_K^2} \right) \ln \left( 1 + \frac{V^2}{4T_K^2} \right) - \frac{V}{2T_K} \arctan \frac{V}{2T_K} \right) \right] \frac{\delta V}{T_K}.$$  

(5.87)

As before, this expression is valid for $V \ll T_K e^{1/(2U)}$ (in addition to requiring $U$ and $\delta V/T_K$ to be small).
Chapter 6

Anderson impurity model

6.1 Setup

We consider the multi-lead Anderson impurity model directly in the infinite volume limit:

\[ H = -i \int dx \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) + \epsilon d_a^\dagger d_a + \left[ \frac{v}{\sqrt{N_{\text{leads}}}} \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(0) d_a + \text{h.c.} \right] + U n_{\uparrow} n_{\downarrow} \]  

(6.1)

Our calculations in this chapter are not as far developed as in the case of the Kondo model. However, we do present the exact many-body scattering states in the limit of infinite Coulomb repulsion \((U \rightarrow \infty)\). We do various checks on the calculation, including computing the wavefunction for small numbers of electrons with arbitrary \(U\), verifying that the same answer is obtained in the limit of \(U \rightarrow \infty\). We also calculate the \(N\)-body wavefunction for small \(U\), use it to calculate the electric current to leading order in \(U\), and find exact agreement with a Keldysh calculation (Appendix D). Finally, we observe that the wavefunction for infinite \(U\) can be used to calculate the current as an expansion in the tunneling parameter, and we find there the standard scaling law of the model.

The calculations of this chapter also serve to illustrate the time-independent version of our formalism, in which the goal is to directly solve for the non-equilibrium steady state (i.e. scattering “in” state, discussed in more detail below) without following its full development in time. Though we largely focused on the time-dependent picture in chapters 4 and 5, the time-independent picture can be used there, as well.

After a unitary transformation, the Hamiltonian (6.1) separates into \(N_{\text{leads}} - 1\) free
fermion fields (with spin) and one copy of the one lead Anderson model:

$$H_e = -i \int dx \, \psi_{e\alpha}^\dagger(x) \frac{d}{dx} \psi_{e\alpha}(x) + c d^\dagger_{\alpha} d_{\alpha} + \left[ \nu \psi_{e\alpha}^\dagger(0) d_{\alpha} + \text{h.c.} \right] + U n_{\uparrow},$$  \hspace{1cm} (6.2)

where $\psi_{e\alpha} = \frac{1}{\sqrt{N_{\text{leads}}}} \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma\alpha}$ is the “even” combination [see the corresponding change of variables in the spinless RLM in Eq. (3.95)].

Let us set up the problem of finding the non-equilibrium steady state, or scattering “in” state, of the model. We write $H = H^{(0)} + H^{(1)}$ with $H^{(1)} = Un_{\uparrow}$, so that $H^{(0)}$ is the multi-lead RLM (with spin). The scattering operators of $H^{(0)}$ can be read off by taking the long time limit [in the usual pointwise way; see Eqs. (3.17) and (3.89a)] of Eq. (3.94b):

$$c_{\gamma k a, \text{in}}^\dagger = c_{\gamma k a}^\dagger + \frac{1}{N_{\text{leads}}} \int dx \, F_{k, \text{in}}(x) \left[ \Theta(0 < x) \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) + \frac{i}{\sqrt{N_{\text{leads}}}} \right] ,$$  \hspace{1cm} (6.3)

where $F_{k, \text{in}}(x) = -iT(k)e^{ikx}$ [recall the RLM notation introduced in Eq. (3.79)]. Note that since we work in infinite volume, we have Dirac delta normalized operators $c_{\gamma k a}^\dagger = \int dx \, e^{ikx} \psi_{a}^\dagger(x)$.

We wish to solve the time-independent Schrodinger equation with the boundary condition of incoming plane waves with quantum numbers $\gamma_N k_N a_N$ (arbitrary for now, later chosen to describe filled Fermi seas). The boundary condition can be stated equivalently by specifying the state $|\Psi_{\gamma_N k_N a_N}\rangle \equiv c_{\gamma_N k_N a_N}^\dagger |0\rangle$, which is an eigenstate of the purely reservoir part of the Hamiltonian: $h = -i \int dx \, \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x)$. With the full Hamiltonian written as $H = h + \mathcal{V}$, the solution $|\Psi_{\gamma_N k_N a_N, \text{in}}\rangle$ of the Schrodinger equation with boundary condition is equivalently characterized by the Lippmann-Schwinger equation [see Eq. (3.93b)]:

$$|\Psi_{\gamma_N k_N a_N, \text{in}}\rangle = |\Psi_{\gamma_N k_N a_N}\rangle + \frac{1}{E - h + i\eta} \mathcal{V} |\Psi_{\gamma_N k_N a_N, \text{in}}\rangle .$$  \hspace{1cm} (6.4)

In the non-interacting case ($H^{(1)} = 0$, i.e. RLM only), the solution is $|\Psi_{\gamma_N k_N a_N, \text{in}}^0\rangle = c_{\gamma_N k_N a_N, \text{in}}^\dagger |0\rangle$. We can use this RLM eigenstate in another formulation of the Lippmann-Schwinger equation in which $H^{(0)}$, rather than $h$, is considered the “free” Hamiltonian [see
Our task is to calculate the many-body eigenstate $|\Psi_{N^kN^aN,\text{in}}\rangle$. We do this for small $U$ or infinite $U$; we have not been able to find a closed form in the case of general $U$. In the case of infinite $U$, it is convenient to use the auxiliary boson technique [67], according to which we write the following Hamiltonian:

$$H = -i \int dx \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) + \epsilon d_{a}^{\dagger} d_{a} + \left[ \frac{v}{\sqrt{N_{\text{leads}}}} \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(0) b^{\dagger} d_{a} + \text{h.c.} \right],$$

where the boson field $b$ is canonical ($[b, b^\dagger] = 1$). This Hamiltonian has a conserved charge $Q = 1$ in this state due to the boson creation operator. In this formulation, we can separate $H = h + \mathcal{V}$, but there is no useful separation $H = H^{(0)} + H^{(1)}$ because the tunneling terms themselves now encode the interaction (due to the presence of the boson field). We therefore have only the first form (6.4) of the Lippmann-Schwinger equation, and not the second (6.5).

To formulate the scattering problem in this case, we note that the incoming plane waves are characterized by the state $|\Psi_{N^kN^aN,\text{in}}\rangle = c_{N^kN^aN}^\dagger b|0\rangle$, which is an eigenstate of $h = -i \int dx \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x)$. Note also that $Q = 1$ in this state due to the boson creation operator. In this formulation, we can separate $H = h + \mathcal{V}$, but there is no useful separation $H = H^{(0)} + H^{(1)}$ because the tunneling terms themselves now encode the interaction (due to the presence of the boson field). We therefore have only the first form (6.4) of the Lippmann-Schwinger equation, and not the second (6.5).

In constructing the scattering states of the infinite-$U$ model (6.1), it is convenient to use essentially the same scattering “in” operators as in the finite $U$ case (6.3), with the boson appearing via the replacement $d_{a}^{\dagger} \rightarrow d_{a}^{\dagger} b$:

$$c_{\gamma k a, \text{in}}^\dagger \equiv c_{\gamma k a}^\dagger + \frac{1}{N_{\text{leads}}} \int dx F_{k,\text{in}}(x) \left[ \Theta(0 < x) \sum_{\gamma=1}^{N_{\text{leads}}} \psi_{\gamma a}^\dagger(x) + i \frac{\sqrt{N_{\text{leads}}}}{v} \delta(x) d_{a}^{\dagger} b \right].$$
Our starting point for the exact “in” state of the infinite-$U$ model (6.6) will be the state produced by a product of these operators:

$$|\Psi^0_{\gamma NkN\alpha N,\text{in}}\rangle = c_{\gamma NkN\alpha N,\text{in}}^\dagger b^\dagger |0\rangle. \quad (6.9)$$

This state satisfies the incoming boundary condition; additional terms $|\Psi^n_{\gamma NkN\alpha N,\text{in}}\rangle$ (with $1 \leq n \leq N$) will be added to get the solution of the Schrodinger equation. In the finite $U$ case, the wavefunction $|\Psi^0_{\gamma NkN\alpha N,\text{in}}\rangle$ has meaning on its own as the solution for the RLM only; however, this is not true of (6.9) because we cannot turn off the interaction in the infinite-$U$ Hamiltonian (6.6) (except for the trivial limit of no tunneling).

Let us recall next the relation of the scattering problem for the multi-lead model [(6.1) or (6.6)] to the scattering problem of the even sector only [(6.2) or (6.7)]. From the calculations of Sec 2.5 (generalized from $N_{\text{leads}} = 2$ to general $N_{\text{leads}}$), we know that the wavefunction of the multi-lead model can be constructed straightforwardly from the wavefunction of the even sector: the crossing states are related by simple prefactors. In particular, the full “in” wavefunction for the multi-lead model is:

$$|\Psi_{\gamma NkN\alpha N,\text{in}}\rangle = \sum_{n=0}^{N} \left( \frac{1}{N_{\text{leads}}} \right)^{n/2} \sum_{m \in \mathbb{Z}_n(N)} (\text{sgn } m) c_{\gamma N/m kN/m\alpha N/m,\text{in}}^\dagger |\Phi_{\text{in}}\rangle, \quad (6.10)$$

where the crossing states $|\Phi_{\text{in}}\rangle$ are given as sums over unsymmetrized crossing states:

$$|\Phi_{\text{in}}\rangle = \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \sum_{p \in \mathbb{P}(m)} |\chi_{\text{ekp}\alpha \text{p}\sigma,\text{in}}\rangle. \quad (6.11)$$

Thus, the problem reduces to finding the crossing states of the even sector. To write down the differential equations that determine the crossing states, we first need to calculate the $A_{\text{in}}$ and $B_{\text{in}}$ operators. These are defined in the usual way:

$$A_{e\text{k}\alpha,\text{in}} \equiv [H, c_{e\text{k}\alpha,\text{in}}^\dagger] - kc_{e\text{k}\alpha,\text{in}}^\dagger, \quad (6.12a)$$

$$B_{e\text{k}_1\alpha_1 e\text{k}_2\alpha_2,\text{in}} \equiv \{[H, c_{e\text{k}_2\alpha_2,\text{in}}^\dagger], c_{e\text{k}_1\alpha_1,\text{in}}^\dagger\}. \quad (6.12b)$$
We present the finite $U$ case first. A short calculation yields:

$$A_{ek_a, in} = \frac{iU}{v} F_{k, in}(0) d^\dagger_a b d_b = \frac{U}{v} \mathcal{T}(k) d^\dagger_a b_d, \quad (6.13a)$$

$$B_{ek_1 a_1 ek_2 a_2, in} = -\frac{U}{v^2} F_{k_1, in}(0) F_{k_2, in}(0) d^\dagger_{a_2} d^\dagger_{a_1} = -\frac{U}{v^2} \mathcal{T}(k_1) \mathcal{T}(k_2) P_{-a_1 a_2} d^\dagger_{b_2} d^\dagger_{b_1}, \quad (6.13b)$$

$$= B^{(red)}_{ek_1 a_1 ek_2 a_2, in} - B^{(red)}_{ek_2 a_2 ek_1 a_1, in}, \quad (6.13c)$$

where:

$$B^{(red)}_{ek_1 a_1 ek_2 a_2, in} = -\frac{U}{2v^2} F_{k_1, in}(0) F_{k_2, in}(0) P b^\dagger_{a_2} b d^\dagger_{b_2} d^\dagger_{b_1} = \frac{U}{2v^2} \mathcal{T}(k_1) \mathcal{T}(k_2) P b^\dagger_{a_1 a_2} d^\dagger_{b_2} d^\dagger_{b_1}, \quad (6.14)$$

where $P_-$ is the antisymmetric spin projection operator:

$$P_- = \frac{1}{2} (I - P), \quad P_{a_1 a_2} = \delta^a_{a_1} \delta^b_{a_2}; \quad P_{a_1 a_0} = \delta^a_{a_1} \delta^b_{a_0}. \quad (6.15)$$

The $B_{in}$ operators commute with the $c^\dagger_{ek_a}$ operators, and the $A_{in}$ operators annihilate $|0\rangle$ (which is the only “fixed impurity state”); thus, the model is of type B. There may seem to be little advantage in using the reduced $B_{in}$ operator here, seeing as $B^{(red)}_{ek_1 a_1 ek_2 a_2, in} = \frac{1}{2} B_{ek_1 a_1 ek_2 a_2, in}$; nevertheless, it is convenient to do so in order to use the general formalism.

In the infinite $U$ case, we find:

$$A_{ek_a, in} = iF_{k, in}(0) \psi^\dagger_{ec}(0) \left[ \delta_{ac}(b^\dagger b - 1) + d^\dagger_a d_c \right] = \mathcal{T}(k) \psi_{ec}^\dagger(0) \left[ \delta_{ac}(b^\dagger b - 1) + d^\dagger_a d_c \right], \quad (6.16a)$$

$$B_{ek_1 a_1 ek_2 a_2, in} = B^{(red)}_{ek_1 a_1 ek_2 a_2, in} - B^{(red)}_{ek_2 a_2 ek_1 a_1, in}, \quad (6.16b)$$

where:

$$B^{(red)}_{ek_1 a_1 ek_2 a_2, in} = \frac{-1}{v} F_{k_1, in}(0) F_{k_2, in}(0) P b^\dagger_{a_2} b d^\dagger_{b_2} b \psi_{eb_1}(0) = \frac{-1}{v} \mathcal{T}(k_1) \mathcal{T}(k_2) P b^\dagger_{a_1 a_2} d^\dagger_{b_2} b \psi_{eb_1}(0), \quad (6.17a)$$

$$B^{(red)}_{ek_1 a_1 ek_2 a_2, in} = \frac{-1}{v} \mathcal{T}(k_1) \mathcal{T}(k_2) P b^\dagger_{a_1 a_2} d^\dagger_{b_2} b \psi_{eb_1}(0). \quad (6.17b)$$

We consider the state $b^\dagger|0\rangle$ (rather than $|0\rangle$) to be the “fixed impurity state” of the model. The operator $A_{in}$ annihilates this state, and $B_{in}$ commutes with every $c^\dagger_{ek_a, in}$; thus, the general formalism for type B models also applies to the infinite $U$ case.

---

\(^1\) As usual, we use the averaging prescription for the delta function (Sec. 3.4). The identities $[\psi_{ec}^\dagger(0)b^\dagger d_c, d^\dagger_a b] = \psi_{ec}^\dagger(0)(\delta_{ac} b^\dagger b + d^\dagger_a d_c)$ and $F_{k, in}(0)(i(\epsilon - k) + v^*/2) = -v^*$ are useful here.
The differential equations that determine the crossing states take a very similar form in the two different cases (finite $U$ and infinite $U$). Let us state the equations for the finite $U$ case. Given a partition $\mathbf{p}$ of $n = (1, \ldots, n)$, we must have:

\[
\begin{align*}
(H - \sum_{m=1}^{n} k_m) |\chi_{ek\mathbf{p}a_n, in}\rangle &= \begin{cases} 
-B_{ek_{n-1}a_{n-1}ek_{a_n, in}}^{(\text{red})} |\chi_{ek_{(n,n-1)}a_{(n,n-1)}, in}\rangle & q = 2 \\
-A_{ek_{a_n}, in} |\chi_{ek_{a_n, in}}\rangle & 3 \leq q \leq n
\end{cases}, \\
|\chi_{ek\mathbf{p}a_n, in}\rangle &= |0\rangle \quad \text{when } \mathbf{p} \text{ is the empty list.}
\end{align*}
\] (6.18a)

Also, each crossing state $|\chi_{ek\mathbf{p}a_n, in}\rangle$ must have no incoming plane waves (since the state $|\Psi^0_{in}\rangle$ already satisfies the boundary condition); this requirement is the time-independent equivalent of the requirement that the time-dependent crossing states vanish at $t = 0$ (which is imposed because the state $|\Psi^0(t)\rangle$ already satisfies the initial condition).

To obtain the differential equations for the infinite $U$ model, we only need to replace $|0\rangle \rightarrow \tilde{b}^\dagger|0\rangle$ in Eq. (6.18b). This “base case” determines the inverse problem for the first crossing state ($n = 2$); the quantity $(H - k_1 - k_2) |\chi_{ek_{1a_1}ek_{2a_2}, in}\rangle$ must either equal $-B_{ek_{1a_1}ek_{2a_2}, in}^{(\text{red})} |0\rangle$ (the finite $U$ case) or $-B_{ek_{1a_1}ek_{2a_2}, in}^{(\text{red})} \tilde{b}^\dagger |0\rangle$ (the infinite $U$ case).

In the next section, we present the solution in the two regimes of small $U$ and large $U$.

### 6.2 Wavefunction

#### 6.2.1 Finite $U$: two electrons, or $N$ electrons to first order in $U$

Our task is to find a state $|\chi_{ek_{1a_1}ek_{2a_2}, in}\rangle$ that has no incoming plane waves and that satisfies:

\[
(H - k_1 - k_2) |\chi_{ek_{1a_1}ek_{2a_2}, in}\rangle = -B_{ek_{1a_1}ek_{2a_2}, in}^{(\text{red})} |0\rangle
\] (6.19a)

\[
= -\frac{U}{2v^2} \mathcal{T}(k_1) \mathcal{T}(k_2) P_{-a_1 a_2} d_{-a_2}^\dagger d_{a_2}^\dagger |0\rangle.
\] (6.19b)

Given such a state, the solution to the two electron scattering problem is:

\[
|\Psi_{ek_{1a_1}ek_{2a_2}, in}\rangle = c_{ek_{2a_2}, in}^\dagger c_{ek_{1a_1}, in}^\dagger |0\rangle + |\chi_{ek_{1a_1}ek_{2a_2}, in}\rangle - |\chi_{ek_{2a_2}ek_{1a_1}, in}\rangle.
\] (6.20)
We make the ansatz:

\[ |\chi_{ek_1a_1ek_2a_2,\text{in}}\rangle = \int dx_1dx_2 \ F^{b_1b_2}_{ek_1a_1ek_2a_2}(x_1,x_2) \left[ \Theta(0 < x_2 < x_1) \psi^\dagger_{eb_2}(x_2) \psi^\dagger_{eb_1}(x_1) + \frac{i}{v}(x_2)\Theta(0 < x_1) d^\dagger_{b_2} \psi^\dagger_{eb_1}(x_1) - \frac{1}{2v^2}\delta(x_1)\delta(x_2) d^\dagger_{b_2} d^\dagger_{b_1} \right] |0\rangle, \tag{6.21} \]

where the function \( F_{ek_1a_1ek_2a_2} \) is determined shortly. By construction, this ansatz vanishes when any position variable is to the left of the origin; this guarantees that there are no incoming waves from \( x = -\infty \). As the model contains only right-movers, there is no possibility of waves coming in from \( x = +\infty \); hence, this ansatz does not disturb the scattering boundary condition satisfied by \( |\Psi_{\text{in}}\rangle \). Furthermore, this ansatz is chosen so that certain terms that are not of the form we want \( (d^\dagger_{b_2} d^\dagger_{b_1} |0\rangle) \) cancel automatically when we act on it with \( H - k_1 - k_2 \). A straightforward calculation yields:

\[
(H - k_1 - k_2) |\chi_{ek_1a_1ek_2a_2,\text{in}}\rangle = \int dx_1dx_2 \left\{ -i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) - k_1 - k_2 \right\} F^{b_1b_2}_{ek_1a_1ek_2a_2}(x_1,x_2) \times \Theta(0 < x_2 < x_1) \psi^\dagger_{eb_2}(x_2) \psi^\dagger_{eb_1}(x_1) |0\rangle \\
+ \frac{i}{v} \int dx_1 \left[ \left( -i \frac{\partial}{\partial x_1} - k_1 - k_2 + z \right) F^{b_1b_2}_{ek_1a_1ek_2a_2}(x_1,0) \right] \Theta(0 < x_1) d^\dagger_{b_2} \psi^\dagger_{eb_1}(x_1) |0\rangle \\
- \frac{1}{2v^2} \left( -k_1 - k_2 + 2z + U \right) F^{b_1b_2}_{ek_1a_1ek_2a_2}(0,0) d^\dagger_{b_2} d^\dagger_{b_1} |0\rangle. \tag{6.22} \]

To get the desired result \( (H - k_1 - k_2) |\chi_{ek_1a_1ek_2a_2,\text{in}}\rangle = -B^{(\text{red})}_{ek_1a_1ek_2a_2,\text{in}} |0\rangle \), we require that the first three terms of Eq. (6.22) all vanish and that the fourth matches Eq. (6.19b):

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) - k_1 - k_2 \right] F^{b_1b_2}_{ek_1a_1ek_2a_2} = 0, \tag{6.23a} \\
\left( -i \frac{\partial}{\partial x_1} - k_1 - k_2 + z \right) F^{b_1b_2}_{ek_1a_1ek_2a_2}(x_1,0) = 0, \tag{6.23b} \\
F^{b_1b_2}_{ek_1a_1ek_2a_2}(0,0) + F^{b_2b_1}_{ek_1a_1ek_2a_2}(0,0) = 0, \tag{6.23c} \\
(-k_1 - k_2 + 2z + U) F^{b_1b_2}_{ek_1a_1ek_2a_2}(0,0) = U \mathcal{T}(k_1) \mathcal{T}(k_2) F^{b_1b_2}_{-a_1a_2}. \tag{6.23d} \]
A function that meets these requirements is:

\[
P_{ek_1a_1ek_2a_2}(x_1,x_2) = -\mathcal{T}(k_1)\mathcal{T}(k_2)\frac{U}{4\Delta} (k_1 + k_2 - U/2) e^{i(k_1+k_2)x_1} e^{-i(x_1-x_2)} \times P_{a_1a_2}^{b_1b_2} \tag{6.24}
\]

The Schrödinger equation with the boundary condition (of incoming plane waves) can be expected to have a unique solution; hence, this is the answer. As a check, we have repeated the calculation in finite volume with the time-dependent formalism and found exactly this answer in the steady state and infinite volume limit (where the limit is taken pointwise, with factors of \( L \) and the free evolution phase factor removed).

In Eq. (6.24), we see a similar structure as appeared in the IRL solution from the previous chapter: the two electrons are bound together over a distance scale of order \( 1/\Delta \) [compare to Eq. (5.16a)]. Collecting all terms of the wavefunction, we have exact agreement with the two electron non-equilibrium steady state found by Imamura et al. in Ref. [47].

**Digression: the time-evolving wavefunction for two electrons.**

Let us take a short detour to present the time-dependent version of the previous calculation. We verify that the long time limit yields the same non-equilibrium steady state.

We consider the finite volume version of the (even sector, i.e. one lead) Hamiltonian:

\[
H_e = -i \int_{-L/2}^{L/2} dx \left( \psi_{ea}^i(x) \frac{d}{dx} \psi_{ea}(x) + \epsilon_a d_a^\dagger d_a + \left[ v \psi_{ea}^i(0) d_a + \text{h.c.} \right] + U n_{\uparrow} n_{\downarrow} \right). \tag{6.25}
\]

Note that we have allowed the dot energy \( \epsilon_a \) to be spin-dependent, as would occur in the presence of a magnetic field on the dot.

In this digression, we return to using Kronecker normalized operators \( c_{e_ka}^\dagger \). The free time evolution of these operators can be read off from the RLM result, Eq. (3.81a), including
now a spin index (and the spectator “even” label $e$):

$$c_{eka}^\dagger(t) = e^{-iH(0)t}c_{eka}^\dagger e^{iH(0)t}$$

$$= e^{-ikt}c_{eka}^\dagger + \frac{1}{\sqrt{L}} \int dx F_{ka}(t - x) \left[ \Theta(0 < x < t)\psi_{ea}^\dagger(x) + \frac{i}{\sqrt{L}} \delta(x)\Theta(0 < t)d^\dagger_a \right],$$

where: $F_{ka}(t) = -iT_a(k)\left(e^{-ikt} - e^{-iz_a t}\right)$, $T_a(k) = \frac{2\Delta}{k - z_a}$, $z_a = \epsilon_a - i\Delta$.

A short calculation yields the time-dependent $A$ and $B$ operators:

$$A_{eka}(t) \equiv [H, c_{eka}^\dagger(t)] - i\frac{\partial}{\partial t}c_{eka}^\dagger(t)$$

$$= \frac{iU}{\sqrt{Lv}} F_{ka}(t)d_0^\dagger d_b^\dagger = \frac{U}{\sqrt{Lv}} T_a(k)\left(e^{-ikt} - e^{-iz_a t}\right),$$

$$B_{ek_1a_1ek_2a_2}(t) = \{A_{ek_2a_2}(t), c_{ek_1a_1}^\dagger(t)\}$$

$$= -\frac{U}{Lv^2} F_{k_1a_1}(t) F_{k_2a_2}(t)d_{a_2}^\dagger d_{a_1}^\dagger = B_{ek_1a_1ek_2a_2}^{(red)}(t) - B_{ek_2a_2ek_1a_1}^{(red)}(t),$$

where:

$$B_{ek_1a_1ek_2a_2}^{(red)}(t) = \frac{U}{2Lv^2} T_{a_1}(k_1) T_{a_2}(k_2) \left(e^{-ik_1 t} - e^{-iz_{a_1} t}\right) \left(e^{-ik_2 t} - e^{-iz_{a_2} t}\right) P_{-a_1a_2} b_{1}^\dagger b_{2}^\dagger d_{a_1}^\dagger d_{a_2}^\dagger.$$

The time evolution of a single electron does not involve the interaction term $U$ at all, and is simply $e^{-iHt}c_{eka}^\dagger(0) = c_{eca}^\dagger(0)|0\rangle$. We proceed to calculate the time evolution of two electrons:

$$|\Psi_{ek_1a_1ek_2a_2}(t)\rangle = e^{-iHt}c_{eka}^\dagger c_{eka}^\dagger |0\rangle.$$ 

Using the general formalism (or just calculating directly), we see that this problem is solved provided that we can find a state $|\chi_{ek_1a_1ek_2a_2}(t)\rangle$ satisfying:

$$\left(H - i\frac{d}{dt}\right)|\chi_{ek_1a_1ek_2a_2}(t)\rangle = -B_{ek_1a_1ek_2a_2}^{(red)}(t)|0\rangle,$$

$$|\chi_{ek_1a_1ek_2a_2}(t = 0)\rangle = 0,$$

for then we have $|\Psi_{ek_1a_1ek_2a_2}(t)\rangle = c_{ek_2a_2}^\dagger(0)c_{ek_1a_1}^\dagger(0)|0\rangle + |\chi_{ek_1a_1ek_2a_2}(t)\rangle - |\chi_{ek_2a_2ek_1a_1}(t)\rangle$. 


We make the following ansatz:

\[ | \chi_{ek_1a_1ek_2a_2}(t) \rangle = \frac{1}{L} \int dx_1 dx_2 F_{ek_1a_1ek_2a_2}^{b_1b_2}(t,x_1,x_2) \left[ \Theta(0 < x_2 < x_1 < t) \psi_{eb_2}^\dagger(x_2) \psi_{eb_1}^\dagger(x_1) \right. \\
\left. + \frac{i}{v} \delta(x_2) \Theta(0 < x_1 < t) d_{b_2}^\dagger \psi_{eb_2}^\dagger(x_1) \right. \\
\left. - \frac{1}{2} \frac{1}{v^2} \delta(x_1) \delta(x_2) \Theta(0 < t) d_{b_2}^\dagger d_{b_1}^\dagger \right] |0\rangle, \quad (6.31) \]

where \( F \) is a function to be determined. As in the similar-looking ansatz in the IRL [see Eq. (5.16a)], the operator structure is chosen so that certain terms in \( (H - i \frac{\partial}{\partial t}) | \chi_{ek_1a_1ek_2a_2}(t) \rangle \) cancel automatically. To see this, we proceed with the calculation. We find:

\[
\left( H - i \frac{\partial}{\partial t} \right) | \chi_{ek_1a_1ek_2a_2}(t) \rangle = \\
\frac{1}{L} \left\{ -i \int dx_1 dx_2 \left[ \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) F^{b_1b_2}(t,x_1,x_2) \right. \\
\left. \times \Theta(0 < x_2 < x_1 < t) \psi_{eb_2}^\dagger(x_2) \psi_{eb_1}^\dagger(x_1) \right. \\
\left. + \frac{i}{v} \int dx_1 \left[ -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + z_{b_2} \right) F^{b_1b_2}(t,x_1,0) \right] \Theta(0 < x_1 < t) d_{b_2}^\dagger \psi_{eb_1}^\dagger(x_1) \right. \\
\left. + \frac{1}{2} \frac{1}{v^2} \left[ F^{b_1b_2} + F^{b_2b_1} \right] (t,0,0) \Theta(0 < t) d_{b_2}^\dagger d_{b_1}^\dagger \right. \\
\left. - \frac{1}{2} \frac{1}{v^2} \left[ -i \left( \frac{\partial}{\partial t} + (z_{b_1} + z_{b_2} + U) \right) F^{b_1b_2}(t,0,0) \right] \Theta(0 < t) d_{b_2}^\dagger d_{b_1}^\dagger \right. \\
\left. + \frac{i}{2} \frac{1}{v^2} F^{b_1b_2}(0,0,0) \delta(t) d_{b_2}^\dagger d_{b_1}^\dagger \right\} |0\rangle, \quad (6.32) \]

where we have temporarily suppressed the subscripts in \( F_{ek_1a_1ek_2a_2}^{b_1b_2} \) to reduce clutter. Thus, it suffices to find a function \( F \) satisfying:

\[
\left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) F^{b_1b_2}(t,x_1,x_2) = 0, \quad (6.33a) \\
-\left( i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + z_{b_2} \right) \right) F^{b_1b_2}(t,x_1,0) = 0, \quad (6.33b) \\
F^{b_1b_2}(t,0,0) + F^{b_2b_1}(t,0,0) = 0, \quad (6.33c) \\
-\frac{1}{2Lv^2} \left[ \left( -i \left( \frac{\partial}{\partial t} + z_{b_1} + z_{b_2} + U \right) \right) F^{b_1b_2}(t,0,0) \right] = -\frac{U}{2Lv^2} T_{a_1}(k_1) T_{a_2}(k_2) \\
\times \left( e^{-ik_1 t} - e^{-iz_{a_1} t} \right) \left( e^{-ik_2 t} - e^{-iz_{a_2} t} \right) P_{-a_1a_2}^{b_1b_2}, \quad (6.33d) \\
F^{b_1b_2}(0,0,0) = 0. \quad (6.33e) 
\]
Let us start with the case of zero magnetic field \([\epsilon_\uparrow = \epsilon_\downarrow = \epsilon]\), hence \(z_a \equiv z\) and \(T_a(k) \equiv T(k)\).

Writing \(F_{e k_1 a_1 e k_2 a_2}^{b_1 b_2}(t, x_1, x_2) = G_{e k_1 e k_2}(t, x_1, x_2) P_{a_1 a_2}^{b_1 b_2}\), we see that the problem reduces to finding \(G\) satisfying (again suppressing subscripts):

\[
\begin{align*}
\left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) G(t, x_1, x_2) &= 0, \\
\left( -i \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x_1} \right) + z \right) G(t, x_1, 0) &= 0, \\
\left( -i \frac{\partial}{\partial t} + (2z + U) \right) G(t, 0, 0) &= U T(k_1) T(k_2) \left( e^{-ik_1 t} - e^{-i z t} \right) \left( e^{-ik_2 t} - e^{-i z t} \right), \\
G(0, 0, 0) &= 0.
\end{align*}
\]

Before presenting the solution, let us consider a limiting case. Taking \(U \to \infty\) turns the third requirement (6.34c) into:

\[
G(t, 0, 0) = T(k_1) T(k_2) \left( e^{-ik_1 t} - e^{-i z t} \right) \left( e^{-ik_2 t} - e^{-i z t} \right).
\]

The \(U \to \infty\) solution is then found to be:

\[
G(t, x_1, x_2) = T(k_1) T(k_2) \left( e^{-i(k_1 + k_2)(t-x_1)} e^{-iz(x_1-x_2)} - e^{-ik_1(t-x_1)} e^{-iz(t-x_2)} \right.
\]
\[
\left. - e^{-ik_2(t-x_1)} e^{-iz(t-x_2)} + e^{-i z(t-x_1)} e^{-i z(t-x_2)} \right). \quad (6.36)
\]

It is not too difficult to read off this solution from the differential equations. The first requirement (6.34a) means that \(G\) has to be a function of differences only \((t - x_1, t - x_2, x_1 - x_2)\). The second requirement (6.34b) means that \(G(t, x_1, 0)\) can contain either \(e^{-i z t}\) or \(e^{-i z t} e^{i z x_1}\) times any function of the difference \(t - x_1\). One can therefore start from the simplified form (6.35) of the third requirement, expand the product on the right-hand side to yield four terms, and replace each \(t\) by either \(t - x_1\) or \(t - x_2\) as appropriate. The fourth requirement (6.34d) is satisfied without further adjustment; in the finite \(U\) case this requirement leads to additional terms, as we see next.

Let us note here a consistency check: in the limit \(U \to \infty\), double occupancy of the dot should not occur. Collecting all terms of the wavefunction, one indeed finds that the
$d_i^ad_i^b|0\rangle$ part vanishes.\(^2\)

For arbitrary $U$, the function $G$ is found to be:

$$G(t,x_1,x_2) = T(k_1)T(k_2) \left[ \frac{U}{2z + U - k_1 - k_2} e^{-i(k_1+k_2)(t-x_1)} e^{-iz(x_1-x_2)} - \frac{U}{z + U - k_1} e^{-ik_1(t-x_1)} e^{-iz(t-x_2)} - \frac{U}{z + U - k_2} e^{-ik_2(t-x_1)} e^{-iz(t-x_2)} + e^{-iz(t-x_1)} e^{-iz(t-x_2)} \right. $$

$$\left. - \left( \frac{U}{2z + U - k_1 - k_2} - \frac{U}{z + U - k_1} - \frac{U}{z + U - k_2} + 1 \right) e^{-i(z+U)(t-x_1)} e^{-iz(t-x_2)} \right]. \quad (6.37)$$

This can be found in much the same manner as in the $U \to \infty$ case discussed above. The first four terms on the right-hand side of (6.37) are the generalizations of (6.36); the finite $U$ version (6.34c) of the third requirement leads to the $U$-dependent prefactors. These prefactors in turn force us to add the fifth and final term on the right-hand side of (6.37) in order for the fourth condition (6.34d) to be satisfied. [Note that the exponents in this last term are such that they have no effect on the third condition (6.34c).] We see that the first term is still the only important one at large time (at least with respect to the calculation of local operators). The length scale at which the electrons are bound to each other is unchanged; only the prefactor is different, being now of order $\frac{U}{T}$ regardless of whether $\epsilon$ is above or below the Fermi level. We will see that higher crossing states introduce more powers of $\frac{U}{T}$, so that this two particle crossing state is sufficient to describe the $N$-particle solution up to order $\frac{U}{T}$.

The corresponding two electron NESS state (obtained by dropping the transients, removing the overall factor of $\frac{1}{L} e^{-i(k_1+k_2)t}$, and extending the Heaviside function to $t = \infty$) agrees with the NESS state found above.

\(^2\)This follows from noting that $G(t,0,0) = F_{k_1}(t)F_{k_2}(t)$. 
What if we put a magnetic field on the dot – that is, allow $\epsilon_\downarrow$ and $\epsilon_\uparrow$ to vary independently? In this case, we need to solve Eqs. (6.33a)-(6.33e). A similar calculation yields:

$$F_{ek1a1ek2a2}^{bb_1b_2}(t, x_1, x_2) =$$

$$\mathcal{T}_{a1}(k_1)\mathcal{T}_{a2}(k_2)\left[ \frac{U}{z_{a1} + z_{a2} + U - k_1 - k_2} e^{-i(k_1 + k_2)(t-x_1)} e^{-iz_{a2}(x_1 - x_2)} - \frac{U}{z_{a1} + k_1} e^{-i(z_{a1} + z_{a2} + k_1)(t-x_1)} e^{-iz_{a2}(t-x_2)} - \frac{U}{z_{a2} + U - k_2} e^{-i(z_{a2} - z_{a1} + k_2)(t-x_1)} e^{-iz_{a2}(t-x_2)} - \frac{U}{z_{a1} + U - k_1} - \frac{U}{z_{a2} + U - k_2} + 1 \right] e^{-i(z_{a1} + U)(t-x_1)} e^{-iz_{a2}(t-x_2)} \mathcal{P}_{-a1a2}^{bb_1b_2}. \quad (6.38)$$

6.2.2 Infinite $U$: full wavefunction

We return to the time-independent problem, and proceed next to calculate the $n = 2$ crossing state in the model (6.7) that has infinite $U$ directly. The result agrees with taking $U \to \infty$ in the previous calculation. This serves as a starting point for calculating all the crossing states in the infinite $U$ case.

Our task is to find a crossing state $|\chi_{ek1a1ek2a2,\text{in}}\rangle$ that has no incoming plane waves and that satisfies:

$$(H - k_1 - k_2)|\chi_{ek1a1ek2a2,\text{in}}\rangle = -B^{(\text{red})}_{ek1a1ek2a2,\text{in}} b_1^\dagger |0\rangle \quad (6.39a)$$

$$= \frac{1}{v} \mathcal{T}(k_1)\mathcal{T}(k_2) \mathcal{P}_{-a1a2}^{bb_1b_2} d_{b_2}^\dagger \psi_{eb_1}^\dagger(0)|0\rangle. \quad (6.39b)$$

We make the ansatz:

$$|\chi_{ek1a1ek2a2,\text{in}}\rangle = \int dx_1 dx_2 F_{ek1a1ek2a2}^{bb_1b_2}(x_1, x_2) \left[ \Theta(0 < x_2 < x_1)\psi_{eb_2}^\dagger(x_2) + i \frac{\delta(x_2)}{v} \Theta(0 < x_1) d_{b_2}^\dagger b_1^\dagger \psi_{eb_1}^\dagger(x_1) b^\dagger |0\rangle, \quad (6.40)\right.$$

where the function $F_{ek1a1ek2a2}$ is determined shortly. As in the finite $U$ case, this ansatz is chosen so that it has no incoming plane waves, and so that certain terms that are not of the
form we want get cancelled automatically in the calculation that follows. A straightforward calculation yields:

\[
(H - k_1 - k_2) |\chi_{ek_1a_1ek_2a_2, in}\rangle = \\
\int dx_1 dx_2 \left\{ \left[ -i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) - k_1 - k_2 \right] F_{ek_1a_1ek_2a_2}^{b_1b_2}(x_1, x_2) \right\} \\
\times \Theta(0 < x_2 < x_1) \psi_{e_{b_2}}^\dagger (x_2) \psi_{e_{b_1}}^\dagger (x_1) b^\dagger |0\rangle \\
+ \frac{i}{v} \int dx_1 \left[ \left(-i \frac{\partial}{\partial x_1} - k_1 - k_2 + z \right) F_{ek_1a_1ek_2a_2}^{b_1b_2}(x_1, 0) \right] \Theta(0 < x_1) d_{a_2}^\dagger \psi_{e_{b_1}}^\dagger (x_1) |0\rangle \\
+ \frac{1}{v} F_{ek_1a_1ek_2a_2}(0, 0) d_{a_2}^\dagger \psi_{e_{b_1}}^\dagger (0) |0\rangle. \tag{6.41}
\]

To get the desired result \( (H - k_1 - k_2) |\chi_{ek_1a_1ek_2a_2, in}\rangle = -B_{ek_1a_1ek_2a_2, in}^{(red)} |0\rangle \), we impose conditions on \( F_{ek_1a_1ek_2a_2} \) so that the first two terms of Eq. (6.41) all vanish and the third matches Eq. (6.39b). In particular, it suffices to require:

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) - k_1 - k_2 \right] F_{ek_1a_1ek_2a_2}^{b_1b_2} = 0, \tag{6.42a}
\]

\[
\left(-i \frac{\partial}{\partial x_1} - k_1 - k_2 + z \right) F_{ek_1a_1ek_2a_2}^{b_1b_2}(x_1, 0), \tag{6.42b}
\]

\[
F_{ek_1a_1ek_2a_2}^{b_1b_2}(0, 0) = T(k_1) T(k_2) P_{-a_1a_2}^{b_1b_2}. \tag{6.42c}
\]

The solution is:

\[
F_{ek_1a_1ek_2a_2}^{b_1b_2}(x_1, x_2) = T(k_1) T(k_2) e^{i(k_1+k_2)x_1} e^{-iz(x_1-x_2)} P_{-a_1a_2}^{b_1b_2}. \tag{6.43}
\]

As a check, we note that \( F_{ek_1a_1ek_2a_2}^{b_1b_2} \) agrees with the \( U \to \infty \) limit of the corresponding function in the finite \( U \) case [Eq. (6.24)]. (The full \( N = 2 \) wavefunctions then agree in the limit.)

\[n = 3\] crossing state.

The next inverse problem is to find a crossing state that has no incoming plane waves and that satisfies:

\[
(H - k_1 - k_2 - k_3) |\chi_{ek_1a_1ek_2a_2ek_3a_3, in}\rangle = -A_{ek_3a_3, in} |\chi_{ek_1a_1ek_2a_2, in}\rangle \tag{6.44a}
\]

\[
= \frac{2i}{v} T(k_3) \int dx_1 F_{ek_1a_1ek_2a_2}^{b_1c_1}(x_1, 0) \Theta(0 < x_1) P_{-c_1a_3}^{b_2b_3} d_{e_{b_2}}^\dagger \psi_{e_{b_1}}^\dagger (x_1) |0\rangle. \tag{6.44b}
\]
We extend the ansatz (6.40) to $n = 3$:

$$\chi_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3},in} = \int dx_{1}dx_{2}dx_{3} F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}b_{3}}(x_{1},x_{2},x_{3}) \left[ \Theta(0 < x_{3} < x_{2} < x_{1}) \psi_{eb_{3}}^{\dagger}(x_{3}) \right.$$  

$$+ \frac{i}{v} \delta(x_{3}) \Theta(0 < x_{2} < x_{1}) d_{b_{1}}^{\dagger} b \left. \psi_{eb_{2}}^{\dagger}(x_{2}) \psi_{eb_{1}}^{\dagger}(x_{1}) \right] b^{\dagger}|0\rangle. \quad (6.45)$$

To ensure the cancellation of certain unwanted terms, we require:

$$\left[ -i \left( \frac{\partial}{\partial x_{1}} + \frac{\partial}{\partial x_{2}} + \frac{\partial}{\partial x_{3}} \right) - k_{1} - k_{2} - k_{3} \right] F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}b_{3}}(x_{1},x_{2},x_{3}) = 0, \quad (6.46a)$$

$$\left[ -i \left( \frac{\partial}{\partial x_{1}} + \frac{\partial}{\partial x_{2}} \right) - k_{1} - k_{2} - k_{3} + z \right] F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}b_{3}}(x_{1},x_{2},0) = 0. \quad (6.46b)$$

Under these conditions, we obtain (see the general $n$ calculation below for more detail):

$$(H - k_{1} - k_{2} - k_{3}) \chi_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3},in} = \frac{1}{v} \int dx_{1} F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}b_{3}}(x_{1},0,0) d_{b_{1}}^{\dagger} \psi_{eb_{2}}(0)$$

$$\times \psi_{eb_{3}}^{\dagger}(x_{1})|0\rangle. \quad (6.47)$$

Comparing to Eq. (6.44b), we see that we must also require:

$$F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}b_{3}}(x_{1},0,0) = 2i T(k_{3}) F_{ek_{1}a_{1}ek_{2}a_{2}}^{b_{1}c_{1}}(x_{1},0) P_{-c_{1}a_{3}} b_{2} b_{3}, \quad (6.48)$$

The solution re-uses the same function that appeared in the $n = 2$ case:

$$F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}b_{3}}(x_{1},x_{2},x_{3}) = 2i T(k_{3}) F_{ek_{1}a_{1}ek_{2}a_{2}}^{b_{1}c_{1}}(x_{1},x_{3}) e^{ik_{3}x_{2}} P_{-c_{1}a_{3}} b_{2} b_{3}, \quad (6.49a)$$

$$= 2i T(k_{1}) T(k_{2}) T(k_{3}) e^{i(k_{1}+k_{2})x_{1}} e^{ik_{3}x_{2}} P_{-a_{1}a_{2}} P_{-c_{1}a_{3}} b_{2} b_{3} e^{-iz(x_{1}-x_{2})}. \quad (6.49b)$$

$n = 4$ crossing state.

Here there are two inverse problems to solve, corresponding to the two partitions $(1,2,3,4)$ and $(1,2,3,4)$:

$$(H - k_{1} - k_{2} - k_{3} - k_{4}) \chi_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}ek_{4}a_{4},in} = -A_{ek_{4}a_{4}in} \chi_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3},in} \quad (6.50a)$$

$$= \frac{2i}{u} T(k_{4}) \int dx_{1}dx_{2} F_{ek_{1}a_{1}ek_{2}a_{2}ek_{3}a_{3}}^{b_{1}b_{2}c_{2}}(x_{1},x_{2},0) \Theta(0 < x_{2} < x_{1}) P_{-c_{2}a_{4}} d_{b_{4}}^{\dagger} \psi_{eb_{3}}^{\dagger}(0)$$

$$\times \psi_{eb_{2}}^{\dagger}(x_{2}) \psi_{eb_{1}}^{\dagger}(x_{1})|0\rangle, \quad (6.50b)$$
and:

\[
(H - k_1 - k_2 - k_3 - k_4)|\chi_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4,\text{in}}\rangle = -B^{(\text{red})}_{ek_3a_3ek_4a_4,\text{in}} b_1^\dagger |0\rangle \tag{6.51a}
\]

\[
= \frac{1}{v} \mathcal{T}(k_3) \mathcal{T}(k_4) \int dx_1 dx_2 F^{b_1b_2}_{ek_1a_1ek_2a_2} P_{-a_3a_4} \Theta(0 < x_2 < x_1) d_{b_4}^\dagger \psi^\dagger_{eb_3}(0) \psi^\dagger_{eb_2}(x_2)
\]

\[
\times \psi^\dagger_{eb_1}(x_1)|0\rangle. \tag{6.51b}
\]

We extend the same ansatz (6.45) to \(n = 4\):

\[
|\chi_{4,\text{in}}\rangle = \int dx_1 dx_2 dx_3 dx_4 F^4_{b_1b_2b_3b_4}(x_1, x_2, x_3, x_4) \left[ \Theta(0 < x_4 < x_3 < x_2 < x_1) \psi^\dagger_{eb_4}(x_4)
\right.
\]

\[
+ \frac{i}{v} \delta(x_4) \Theta(0 < x_3 < x_2 < x_1) d_{b_3}^\dagger b_4 |0\rangle, \tag{6.52}
\]

where \(|\chi_{4,\text{in}}\rangle\) stands for either \(|\chi_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4,\text{in}}\rangle\) or \(|\chi_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4,\text{in}}\rangle\), corresponding to \(F^4_{b_1b_2b_3b_4}\) standing for \(F^{b_1b_2b_3b_4}_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4}\) or \(F^{b_1b_2b_3b_4}_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4}\). In order to cancel unwanted terms, we require each \(F_4\) to satisfy:

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3} + \frac{\partial}{\partial x_4} \right) - k_1 - k_2 - k_3 - k_4 \right] F^b_{b_1b_2b_3b_4}(x_1, x_2, x_3, x_4) = 0, \tag{6.53a}
\]

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3} \right) - k_1 - k_2 - k_3 - k_4 + z \right] F^b_{b_1b_2b_3b_4}(x_1, x_2, x_3, 0) = 0. \tag{6.53b}
\]

Under these conditions, we obtain (see the general \(n\) calculation below for more detail):

\[
(H - k_1 - k_2 - k_3 - k_4)|\chi_{4,\text{in}}\rangle = \frac{1}{v} \int dx_1 dx_2 F^b_{b_1b_2b_3b_4}(x_1, x_2, 0, 0) \Theta(0 < x_2 < x_1)
\]

\[
\times d_{b_4}^\dagger \psi^\dagger_{eb_3}(0) \psi^\dagger_{eb_2}(x_2) \psi^\dagger_{eb_1}(x_1)|0\rangle. \tag{6.54}
\]

Thus, Eqs. (6.50b) and (6.51b) hold provided that:

\[
F^{b_1b_2b_3b_4}_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4}(x_1, x_2, 0, 0) = 2i \mathcal{T}(k_4) F^{b_1b_2}_{ek_1a_1ek_2a_2} P_{b_3b_4}, \tag{6.55a}
\]

\[
F^{b_1b_2b_3b_4}_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4}(x_1, x_2, 0, 0) = \mathcal{T}(k_3) \mathcal{T}(k_4) F^{b_1b_2}_{ek_1a_1ek_2a_2}(x_1, x_2) P_{b_3b_4} \tag{6.55b}
\]
The solutions are:

\[
F_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4}(x_1, x_2, x_3, x_4) = 2iT(k_4)e^{ik_4x_3}F_{ek_1a_1ek_2a_2ek_3a_3}(x_1, x_2, x_4)P_{-c_2a_3}
\]

\[
= (2i)^2T(k_1)T(k_2)T(k_3)T(k_4)e^{i(k_1+k_2)x_1}e^{ik_3x_2}e^{ik_4x_4}P_{-a_1a_2}P_{-a_3a_4}e^{-iz(x_1-x_4)},
\]

and:

\[
F_{ek_1a_1ek_2a_2ek_3a_3ek_4a_4}(x_1, x_2, x_3, x_4) = F_{ek_1a_1ek_2a_2}(x_1, x_2)F_{ek_3a_3ek_4a_4}(x_3, x_4).
\]

Crossing states for general \( n \)

The above cases are enough to show the general pattern, which we describe first before proving in detail. The ansatz for the crossing state [Eq. (6.40), (6.45), and (6.52)] extends to general \( n \) straightforwardly. The function \( F_{ek_1a_1} \), with \( k_1 \) being a partition of \( n = (1, \ldots, n) \), is a product over cells of a single function \( F_{ek_1a_1}(x) \), where \( \ell = (1, \ldots, \ell) \) is a list representing the quantum numbers of a single cell. A \( B_{in}^{(red)} \) operator adds a new cell [as in Eq. (6.57a)], while an \( A_{in} \) operator increases the cell length by 1. The single-celled function has already been constructed for \( \ell = 2, 3, \) and \( 4 \) [Eqs. (6.43), (6.49b), and (6.56b)], and is given in general by:

\[
F_{ek_1a_1}(x) = (2i)^{\ell-1}\delta_{c_1}^{\ell-1}T(k_1)e^{ik_1x_1}\left[\prod_{m=2}^{\ell}T(k_m)P_{-c_{m-1}a_m}e^{ik_mx_{m-1}}\right]e^{-iz(x_1-x_{\ell})}.
\]

Note that the spin matrices multiply in the same diagonal manner as in the Kondo solution (chapter 4). Note also that we have a factor of \( e^{-iz(x_1-x_{\ell})} \), indicating electrons bound together on a distance scale \( 1/\Delta \). The single-celled function describes \( \ell \) electrons bound together, and the full function with a general partition has some number of these cells.

We now present the formal proof. We make the following ansatz for the \( n \)-electron
crossing state (where $p$ is a given partition of $n$):

$$\left| \chi_{ekpap, in} \right| = \int dx_n F_{ekpap}^{bn}(x_n) \left[ \Theta(0 < x_n < \cdots < x_1) \psi_{ebn}^\dagger(x_n) \right. $$

$$+ \frac{i}{\nu} \delta(x_n) \Theta(0 < x_{n-1} < \cdots < x_1) d_{bn}^\dagger b \left. \psi_{ebn-2}^\dagger(x_{n-2}) b^\dagger \right| 0 \rangle, \quad (6.59)$$

where $F$ is to be determined. By construction, the wavefunction vanishes to the left of the origin; hence, there are no incoming plane waves, so these states satisfy the required boundary condition. What remains to be shown is that for any partition $p$ whose last cell has length $q$, we have:

$$\left( H - \sum_{\ell=1}^{n} k_{\ell} \right) \left| \chi_{ekap, in} \right| = \begin{cases} -A_{ekn, in} \left| \chi_{ekp/nap, in} \right| & q \geq 3 \\ -B_{ekn-1, in} \left| \chi_{ekp/(n-1)a, in} \right| & q = 2 \end{cases} \quad (6.60)$$

Computing the right-hand side, we obtain:

$$-B_{ekn-1, in} \left| \chi_{ekp/(n-1)a, in} \right| = \frac{1}{\nu} T(k_{n-1}) T(k_n)$$

$$\times \int dx_{n-2} F_{ekp/(n-1)a}^{bn-2}(x_{n-2}) P_{a_{n-1}a_n}^{bn-1bn} \Theta(0 < x_{n-2} < \cdots < x_1)$$

$$\times d_{bn}^\dagger \psi_{ebn-2}^\dagger (0) \psi_{ebn-2}^\dagger (x_{n-2}) |0 \rangle, \quad (6.61)$$

and:

$$-A_{ekn, in} \left| \chi_{ekp/nap, in} \right| = \frac{1}{\nu} 2i T(k_n) \int dx_{n-2} F_{ekp/n}^{bn-2c}(x_{n-2}, 0) P_{c a_n}^{bn-1bn}$$

$$\times \Theta(0 < x_{n-2} < \cdots < x_1) d_{bn}^\dagger \psi_{ebn-1}^\dagger (0) \psi_{ebn-2}^\dagger (x_{n-2}) |0 \rangle. \quad (6.62)$$
For the left-hand side of (6.60), we obtain:

\[
\left(H - \sum_{m=1}^{n} k_m \right) |\chi_{ekp_{ap,m}}\rangle = \int dx_n \left\{ \left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_n} \right) - \sum_{m=1}^{n} k_m \right] F_{ekp_{ap,m}}^{bn}(x_n) \right\} \\
\times \Theta(0 < x_n < \cdots < x_1)\psi_{ebn}^{\dagger}(x_n)b^{\dagger}|0\rangle \\
+ \frac{i}{v} \int dx_{n-1} \left\{ \left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_{n-1}} \right) - \sum_{m=1}^{n} k_m + z \right] F_{ekp_{ap}}^{bn}(x_{n-1}, 0) \right\} \\
\times \Theta(0 < x_{n-1} < \cdots < x_1)d_{bn}^{\dagger}\psi_{ebn-1}^{\dagger}(x_{n-1})|0\rangle \\
+ \frac{1}{v} \int dx_{n-2} F_{ekp_{ap}}^{bn}(x_{n-2}, 0, 0) \Theta(0 < x_{n-2} < \cdots < x_1)d_{bn}^{\dagger}\psi_{ebn-1}^{\dagger}(0)\psi_{ebn-2}^{\dagger}(x_{n-2})|0\rangle.
\]

(6.63)

Comparing, we see that the crossing state condition (6.60) holds provided that \( F \) satisfies the following conditions:

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_n} \right) - \sum_{m=1}^{n} k_m \right] F_{ekp_{ap}}^{bn}(x_n) = 0, \quad \text{(6.64a)}
\]

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_{n-1}} \right) - \sum_{m=1}^{n} k_m + z \right] F_{ekp_{ap}}^{bn}(x_{n-1}, 0) = 0, \quad \text{(6.64b)}
\]

\[
F_{ekp_{ap}}^{bn}(x_{n-2}, 0, 0) = \begin{cases} 
\mathcal{T}(k_{n-1})\mathcal{T}(k_n)F_{ekp_{ap}}^{bn}(x_{n-2})P_{e_{n-1}a_n}^{b_{n-1}b_n} & q = 2 \\
2i\mathcal{T}(k_n)F_{ekp_{ap}}^{bn}(x_{n-2}, 0)P_{c_{a_n}}^{b_{n-1}b_n} & q \geq 3
\end{cases} \quad \text{(6.64c)}
\]

We take as an ansatz that \( F_{ekp_{ap}}^{bn} \) separates into a product over cells. That is, we write \( p = (p(1), \ldots, p(s)) \), where \( s \) is the number of cells in \( p \) and each \( p(j) \) is a list. The full function \( F_{ekp_{ap}}^{bn} \) will be built from a “single-celled” function \( F_{ekp_{ae}}^{bn} \), called such because its quantum numbers are in a simple list \( \ell = (1, \ldots, \ell) \) (with \( \ell \geq 2 \)) rather than a partition.

We write:

\[
F_{ekp_{ap}}^{bn}(x_n) = \prod_{j=1}^{s} F_{ekp_{ae}}^{bn}(x_{p(j)}), \quad \text{(6.65)}
\]

where the single-celled function \( F_{ekp_{ae}}(x_{\ell}) \) is to be determined shortly. The problem now
reduces to showing certain properties of the single-celled function. For instance, we have:

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_n} \right) - \sum_{m=1}^{n} k_m \right] F_{e k p a p}^b (x_n) = \sum_{j'=1}^{s} \prod_{j=1, j \neq j'}^{s} F_{e k_{p(j)} a_{p(j)}}^b (x_{p(j)}) \\
\times \sum_{m \in p(j')} \left( -i \frac{\partial}{\partial x_m} - k_m \right) F_{e k_{p(j')} a_{p(j')}}^b (x_{p(j')}). \tag{6.66}
\]

Thus, the first requirement, Eq. (6.64a), holds for a general partition provided that it holds for a single cell. A similar calculation shows that the same is true for the second requirement, Eq. (6.64b). In the third requirement, Eq. (6.64c), the first \( n - 2 \) coordinates contribute the same constant factor on both sides, which factors out. All together, we find that the single-celled function must satisfy:

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_\ell} \right) - \sum_{m=1}^{\ell} k_m \right] F_{e k_{\ell a \ell}}^b (x_{\ell}) = 0, \tag{6.67a}
\]

\[
\left[ -i \left( \frac{\partial}{\partial x_1} + \cdots + \frac{\partial}{\partial x_{\ell-1}} \right) - \sum_{m=1}^{\ell} k_m + z \right] F_{e k_{\ell a \ell}}^b (x_{\ell-1}, 0) = 0, \tag{6.67b}
\]

\[
F_{e k_{\ell a \ell}}^b (x_{\ell-2}, 0, 0) = \begin{cases} 
T(k_1)T(k_2)P_{-a_1 a_2}^{b_1 b_2} & \ell = 2 \\
2iT(k_\ell)F_{e k_{\ell j a_{\ell j}}}^{b_{\ell-2}c} (x_{\ell-2}, 0)P_{-c a_\ell}^{b_{\ell-1} b_\ell} & \ell \geq 3 
\end{cases} \tag{6.67c}
\]

In the last equation, we have relabelled the quantum numbers that were originally the last cell \( (n - q + 1, \ldots, n) \) to \( \ell = (1, \ldots, \ell) \). The solution is the function stated earlier in Eq. (6.58).

The exact scattering “in” wavefunction of the infinite-\( U \) multi-lead Anderson model (6.6), with any \( N \) quantum numbers, is thus defined by Eqs. (6.58), (6.65), (6.59), (6.11), and (6.10).

### 6.3 Electric current

#### 6.3.1 Setup

We consider the two lead model, \( N_{\text{leads}} = 2 \). We formulate the calculation for the finite \( U \) Hamiltonian (6.1), then specialize to either small \( U \) (first order) or infinite \( U \) with small
The latter case can also be done using the wavefunction for the infinite $U$ Hamiltonian (6.6).

The wavefunction we need is in the non-equilibrium steady state $|\Psi_{\text{in}}\rangle \equiv |\Psi_{\gamma_{N}k_{N}a_{N,\text{in}}}\rangle$ given by Eq. (6.4), with the quantum numbers $\gamma_{N}k_{N}a_{N}$ later specialized to describe two filled Fermi seas. (As usual, we do the calculation at zero temperature, then generalize to allow the lead temperatures to be arbitrary.) Our task is to evaluate the expectation value of the current operator in this state. We keep only the first crossing state in the wavefunction, which restricts the calculation to particular regimes.

The setup of this calculation is essentially the same as in the two lead RLM calculation, now with a spin index and with a more complicated “in” state. We summarize the main equations here; see Sec. 3.3.3 for more detail. The symmetrized current operator is:

$$\hat{I}_{\text{Sym}} = \frac{i}{2\sqrt{2}} v \left( \psi_{1a}^\dagger(0) - \psi_{2a}^\dagger(0) \right) d_a + \text{h.c.} \quad (6.68)$$

We wish to evaluate the expectation value of the current directly in the steady state:

$$\langle \hat{I}_{\text{Sym}} \rangle \equiv \frac{\langle \Psi_{\text{in}}|\hat{I}_{\text{Sym}}|\Psi_{\text{in}}\rangle}{\langle \Psi|\Psi \rangle}, \quad (6.69)$$

where $|\Psi\rangle = c_{\gamma_{N}k_{N}a_{N}}^\dagger|0\rangle$ is the free state encoding the incoming plane waves in Eq. (6.4). To write the numerator in terms of an overlap, we consider the following $\bar{\phi}$-dependent Hamiltonian:

$$\bar{H} = H + \left[ \frac{v}{\sqrt{2}} \left( e^{i\frac{1}{2}\bar{\phi}} - 1 \right) \psi_{1a}^\dagger(0)d_a + \frac{v}{\sqrt{2}} \left( e^{-i\frac{1}{2}\bar{\phi}} - 1 \right) \psi_{2a}^\dagger(0)d_a + \text{h.c.} \right]. \quad (6.70)$$

Then we can write the expectation value of $\hat{I}_{\text{Sym}}$ (in any eigenstate $|\Psi(E)\rangle$ of the original $H$ with energy $E$) in terms of an overlap; the derivative formula (2.191) yields:

$$\langle \Psi(E)|\hat{I}_{\text{Sym}}|\Psi(E)\rangle = \lim_{E'\to E} \left( E - E' \right) \frac{\partial}{\partial \bar{\phi}} \bigg|_{\bar{\phi}=\phi} \langle \Psi(E')|\Psi(E)\rangle. \quad (6.71)$$

We define the usual set of $\bar{\phi}$-dependent fields [Eqs. (3.55) and (3.60a), now with a spin index]:

$$\begin{pmatrix} c_{0ka} \\ c_{1ka} \\ c_{2ka} \end{pmatrix} \equiv \mathcal{U} \begin{pmatrix} \bar{c}_{oka} \\ \bar{c}_{1ka} \\ \bar{c}_{2ka} \end{pmatrix}, \quad \begin{pmatrix} \bar{c}_{1ka} \\ \bar{c}_{2ka} \end{pmatrix} \equiv \mathcal{U}^\dagger \begin{pmatrix} c_{oka} \\ c_{eka} \end{pmatrix}, \quad \mathcal{U} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\frac{1}{2}\bar{\phi}} & -e^{i\frac{1}{2}\bar{\phi}} \\ e^{i\frac{1}{2}\bar{\phi}} & e^{-i\frac{1}{2}\bar{\phi}} \end{pmatrix}. \quad (6.72)$$
with corresponding fields in position space \( \overline{\psi}_{\gamma a}^\dagger(x) = \int \frac{dk}{2\pi} e^{-ikx} \tau_{\gamma ka} \) (\( \gamma = 1, 2, o, \) or \( e \)). Then we have:

\[
\mathcal{H} = -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1}^2 \overline{\psi}_{\gamma a}^\dagger(x) \frac{d}{dx} \psi_{\gamma a}(x) + c d^a d^\dagger_a + \left[ \frac{\psi}{\sqrt{2}} \sum_{\gamma=1}^2 \overline{\psi}_{\gamma a}(0) d^a + \text{h.c.} \right] + U n^a n^a, \quad (6.73)
\]

which is the same Hamiltonian already considered (6.1), with each unbarred electron field replaced by the corresponding barred field. We know the “in” states of this Hamiltonian (for small or large \( U \)) provided that the incoming plane waves are in the barred basis. Hence, it is convenient to let the \( \bar{\phi} \)-dependent family of eigenstates states be scattering states defined in the same way as in Eq. (6.4) (now with the barred Hamiltonian):

\[
|\Psi(E)\rangle \equiv |\Psi_{\text{in}}\rangle = |\Psi\rangle + \frac{1}{E - \hbar + i\eta} \nabla |\Psi\rangle, \quad (6.74)
\]

where \( |\Psi\rangle = \overline{\tau}_{\gamma N a a N}^\dagger |0\rangle \). By construction, these states satisfy the required condition, namely they reduce to the original state of interest \( |\Psi_{\text{in}}\rangle \) at \( \bar{\phi} = 0 \).

We write \( |\Psi_{\text{in}}\rangle \) for same Lippmann-Schwinger state \( |\Psi_{\text{in}}\rangle \) with momenta \( k_1, \ldots, k_N \) replaced by \( k'_1, \ldots, k'_N \). Then the energy \( E' = \sum_{j=1}^N k'_j \) varies continuously, so we can write \( \langle \Psi(E') \rangle = \langle \Psi_{\text{in}} \rangle \) in Eq. (6.71) to find:

\[
\langle \Psi_{\text{in}} | \hat{I}_{\text{Sym}} | \Psi_{\text{in}} \rangle = \lim_{\text{all } k'_j \to k_j} \left( E - E' \right) \frac{\partial}{\partial \bar{\phi}} \bigg|_{\bar{\phi} = 0} \langle \Psi_{\text{in}} | \Psi_{\text{in}} \rangle. \quad (6.75)
\]

Thus, the calculation reduces to finding the overlap \( \langle \Psi_{\text{in}}' | \overline{\Psi}_{\text{in}} \rangle \) for \( \bar{\phi} \) near 0 and \( E' \) near \( E \).

### 6.3.2 Evaluation with first crossing state

We evaluate the right-hand side of Eq. (6.75) with the wavefunction truncated so that only the first crossing state is kept – that is, \( |\Psi_{\text{in}}\rangle = |\overline{\Psi}_{\text{in}}^0\rangle + |\overline{\Psi}_{\text{in}}^2\rangle \) and \( \langle \Psi' \rangle = \langle \Psi^0 \rangle + \langle \Psi^2 \rangle \).

We work to first order in the crossing, i.e.:

\[
\langle \hat{I}_{\text{Sym}} \rangle = \langle \hat{I}_{\text{Sym}} \rangle^{(0,0)} + \langle \hat{I}_{\text{Sym}} \rangle^{(0,2)} + \langle \hat{I}_{\text{Sym}} \rangle^{(2,0)}, \quad (6.76)
\]

where:

\[
\langle \hat{I}_{\text{Sym}} \rangle^{(\ell_1, \ell_2)} = \left[ \langle \Psi | \Psi \rangle \right]^{-1} \lim_{\text{all } k'_j \to k_j} \left( E - E' \right) \frac{\partial}{\partial \bar{\phi}} \bigg|_{\bar{\phi} = 0} \langle \Psi_{\text{in}}^{\ell_1} | \overline{\Psi}_{\text{in}}^{\ell_2} \rangle. \quad (6.77)
\]
The term \( \langle \hat{I}_{\text{Sym}} \rangle^{(2,2)} \) is not kept as it involves two crossings. We will see below that in the small \( U \) regime, expanding in crossings amounts to expanding in \( U \), and our calculation is to first order. For \( U \to \infty \), the expansion in crossings appears to be an expansion in powers of \( \Delta \).

The terms of the wavefunction that we need are:

\[
|\Psi_\text{in}^0\rangle = c^\dagger_{N_k N_a N, \text{in}} |0\rangle, \quad (6.78)
\]

and:

\[
|\Psi_{\text{in}}^2\rangle = \frac{1}{2} \sum_{m \in \mathcal{L}_2(N)} (\text{sgn } m) c^\dagger_{N/m N/m a N/m, \text{in}} |\Phi_{km am, \text{in}}\rangle, \quad (6.79a)
\]

where:

\[
|\Phi_{ek_1 a_1 ek_2 a_2, \text{in}}\rangle = \langle \bar{x}_{ek_1 a_1 ek_2 a_2, \text{in}} - |x_{ek_2 a_2 ek_1 a_1, \text{in}}\rangle. \quad (6.79b)
\]

(We can take the adjoint and relabel each \( k_j \to k'_j \) to get \( |\Psi'_{\text{in}}\rangle = |\Psi_{\text{in}}^0\rangle + |\Psi_{\text{in}}^2\rangle \). Let us recall the explicit form of the unsymmetrized crossing state [Eq. (6.21), now with barred fields]:

\[
|\bar{x}_{ek_2 a_2 ek_1 a_1, \text{in}}\rangle = \int dx_1 dx_2 F_{b_1 b_2}^{j_1 j_2}(x_1, x_2) \left[ \Theta(0 < x_2 < x_1) \bar{\psi}_{eb_2}(x_2) \bar{\psi}_{eb_1}(x_1) + \frac{i}{v} \delta(x_2) \Theta(0 < x_1) d^\dagger_{b_2} \psi_{eb_1}(x_1) - \frac{1}{2v^2} \delta(x_1) \delta(x_2) d^\dagger_{b_2} d^\dagger_{b_1} \right] |0\rangle, \quad (6.80)
\]

where the function \( F \) is given in Eq. (6.24).

The first contribution to the current, involving only the scattering operators and no crossings, just yields twice the RLM answer (one for each spin; see Sec. 3.3.3 for the RLM calculation):

\[
\langle \hat{I}_{\text{Sym}} \rangle^{(0,0)} = \frac{1}{2\pi \delta(0)} \sum_{j=1}^{N} (-1)^{\gamma_j - 1} \delta_{\alpha_j \alpha_j} \frac{|T(k_j)|^2}{4} \quad (6.81a)
\]

\[
= \frac{1}{2\pi \delta(0)} \sum_{\gamma=1,2} \sum_{k \in \mathcal{K}_\gamma} \sum_{a} (-1)^{\gamma - 1} \frac{|T(k)|^2}{4} \quad \text{(setting } \gamma_k a \text{ = Fermi seas)} \quad (6.81b)
\]

\[
\lim_{\text{therm. limit}} \int_{-D}^{D} \frac{dk}{2\pi} [f_1(k) - f_2(k)] \frac{|T(k)|^2}{2} \quad \text{[recall (3.115)].} \quad (6.81c)
\]
We proceed to calculate the contribution from the first crossing. We only need to calculate \( \langle \tilde{I}_{\text{Sym}} \rangle^{(0,2)} \), since the calculation below will show that \( \langle \tilde{I}_{\text{Sym}} \rangle^{(2,0)} \) is the complex conjugate.

The calculation reduces to the evaluation of the following overlap:

\[
\Omega_{(0,2)}^{(0)}[\gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] \equiv \langle 0 | c_{\gamma_1 a_1}^* c_{\gamma_2 a_2} | \Phi_{ek_1 e k_2 a_2} \rangle. \tag{6.82}
\]

In the overlap \( \langle \Psi | \Phi \rangle \) that appears in \( \langle \tilde{I}_{\text{Sym}} \rangle^{(0,2)} \), we must contract the \( c_{\gamma N/m N a_N/m}^* \) operators with the \( c_{\gamma N/m N a_N/m}^* \) operators (which cancels the sign factor \( \text{sgn} \, m \)). This produces a factor of \( [2 \pi \delta(0)]^{N-2} \) which is mostly cancelled by the normalization factor \( \langle \Psi | \Psi \rangle = [2 \pi \delta(0)]^N \), leaving:

\[
\langle \tilde{I}_{\text{Sym}} \rangle^{(0,2)} = [2 \pi \delta(0)]^{-2} \sum_{m_1, m_2 = 1}^N \left( k_{m_1} + k_{m_2} - k'_{m_1} - k'_{m_2} \right) \times \frac{\partial}{\partial \phi} \bigg |_{\phi = 0} \Omega_{(0,2)}^{(0)}[\gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2], \tag{6.83}
\]

where we have used the antisymmetry of the operators and crossing state to replace the original sum over \( m_1 < m_2 \) with an unrestricted sum with an extra factor of \( 1/2 \).

Again by antisymmetry, the overlap \( \Omega_{(0,2)}^{(0)} \) can be written as the antisymmetrization of some “reduced” overlap \( \Omega_{(0,2)}^{(\text{red})} \):

\[
\Omega_{(0,2)}^{(0)}[\gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] = \sum_{\sigma, \sigma' \in \text{Sym}(2)} (\text{sgn} \, \sigma)(\text{sgn} \, \sigma') \times \Omega_{(0,2)}^{(\text{red})}[\gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2], \tag{6.84}
\]

where \( \Omega_{(0,2)}^{(\text{red})} \) is only defined modulo antisymmetrization. To specialize the quantum numbers \( \gamma N k_N a_N \) to the case of two filled Fermi seas, we replace the sums over quantum numbers via \( \sum_{m=1}^N X(\gamma_m, k_m, a_m) \rightarrow \sum_{\gamma=1,2} \sum_{k \in K_{\gamma}} \sum_{a} X(\gamma, k, a) \), where \( K_{\gamma} \) is the set of allowed momenta\(^3\) in lead \( \gamma \) and \( X \) is any function. Relabelling summation indices, we then obtain:

\(^3\)Since we work in infinite volume, the momenta \( m \) vary continuously. However, recall from (3.115) and the discussion there that we identify \( 2 \pi \delta(0) \leftrightarrow L \). The primed momenta \( k'_j \) vary continuously so that we can take the limit \( k'_j \rightarrow k_j \), after which we take the thermodynamic limit \( L \rightarrow \infty \) with fixed density. With the \( k_j \) quantized with spacing \( \frac{1}{2 \pi (0)} \leftrightarrow \frac{\pi}{L} \) this procedure is a shortcut way of getting the same answer as taking the limit of the more careful calculation (with finite time and finite volume at first, later sent to infinity).
\[
\langle \hat{I}_{\text{Sym}} \rangle^{(0,2)} = [2\pi \delta(0)]^{-1} \frac{1}{2} \sum_{\gamma_1, \gamma_2 = 1, 2} \sum_{k_1 \in \mathcal{K}_{\gamma_1}} \sum_{k_2 \in \mathcal{K}_{\gamma_2}} \sum_{a_1, a_2 \in \text{Sym}(2)} (\text{sgn } \sigma) \lim_{k_1 \to k_1, k_2 \to k_2} (k_1 + k_2 - k_1' - k_2') \\
\times \frac{\partial}{\partial \phi} \bigg|_{\bar{\varphi} = 0} \tilde{\Omega}^{(\text{red})}_{(0, 2)} [\gamma_1 k_1' a_1, \gamma_2 k_2' a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] \quad (6.85a)
\]

\[
\text{therm, limit} \quad \frac{1}{2} \sum_{\gamma_1, \gamma_2 = 1, 2} \int_{-D}^{D} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} f_{\gamma_1}(k_1) f_{\gamma_2}(k_2) \sum_{a_1, a_2 \in \text{Sym}(2)} (\text{sgn } \sigma) \\
\times \lim_{k_1 \to k_1, k_2 \to k_2} (k_1 + k_2 - k_1' - k_2') \frac{\partial}{\partial \phi} \bigg|_{\bar{\varphi} = 0} \tilde{\Omega}^{(\text{red})}_{(0, 2)} [\gamma_1 k_1' a_1, \gamma_2 k_2' a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] \quad (6.85b)
\]

We proceed to evaluate the reduced function \( \tilde{\Omega}^{(\text{red})}_{(0, 2)} \). Any terms that are finite in the limit of equal momenta \((k_j' \to k_j)\) can be dropped; we are looking for a \textit{real} pole, such as \(1/(k_1 + k_2 - k_1' - k_2')\) (as opposed to a pole off the real axis). Such a pole is not present in the \(\mathcal{T}\)-matrix prefactors that appear explicitly in the “in” operators and crossing state (since \(\text{Im } z = -\Delta \neq 0\), so it can only be produced by the position integral in the overlap itself (see below). From Eq. (6.82) and the form of the crossing state, we can read off:

\[
\tilde{\Omega}^{(\text{red})}_{(0, 2)} [\gamma_1 k_1' a_1', \gamma_2 k_2' a_2'; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] = \int dx_1 dx_2 F_{\gamma_1 k_1 a_1, \gamma_2 k_2 a_2} (x_1, x_2) \Theta(0 < x_2 < x_1) \\
\times \{c_{\gamma_1 k_1 a_1', in}^\dagger, \psi_{eb_1}^\dagger (x_1)\} \{c_{\gamma_2 k_2 a_2', in}^\dagger, \psi_{eb_2}^\dagger (x_2)\} + \text{(regular)}, \quad (6.86)
\]

where “regular” indicates omitted terms that are finite in the limit of equal momenta.

These are the terms involving the anticommutators \(\{c_{\gamma_1 k_1 a_1', in}^\dagger, \psi_{eb_1}^\dagger (x_1)\}\)\{c_{\gamma_2 k_2 a_2', in}^\dagger, \psi_{eb_2}^\dagger (x_2)\} and \(\{c_{\gamma_1 k_1 a_1', in}^\dagger, d_{\gamma_1 b_1}^\dagger\}\{c_{\gamma_2 k_2 a_2', in}^\dagger, d_{\gamma_2 b_2}^\dagger\}. In the former case, we get a single integral over \(x_1\) involving \(F(x_1, 0)\), which (due to the factor of \(z\) in the exponent in \(F\)) produces a momentum denominator with a complex poles; in the latter case, we just get a constant again with complex poles.

To take the \(\bar{\varphi}\) derivative, we recall that \(\frac{\partial}{\partial \varphi} \bigg|_{\bar{\varphi} = 0} \psi_{eb}^\dagger (x) = \frac{i}{2} \psi_{eb}^\dagger (x)\). This derivative can act on either one of the anticommutators, setting \(\psi_{eb}^\dagger = \psi_{eb}^\dagger\) in the other one. In the calculation that follows, we do this derivative, then relabel variables in one term (using the
fact that \( \Omega^{(\text{red})}_{\text{(0,2)}} \) is only defined up to antisymmetrization, then recall the anticommutators
\[ \{c_{\gamma'k'a',\text{in}}, \psi^\dagger_{eb}(x)\} = \frac{1}{\sqrt{2}} S^\ast(k') \delta_{ba'} e^{-ik'x} \] (where \( S(k) = 1 - i T(k) \) is the \( S \)-matrix) and
\[ \{c_{\gamma'k'a',\text{in}}, \psi^\dagger_{ob}(x)\} = \frac{1}{\sqrt{2}} (-1)^{\gamma'} \delta_{ba} e^{-ik'x}, \] then put in the explicit form of \( F \). The “regular”
part is dropped throughout. Following these steps, we find:

\[
\frac{\partial}{\partial \phi} \bigg|_{\phi=0} \Omega^{(\text{red})}_{\text{(0,2)}}[\gamma'_1 k'_1 a'_1, \gamma'_2 k'_2 a'_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] = \frac{i}{2} \int dx_1 dx_2 \, F_{eb,1 e k_2 a_2}^{b_1 b_2}(x_1, x_2) \times \Theta(0 < x_2 < x_1) \left[ \{c_{\gamma'_1 k'_1 a'_1, \text{in}}, \psi^\dagger_{eb_1}(x_1)\} \{c_{\gamma'_2 k'_2 a'_2, \text{in}}, \psi^\dagger_{ob_2}(x_2)\} + (o \leftrightarrow e) \right]
\]
(6.87a)
up to antisym. \[ = \frac{i}{2} \int dx_1 dx_2 \, F_{eb,1 e k_2 a_2}^{b_1 b_2}(x_1, x_2) \Theta(0 < x_2 < x_1) \times \left[ \{c_{\gamma'_1 k'_1 a'_1, \text{in}}, \psi^\dagger_{eb_1}(x_1)\} \{c_{\gamma'_2 k'_2 a'_2, \text{in}}, \psi^\dagger_{ob_2}(x_2)\} - (b_1 \leftrightarrow b_2, x_1 \leftrightarrow x_2) \right]
\]
(6.87b)
\[ = \frac{i}{2} \int dx_1 dx_2 \, F_{eb,1 e k_2 a_2}^{b_1 b_2}(x_1, x_2) \Theta(0 < x_2 < x_1)
\times \frac{1}{\sqrt{2}} S^\ast(k'_1) \frac{1}{\sqrt{2}} (-1)^{\gamma'_2 - 1} \left[ \delta_{b_1 a'_1} \delta_{b_2 a'_2} e^{-ik'x_1} e^{-i k'_2 x_2} - (b_1 \leftrightarrow b_2, x_1 \leftrightarrow x_2) \right]
\]
(6.87c)
\[ = \frac{i}{2} \int dx_1 dx_2 \left[ -T(k_1) T(k_2) \frac{U T [(k_1 + k_2 - U)/2]}{4 \Delta} \right] e^{i(k_1 + k_2) x_1} e^{-iz(x_1 - x_2)}
\times P_{-a'_1 a'_2} \Theta(0 < x_2 < x_1) \frac{1}{2} S^\ast(k'_1) (-1)^{\gamma'_2 - 1} \left(e^{-ik'x_1} e^{-i k'_2 x_2} + e^{-i k'x_1} e^{-ik'_2 x_2}\right).
\]
(6.87d)

The integration over position yields a real pole:
\[ \int dx_1 dx_2 \, e^{i(k_1 + k_2 - k'_1 - k'_2) x_1} e^{i(z - k'_2) x_2} \Theta(0 < x_2 < x_1) = -\frac{T(k'_2)}{2 \Delta} \text{P.V.} \frac{1}{k_1 + k_2 - k'_1 - k'_2}, \]
(6.88)

Thus, we obtain:

\[
\lim_{\substack{k'_1 \to k_1 \\ k'_2 \to k_2}} (k_1 + k_2 - k'_1 - k'_2) \frac{\partial}{\partial \phi} \bigg|_{\phi=0} \Omega^{(\text{red})}_{\text{(0,2)}}[\gamma'_1 k'_1 a'_1, \gamma'_2 k'_2 a'_2; \gamma_1 k_1 a_1, \gamma_2 k_2 a_2] = \frac{i}{32 \Delta^2} (-1)^{\gamma'_2 - 1} T(k_1) T(k_2) U T [(k_1 + k_2 - U)/2] S^\ast(k'_1) T(k'_1) ] + T(k'_2) ] P_{-a'_1 a'_2}, \]
(6.89)

and then Eq. (6.85b) yields [using \( S^\ast(k) = T^\ast(k)/T(k) \) and the spin sums \( P_{-a'_1 a'_2} = 1 \) and \( P_{-a'_1 a'_2} = 1 \):]

\[
\langle \tilde{I}_{\text{Sym}} \rangle^{(0,2)} \text{ therm. limit } \frac{i}{32 \Delta^2} \int_{-D}^{D} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} \left[ f_1(k_1) + f_2(k_2) \right] \left[ f_1(k_2) - f_2(k_2) \right]
\times T^\ast(k_1) T(k_2) U T [(k_1 + k_2 - U)/2] \left(T(k_1) + T(k_2)\right). \]
(6.90)
By taking the adjoint and relabelling, we can read off that \( \langle \hat{I}_{\text{Sym}} \rangle^{(2,0)} = \langle \hat{I}_{\text{Sym}} \rangle^{(0,2)*} \). Collecting terms, we find the following answer for the current in the wavefunction including only the first crossing:

\[
\langle \hat{I}_{\text{Sym}} \rangle = \int_{-D}^{D} \frac{dk}{2\pi} \left[ f_1(k) - f_2(k) \right] \frac{1}{2} |\mathcal{T}(k)|^2 - \frac{1}{16\Delta^2} \int_{-D}^{D} \frac{dk_1 dk_2}{2\pi} \left[ f_1(k_1) + f_2(k_2) \right] \\
\times |f_1(k_2) - f_2(k_2)| \Im \left\{ U \mathcal{T} \left[ \frac{k_1 + k_2 - U}{2} \right] \mathcal{T}^*(k_1) \mathcal{T}(k_2) \left[ \mathcal{T}(k_1) + \mathcal{T}(k_2) \right] \right\}. \tag{6.91}
\]

What does this “expansion in crossings” really mean? While we cannot give a general answer, we can at least understand this result for the current by examining the limits of small and large \( U \).

**Small \( U \) regime**

Expanding to first order in \( U \) replaces \( U \mathcal{T} \left[ (k_1 + k_2 - U)/2 \right] \to U \mathcal{T} \left[ (k_1 + k_2)/2 \right] \). Then, using the simple identities \( \mathcal{T} \left[ (k_1 + k_2)/2 \right] \left[ \mathcal{T}(k_1) + \mathcal{T}(k_2) \right] = 2\mathcal{T}(k_1)\mathcal{T}(k_2) \) and \( \Im \left[ \mathcal{T}(k)^2 \right] = |\mathcal{T}(k)|^2 \Re \left[ \mathcal{T}(k) \right] \), we obtain:

\[
\langle \hat{I}_{\text{Sym}} \rangle = \int_{-D}^{D} \frac{dk}{2\pi} \left[ f_1(k) - f_2(k) \right] \frac{1}{2} |\mathcal{T}(k)|^2 \\
+ \frac{U}{8\Delta^2} \int_{-D}^{D} \frac{dk_1 dk_2}{2\pi} \left[ f_1(k_1) + f_2(k_1) \right] \left[ f_1(k_2) - f_2(k_2) \right] \\
\times |\mathcal{T}(k_1)|^2 \mathcal{T}(k_2)^2 \Re \left[ \mathcal{T}(k_2) \right] + O(U^2). \tag{6.92}
\]

This calculation mainly serves as a check on our formalism. In Appendix D, we calculate the steady state current using Keldysh perturbation theory, arriving at precisely the same answer. The result in the Appendix allows a spin-dependent dot energy \( \epsilon_a \); repeating the above calculation in this more general case [using the more general crossing state (6.38)], we again find exact agreement between the two answers.

We note that the small \( U \) expansion of the AIM has been used in the literature to explore the neighborhood of the strong coupling fixed point of the Kondo model both in and out of equilibrium. This proceeds by, e.g., assuming the impurity is in a singlet state by a choice
of Green’s function [68], expanding about the Hartree-Fock solution [69], or using a Fermi liquid theory approach [34]. In contrast, our result (6.92) describes the AIM itself in the regime of small $U/\Delta$.

Since $\mathcal{T}(k) \sim 1/k$ for large $|k|$, there are no divergences as the bandwidth $D$ is sent to infinity. This is consistent with prior work on the Anderson model (see, e.g., Ref. [70]).

**Infinite U regime – expansion in crossings**

If we instead send $U \rightarrow \infty$, then $U\mathcal{T}[(k_1 + k_2 - U)/2] \rightarrow -4\Delta$, leaving:

\[
\langle \hat{I}_{\text{Sym}} \rangle = \int_{-D}^{D} \frac{dk}{2\pi} \left[ f_1(k) - f_2(k) \right] \frac{1}{2} |\mathcal{T}(k)|^2 \\
+ \frac{1}{4\Delta} \int_{-D}^{D} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} \left[ f_1(k_1) + f_2(k_2) \right] [f_1(k_2) - f_2(k_2)] \\
\times \text{Im} \{ \mathcal{T}^*(k_1)\mathcal{T}(k_2) [\mathcal{T}(k_1) + \mathcal{T}(k_2)] \} + \text{(higher crossings)}. \quad (6.93)
\]

This expansion in crossings appears to capture the regime of small $\Delta$. We note first that Eq. (6.93) satisfies the following Callan-Symanzik equation:

\[
\left( D \frac{\partial}{\partial D} + \beta_\epsilon \frac{\partial}{\partial \epsilon} \right) \langle \hat{I}_{\text{Sym}} \rangle = O(1/D), \quad (6.94a)
\]

where: $\beta_\epsilon = -\frac{\Delta}{\pi\epsilon} + O \left( \frac{\Delta^2}{\epsilon^2} \right). \quad (6.94b)$

To show this, we proceed similarly as in Eq. (5.75) and below from the multi-lead IRL calculation. Under $D \frac{\partial}{\partial D}$, the only terms that survive for large bandwidth are those with $k_1$ integrated (since the $k_2$ Fermi functions cancel at $k_2 = -\infty$) and a single $\mathcal{T}$-matrix in $k_1$ (since $\mathcal{T}(k) \sim 2\Delta/k$ for large $|k|$). Thus, we obtain:

\[
D \frac{\partial}{\partial D} \langle \hat{I}_{\text{Sym}} \rangle \xrightarrow{D \rightarrow \infty} -\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \left[ f_1(k_2) - f_2(k_2) \right] \text{Im} \left[ |\mathcal{T}(k_2)|^2 \right]. \quad (6.95)
\]

Then (6.94b) follows from the identity $\frac{\partial}{\partial \epsilon} |\mathcal{T}(k)|^2 = \frac{1}{\Delta} |\mathcal{T}(k)|^2 \text{Re} \mathcal{T}(k) = -\frac{1}{\Delta} \text{Im} [\mathcal{T}(k)]^2$.

The associated scaling invariants are $\Delta$ and:

\[
\epsilon_d \equiv \epsilon + \frac{\Delta}{\pi} \ln \frac{D}{\Delta}, \quad (6.96)
\]
which is the standard result \[71, 9\].

To clarify the meaning of the expansion in crossings, we consider the zero temperature limit with a voltage drop across the leads: \(\mu_1 = 0\) and \(\mu_2 = -V\). Then the conductance is given by:

\[
\frac{dI}{dV} = \frac{1}{\pi} \frac{\Delta^2}{(\epsilon + V)^2 + \Delta^2} \left[ 1 - \frac{\Delta(\epsilon + V)}{\pi^2(\epsilon + V)^2 + \Delta^2} \times \left( \ln \frac{D}{\sqrt{(\epsilon + V)^2 + \Delta^2} + \ln \frac{D}{\sqrt{\epsilon^2 + \Delta^2} + \text{finite}} \right) \right], \tag{6.97}
\]

where the omitted terms are finite as \(D \to \infty\) (or involve more crossings). It is seen here that the contribution from the first crossing starts at the third order in \(\Delta\), while the RLM contribution is second order (though it becomes a delta function in the limit \(\Delta \to 0\)). Continuing the calculation to one order higher, we find that the contribution of two crossings starts at another order higher (\(\Delta^4\)).

Strictly speaking, our result should be interpreted as a power series in \(\Delta\), meaning that we should keep only up to order \(\Delta^3\). It is interesting to note, however, that when \(\langle \tilde{I}_{\text{Sym}} \rangle\) is calculated with only zero or one crossing allowed (as we did above), the Callan-Symanzik equation (6.94a) holds to all orders in \(\Delta\). Our demonstration of the Callan-Symanzik equation did not expand in \(\Delta\). The expansion in crossings can be thought of as a particular resummation of terms of the \(\Delta\) expansion; the fact that the Callan-Symanzik equation holds exactly suggests that this resummation may be a useful one. This may be worth further study.

While much work has been done on the infinite-\(U\) Anderson model, the most direct comparison we can make to the literature is to Ref. \[72\], in which the current is calculated analytically for \(U \to \infty\) up to order \(\Delta^3\). Our result here disagrees beyond the first order in \(\Delta\). In particular, Ref. \[72\] finds a small Kondo peak beginning to develop at zero bias, which we do not. However, a true comparison can only be made once both answers are expressed in terms of RG invariants, and the result of Ref. \[72\] does not seem to have the standard quantity given in Eq. (6.96) as a scaling invariant.
Chapter 7
Conclusion and outlook

The two main outcomes of this thesis are (1) the development of a new method for calculating the many-body wavefunction and expectation values in quantum impurity systems out of equilibrium and (2) the application of this method to the Kondo model with the prediction of universality in the regime of strong ferromagnetic coupling. The applications of the method to the IRL and AIM show – notwithstanding that the expectation values calculated in these cases are in regimes that have already been explored perturbatively – that the method has a wider scope beyond the Kondo model.

The work on the $1/J$ series in the Kondo model in particular has wider implications for our understanding of renormalization and universality. The main conclusion is that a large bare coupling constant is not the same as a running coupling constant that becomes large under RG flow (a distinction that is often blurred in the literature). Indeed, the limit of strong bare coupling is of little use in understanding the low energy regime of the model with weak bare coupling, contrary to intuitive expectation. The only identification that can be made is the extreme point – infinite bare coupling appears to correspond precisely the zero energy limit of the model with weak bare coupling. Equivalently, we can say that the large bare coupling series captures the correct fixed point, but not the detailed approach to the fixed point. The proper use of the strong coupling series is to identify a new universal regime, corresponding to models that have large (bare) ferromagnetic coupling.

It would be interesting to see if the new method for calculating wavefunctions has applicability beyond quantum impurities. Much of the machinery consists of rewriting the
many-body Schrödinger equation in a convenient way as a set of differential equations constituting the hard part of the many-body problem. The assumptions required up to this point are mild – the Hamiltonian is taken to be one-dimensional with linear spectrum only once we attempt to solve the differential equations exactly. It is an open question, then, if this reformulation of the Schrödinger equation could be useful in a numerical implementation.

To conclude this thesis, I present a discussion of a number of questions or possible future directions raised by this work.

Other observables in the Kondo model.

It would be interesting to explore other observables, particularly in the large negative $J$ regime (and the small $J$ regime would also be accessible as a check). One natural candidate is the $S$-matrix\footnote{Some work in this direction was done by C. Munson (unpublished), in collaboration with N. Andrei and I.} – not the bare $S$-matrix that we used in our calculations, but the physical $S$-matrix for excitations above a filled Fermi sea. The NESS we obtained in the Kondo model is a many-body scattering “in” state; it straightforward to obtain the corresponding “out” state by considering evolution to large negative times. Since the initial quantum numbers are completely arbitrary, we are free to construct a state consisting of a Fermi sea with one electron above it with momentum $p$ and spin $a$; schematically, $|\text{FS}, pa\rangle_{\text{in}}$. The $S$-matrix for elastic single particle scattering is then given by $\langle \text{FS}, pa'|\text{FS}, pa\rangle_{\text{in}}$. (Although this naive construction some modification; see next paragraph.) The calculation of the $S$-matrix can proceed using some of the same technology developed here, such as the reduction of a general overlap to a sum of normal ordered overlaps. If necessary, the calculation could be done by considering the finite time first and then taking the limit of large time. More complicated scattering processes involving particle-hole pairs could be considered by making different choices of the initial and final quantum numbers.

Though there appear to be no technical obstacles to this calculation, there is a curious
conceptual obstacle: in the overlap, the theory does not “know” which momenta belong to the Fermi sea and which momenta are the scatterers. Consider elastic single particle scattering in the RLM. The $S$-matrix is given naively by the $\langle \text{FS}, p | \text{FS}, p \rangle_{\text{in}} = \left[ \prod_{k \in \text{FS}} S(k) \right] S(p)$, where $S(q)$ is the bare $S$-matrix. As this is a single particle problem, we would expect the answer to be $S(p)$. Clearly, the solution in this case is to divide by the phase factor coming from the Fermi sea momenta, i.e. $\langle \text{FS} | \text{FS} \rangle_{\text{in}} = \prod_{k \in \text{FS}} S(k)$. This prescription seems to be a version of the dividing out of vacuum bubbles that occurs in the standard field theory approach to calculating the $S$-matrix. While it is clear that the same prescription can be implemented with interactions included (e.g. IRL or AIM), it is less clear what do in the Kondo model. The difficulty is that the corresponding object to be divided out, $\langle \text{FS}, a_0 | \text{FS}, a_0 \rangle_{\text{in}}$, is no longer a phase factor, but is instead one of the diagonal components of a unitary matrix (due to the fixed impurity spin $a_0$).

Aside from the $S$-matrix, other good candidates to calculate are likely to be expectation values, or 1-point correlators; any higher correlators appear too difficult at present due to the need to carry out another round of time evolution. The method seems to work best on local observables, meaning that there are field operators evaluated at fixed points.\footnote{Although, R. Tourani has been working in collaboration with N. Andrei and I on calculating the time-dependent magnetization, or expectation value of $S^z$, in the Kondo model.} It would be interesting to see, for instance, if the method can yield any insight into the “Kondo cloud” by calculating, e.g., some density as a function of distance from the impurity.

Modifying the cutoff scheme.

As discussed in the introduction, it is a standard technique in problems with many scales to modify the behavior of theory at high energies (i.e. choose the cutoff scheme) in some convenient way. The way pursued in this thesis, with the cutoff on the initial state but not on the Hamiltonian, evidently produces the correct results for the leading log series ($g^2$, $g^3 \ln \frac{D}{\text{scale}}$, etc.) and the next two sub-leading constants ($g^3$ and $g^4$), but something is amiss at the sub-leading logarithmic level ($g^4 \ln \frac{D}{\text{scale}}$, $g^5 \ln^2 \frac{D}{\text{scale}}$, etc.). In Sec. A.5, we see that
the fact that the Hamiltonian is unregulated is probably the culprit; the support for this is that in a simpler calculation – the magnetization at one loop order – it can be clearly shown that removing the regulator on the Hamiltonian changes the first log divergence. It seems more likely that our scheme would break down (perhaps the Callan-Symanzik equation would cease to hold) at some sufficiently high order, rather than that our scheme yields an internally-consistent physical answer distinct from that of conventional schemes.

The task, then, is to modify the scheme so as to reproduce the standard answer at the sub-leading logarithmic order. Solving for the wavefunction with a cutoff on the Hamiltonian seems to be too difficult (see Appendix E). However, another option is to define a projection operator \( P_D \) that projects onto the modes within the cutoff region, then calculate the expectation value in the projected state \( P_D|\Psi(t)\rangle \). This procedure works in the magnetization example (Sec. A.5), so it is worth attempting in the calculation of the current.

Including a magnetic field on the dot.

Chapter 4 presented the Kondo wavefunction given a local magnetic field term, \(-BS^z\), in the Hamiltonian; however, this field was set to 0 in the calculation of the current. This was done for more than just simplicity, but also to avoid certain infrared subtleties that are known to occur in the case of a non-zero magnetic field. The essential point is one of order of limits: the spin occupancy does not revert its free value as one sends the coupling constants to zero, but instead has some “memory” of the ratios of coupling constants (for instance, the coupling between leads vs. the coupling within a lead). The way to deal with this problem is to set up a self-consistent equation, either by means of a Dyson equation [73] or a Boltzmann equation [29]. These constructions seem to be based on a correlation function (a pseudo-fermion self-energy), and so it is not obvious how to reproduce them in the wavefunction approach (in which so far we only have access to expectation values).
Integrability?

The machinery of integrability as it appears in Bethe Ansatz – in particular, the Yang-Baxter equation for consistent factorization of scattering amplitudes – does not appear to play any role in the wavefunctions constructed in this thesis. Is the Yang-Baxter equation playing some hidden role in the calculation? One way to resolve this would be to calculate the wavefunction in a theory that is not known (in the equilibrium case) to have a Bethe Ansatz solution. The solution of the wavefunction with a magnetic field on the dot would seem to satisfy this requirement, seeing as there does not appear to be any Bethe Ansatz solution for non-zero field in the literature. Complicating this picture, however, is the work of P. Pasnoori in collaboration with N. Andrei (unpublished) that does find a Bethe Ansatz solution in the model with non-zero field.

Prospects for calculating the full crossover.

The final answers obtained in this thesis are confined (in the Kondo model) to the regime in which one or more of external scales is $\gg T_K$. In contrast, the Bethe Ansatz approach to the equilibrium problem permits the evaluation of complete curves for some physical quantities, including $\sim T_K$ and down to the lower scales, $\ll T_K$, at which Fermi liquid behavior takes over. The difference is due to the fact that a lot of technology has been developed over the decades for calculating the partition function using Bethe Ansatz wavefunctions; the technology presented in this thesis, for use in the new nonequilibrium wavefunctions, is not as powerful. One reason for this is the relative infancy of the new technique (recall that the Bethe Ansatz dates to 1931 [74]). Probably the more important factor, though, is that the partition function requires “only” the enumeration, or counting, of states at different energies. A nonequilibrium problem, or even a more detailed equilibrium problem like the calculation of correlation functions, requires more information than is available in the enumeration of states.

To achieve a calculation of the full crossover out of equilibrium, one needs to find an
alternative way of taking the thermodynamic limit of the expression found in this thesis (modulo some correction for fixing the cutoff scheme; see previous bold heading) for the current given \(N\) electrons. The strategy taken in this thesis, of expanding in \(J\) or \(1/J\), is not sufficient for obtaining the full curve at all scales.\(^3\) It seems that some new idea is needed in order to reorganize the \(N\) particle current into a form that permits efficient evaluation of the thermodynamic limit throughout the full range of scales. If you have read this far, I encourage you to find this new idea!

\(^3\)It would be formally sufficient if the expansion could be summed to all orders; however, it may be the case that the series is asymptotic and that some features of the full curve are not captured. On the other hand, Ref. [75] argues that the full answer (for an equilibrium quantity) is expressible as a Borel summation of a series in powers of \(J\).
References


Appendix A

Additional topics in the Kondo model

A.1 Including anisotropy and potential scattering

We can solve the quench problem in a more general version of the one lead Kondo model:

\[ H = -i \int_{-L/2}^{L/2} dx \psi_\alpha^\dagger(x) \frac{d}{dx} \psi_\alpha(x) - B S^z + \psi_\alpha^\dagger(0) \left[ J_2 \sigma_{ab}^j S^j + J'_2 \delta_{ab} \right] \psi_b(0), \quad (A.1) \]

where summation over \( j = 1, 2, 3 \) is implied. Let us do the calculation in the \( J = 0 \) basis.

We can include the potential scattering \( J'_2 \) term either in \( H^{(1)} \) or in \( H^{(0)} \). We pursue the first option, since then the wavefunction is the same as in the main text, just with a more general \( T \)-matrix (or in the notation used here, the matrix \( M = iT \)).

With the potential scattering term taken to be in \( H^{(1)} \), we do not need to make any change in the \( c^\dagger(t) \) operators. The model remains type A with:

\[ A_{k_1 a_1}(t) = e^{-i k_1 t} \left[ J_j \sigma_{b_1 a_1}^j S^j + J'_2 \delta_{b_1 a_1} \right] \psi_{b_1}^\dagger(0). \quad (A.2) \]

Making the same ansatz (4.27) for the crossing states, we find that the function \( F \) must satisfy:

\[ -i F^{b_1 b_0}_{c_1 c_0} (t) e^{i b_1 a_0 B t} + \left[ J_j \sigma_{b_1 c_1}^j S_{b_0 c_0}^j + J'_2 \delta_{b_1 c_1} \delta_{b_0 c_0} \right] \frac{1}{2} F^{c_1 c_0}_{k_1 a_1 a_0} (t) e^{i a_0 B t} = -e^{-i k_1 t} \left[ J_j \sigma_{b_1 a_1}^j S_{b_0 a_0}^j + J'_2 \delta_{b_1 a_1} \delta_{b_0 a_0} \right] e^{i a_0 B t}. \quad (A.3) \]

In matrix form, this equation reads:

\[ \left[ I + i \frac{1}{2} \left( \frac{1}{2} J_j \sigma_j \otimes \sigma_j + J' I \right) \right]^{b_1 b_0}_{c_1 c_0} F^{c_1 c_0}_{k_1 a_1 a_0} (t) e^{i a_0 B t} = -i e^{-i k_1 t} \left[ \frac{1}{2} J_j \sigma_j \otimes \sigma_j + J' I \right]^{b_1 b_0}_{a_1 a_0} e^{i a_0 B t}. \quad (A.4) \]
Isolating $F$, we find:

$$F_{k_1a_1, a_0}^{b_1, b_0}(t) = \mathcal{M}_{a_1 a_0}^{b_1 b_0} e^{-i(k_1+(a_0–b_0)B)t}, \quad (A.5)$$

where the matrix $\mathcal{M}$ takes a more general form:

$$\mathcal{M}_{a_1 a_0}^{b_1 b_0} = -i \left[ I + i \frac{1}{2} \left( \frac{1}{2} J_j \sigma^j \otimes \sigma^j + J' I \right) \right]^{-1}{}_{c_1 c_0}^{b_1 b_0} \left( \frac{1}{2} J_j \sigma^j \otimes \sigma^j + J' I \right)_{a_1 a_0}^{c_1 c_0}. \quad (A.6)$$

It is straightforward to prove the following matrix inversion formula:

$$\left[ \sum_{j=0}^{3} \alpha_{j} \sigma^j \otimes \sigma^j \right]^{-1} = \frac{1}{4} \sum_{j=0}^{3} \left( \sum_{n=0, n \neq j}^{3} \frac{1}{\alpha_{\text{tot}} - 2 \alpha_{n}} - \frac{1}{\alpha_{\text{tot}} - 2 \alpha_{j}} \right) \sigma^j \otimes \sigma^j, \quad (A.7)$$

where $\alpha_{\text{tot}} \equiv \sum_{j=0}^{3} \alpha_{j}$ and $\alpha_{a_1 a_0}^{0} \equiv \delta_{a_1 a_0}^{0}$, which yields a complicated result for $\mathcal{M}$. If two of the Kondo coupling constants are equal (call this value $J_\perp$) with the remaining coupling being $J_m$ ($m = 1, 2, 3$), then we obtain:

$$\mathcal{M} = \left[ -2I + \frac{1}{1 + i \frac{1}{2} (J_m + J')} P_+ (I + \sigma^m \otimes \sigma^m) + \frac{1}{1 + i \frac{1}{2} (J_\perp - \frac{1}{2} J_m + J')} P_+ (I - \sigma^m \otimes \sigma^m) + \frac{1}{1 - i \frac{1}{2} (2 J_\perp - \frac{1}{2} J_m - J')} P_- (I + \sigma^m \otimes \sigma^m) + \frac{1}{1 - i \frac{1}{2} (J_\perp + \frac{1}{2} J_m - J')} P_- (I - \sigma^m \otimes \sigma^m) \right]_{a_1 a_0}^{c_1 c_0}, \quad (A.8)$$

where $P_{\pm} = \frac{1}{2} (I \pm P)$ and $m$ is not summed.

In the fully isotropic case ($J_x = J_y = J_z = J$), we obtain:

$$\mathcal{M} = 2 \left( -I + \frac{1}{1 + i \frac{1}{2} (J + J')} P_+ + \frac{1}{1 - i \frac{1}{2} (J - J')} P_- \right). \quad (A.9)$$

A short calculation then shows that the corresponding $S$-matrix $S = I + \mathcal{M}$ agrees exactly with the electron-impurity $S$-matrix of the Bethe Ansatz solution (see. Ref. [41]), bearing in mind that the coupling constant $J$ used there is $\frac{1}{2} J$ in our convention.

Let us now solve the model with the potential scattering term included in $H^{(0)}$ instead
of $H^{(1)}$. This affects the time-evolving creation operators:

$$c_{ka}^\dagger(t) = \int_{-L/2}^{L/2} dx \ e^{-ik(t-x)} \left[ 1 + \mathcal{M}'\Theta(0 < x < t) + \mathcal{M}'^*\Theta(t < x < 0) \right]\psi^\dagger_a(x), \quad (A.10a)$$

$$\mathcal{M}' = \frac{-iJ'}{1 + i\frac{1}{2}J'}. \quad (A.10b)$$

The $A(t)$ operator is then:

$$A_{k_1a_1}(t) = J \left( 1 + \frac{1}{2}\mathcal{M}' \right) \sigma_{b_1a_1} \cdot S \psi_{b_1}^\dagger(0). \quad (A.11)$$

It is then clear that the same auxiliary states $|\chi(t)\rangle$ will still work, provided that we include in each $|\chi_{k_1a_1...k_na_na_0}(t)\rangle$ an additional prefactor of $(1 + \frac{1}{2}\mathcal{M}')^n$. In this way of writing the wavefunction, the constant $J'$ appears in both the time-evolving creation operators and in the crossing states. It seems more convenient, then, to use the previous way of writing the wavefunction, in which $J'$ appears only in the crossing states.

### A.2 Alternate calculations of the current

It is stated in the main text that there are several different equivalent forms of the average current [see Eq. (4.50)] and following. This section calculates some of the alternate forms, yielding the same answer as found in the main text.

**Local form, direct calculation.**

It is convenient to write the local form of the current, Eq. (4.51b), in the odd/even basis:

$$\hat{I} = i\frac{1}{2}J\psi_{aa}^\dagger(0)\sigma_{aa'}\psi_{ea'}(0) \cdot S + \text{ h.c.} \quad (A.12)$$

Then the expectation value we are interested in becomes:

$$\langle \Psi_{\gamma N k\alpha N\alpha_0}(t) | \hat{I} | \Psi_{\gamma N k\alpha N\alpha_0}(t) \rangle = \text{Re} \left[ iJ\psi_{aa}^\dagger(0)\sigma_{aa'}\psi_{ea'}(0) \cdot S \right]. \quad (A.13)$$
The general result Eq. (2.166) yields:

\[
\langle \Psi_{NkN^N,a_0}(t) | \psi^\dagger_{0a}(0)\psi_{ea'}(0)S|\Psi_{NkN^N,a_0}(t) \rangle =
\sum_{n=1}^{N} \frac{1}{2^n(n-1)!} \sum_{m_1,\ldots,m_n=1}^{N} (-1)^{\gamma_{mn}-1}\{c_{ok_{mn}a_{mn}}(t), \psi^\dagger_{0a}(0)\}
\times \langle \langle \psi_{ek_{m/m_n}a_{m/m_n}a_0}(t)|\psi_{ea'}(0)S|\Psi_{ek_{m/m_n}a_{m/m_n}a_0}(t) \rangle : \rangle +
\sum_{\ell \in I_1(m)} (\tilde{\text{sgn}} \ell) \{\psi_{ea'}(0), c_{ek_{(1)}}a_{(1)}(t)\} : \langle \psi_{ek_{m/m_n}a_{m/m_n}a_0}(t)|S|\Psi_{ek_{m/m_n}a_{m/m_n}a_0}(t) \rangle : \rangle.
\]

(A.14)

Thus, we obtain:

\[
\langle \Psi_{NkN^N,a_0}(t) | \tilde{T}\Psi_{NkN^N,a_0}(t) \rangle =
Re \left[ iJ_{aa'}^{ij} \sum_{n=1}^{N} \frac{1}{2^n(n-1)!} \sum_{m_1,\ldots,m_n=1}^{N} (-1)^{\gamma_{mn}-1}\{c_{ok_{mn}a_{mn}}(t), \psi^\dagger_{0a}(0)\}
\times \langle \langle \psi_{ek_{m/m_n}a_{m/m_n}a_0}(t)|\psi_{ea'}(0)S|\Psi_{ek_{m/m_n}a_{m/m_n}a_0}(t) \rangle : \rangle +
\sum_{\ell \in I_1(m)} (\tilde{\text{sgn}} \ell) \{\psi_{ea'}(0), c_{ek_{(1)}}a_{(1)}(t)\} : \langle \psi_{ek_{m/m_n}a_{m/m_n}a_0}(t)|S|\Psi_{ek_{m/m_n}a_{m/m_n}a_0}(t) \rangle : \rangle \right].
\]

(A.15)

Our task is to show that this is exactly equal to the expression (4.114) found in the main text. We evaluate the first term using the technology for normal ordered overlaps developed in Sec. 4.2.2. The main point is to notice that the \(\psi(0)\) operator must contract with the \(x_n\) coordinate – which must be a crossing state, due to normal ordering – leading to a factor of 1/2 from \(\delta(x_n)\Theta(0 < x_n < \cdots < x_1 < t) = \frac{1}{2}\delta(x_n)\Theta(0 < x_{n-1} < \cdots < x_1 < t)\) (the
averaging prescription). We obtain:

\[
\langle \Psi_{ekn',a'_{n,n},a_0}(t)|\psi_{ea'}(0)S^j|\Psi_{ekn,a_0}(t) \rangle := 1 \frac{1}{L-n-1/2} \sum_{\sigma' \in \text{Sym}(n)}(\text{sgn } \sigma)(\text{sgn } \sigma')e^{-ik_{ea}t}Q_n(t; k_{\sigma_0(n/n)} - k_{\sigma'(n/n)})
\]

(\text{A.16})

The spin-dependent terms in the second line simplify to \(\Xi_{n-1}[a_{\sigma'(n/n)}; a_{\sigma_0(n/n)}]S_{a_0} b_0 b_0 \times M^a_{\sigma_0} b_0 \). We then note that \(e^{-i(k_{ea} - k_{ea}')t}Q_{n-1}(t; k_{\sigma_0(n/n)} - k_{\sigma'(n/n)}) = \frac{\partial}{\partial t}Q_n(t; k_{\sigma_0} - k_{\sigma't}) \), which yields:

\[
\{c_{ao_0}(0)\} : \langle \Psi_{ekn',a'_{n,n},a_0}(t)|\psi_{ea'}(0)S^j|\Psi_{ekn,a_0}(t) \rangle := 1 \frac{1}{L^n} \sum_{\sigma' \in \text{Sym}(n)}(\text{sgn } \sigma)
\]

(\text{A.17})

From Eq. (4.109), we get:

\[
\langle \Psi_{k_{n',a'_{n,n},a_0}}(t)|S|\Psi_{kn,a_0}(t) \rangle := 1 \frac{1}{L-n-1} \sum_{\sigma,\sigma' \in \text{Sym}(n-1)}(\text{sgn } \sigma)(\text{sgn } \sigma')
\]

(\text{A.18})

Relabeling \(\ell(1) \to \sigma_n\) then yields:

\[
\{c_{ao_0}(0)\} \sum_{\ell \in S_{(n)}}(\text{sgn } \ell) \{\psi_{ea'}(0), c_{ek\ell(1)\ell(1)}(t)\}
\]

(\text{A.19})
Returning to Eq. (A.15) and doing some relabeling, we obtain:

\[
\langle \Psi_{\gamma NkN aN, a_0}(t) \mid \hat{H} \mid \Psi_{\gamma NkN aN, a_0}(t) \rangle = -\text{Re} \left[ \sum_{n=1}^{N} \frac{1}{L} \sum_{m_1, \ldots, m_n=1}^{N} (-1)^{\gamma_{mn} - 1} \sigma \in \text{Sym}(n) \right. \\
\times \frac{\partial}{\partial t} Q_n(t; k_{m\sigma} - k_m) \sum_{a_i} \left[ a_{m/m_n} ; a_{(m/m_n)\sigma} \right]_{a_0 a_0}^{b_i' b_0} \\
\times (-iJ) \left( \frac{1}{2} \sigma_{a_m a'} \mathcal{M}_{a\sigma m n, b_0}^{a' b_0} + \frac{1 + \xi}{2} \sigma_{a_m a_{\sigma m n} a_{\sigma m n} \delta b_0 c_0} \right) \cdot S_{b_0 c_0}. \quad (A.20)
\]

To show that we have exact agreement with Eq. (4.114) from the main text, we recall that \( \mathcal{M} = \xi(S - I) \) and use the following identity:

\[
\frac{-iJ}{2} \left( \sigma_{a_i', a'} \xi S_{a_n b_0}^{a' c_0} + \sigma_{a_i', a_{\sigma n} \delta b_0 c_0} \right) \cdot S_{b_0 c_0} = \xi S_{a_n b_0}^{a' c_0} - I_{a_n b_0}^{a' c_0}, \quad (A.21)
\]

which is easily shown from Eqs. (4.43a)-(4.43c).

**Boundary terms.**

First, we write the lead 1 density in the odd/even basis:

\[
\psi_{1a}^\dagger(x) \psi_{1a}(x) = \frac{1}{2} \left[ \psi_{oa}^\dagger(x) \psi_{oa}(x) + \left( \psi_{oa}^\dagger(x) \psi_{ea}(x) + \text{h.c.} \right) + \psi_{ea}^\dagger(x) \psi_{ea}(x) \right]. \quad (A.22)
\]

We are interested in the discontinuity at zero – i.e. we evaluate the density at \( x = 0^- \) minus the density at \( x = 0^+ \). The odd-odd part has no discontinuity and so makes no contribution; the even-even part leads to three terms that cancel due to unitarity, again leading to no contribution.

There remains the odd-even term. We start from Eqs. (4.55a)-(4.55b) in the main text. Eq. (4.56b) yields:

\[
\text{Re} \left[ (i)|_{x=0^-} - (i)|_{x=0^+} \right] = \frac{1 - \xi}{2} \frac{1}{L} \sum_{m=1}^{N} (-1)^{\gamma_m - 1}, \quad (A.23)
\]

which agrees exactly with (4.56c).

Due to normal ordering, we have \( (ii)|_{x=0^-} \). Using the technology of Sec. 4.2.2, we
evaluate the normal ordered overlap that appears in \( (ii) \mid_{x=0^+} \):

\[
\langle \Psi_{e k_n'/n', a_n', a_0'}(t) | \psi_{ea}(0^+) \rangle | \Psi_{e k_n a_n, a_0}(t) \rangle = \sum_{\sigma, \sigma' \in \text{Sym}(n)} \sum_{(\sigma') = n} \left( \text{sgn} \sigma \right) \left( \text{sgn} \sigma' \right) e^{-ik_{\sigma n}t} Q_n(t; k_{\sigma n}(n/n) - k_{\sigma' n}(n/n))
\]

\[
\times \int \mathcal{D}_a c_{n} \mathcal{D}_a c_{n} \mathcal{D}_a c_{n} \mathcal{D}_b c_{n} \prod_{j=1}^{n-1} \left( S_{\alpha j}^{b j} c_{j-1} - S_{\alpha j}^{a_j} c_{j-1} M_{\alpha j}^{b_j, c_j} \right) \int a_{n} c_{n} \mathcal{M}_{a_n, c_n}^{b_n, c_n}.
\]

(A.24)

The spin-dependent terms in the second line simplify to \( \Xi_{n-1}[a_{\sigma' o(n/n)}; a_{\sigma o(n/n)}] = \Xi_{n-1}[a_{\sigma' o(n/n)}; a_{\sigma o(n/n)}] \). We then note that

\[
e^{-i(k_{\sigma n} - k_{\sigma' n}) t} Q_n(t; k_{\sigma n}(n/n) - k_{\sigma' n}(n/n)) = \frac{\partial}{\partial t} Q_n(t; k_{\sigma n} - k_{\sigma' n}),
\]

which yields:

\[
\{ c_{n} a_{n}(t), \psi_{ea}(0^+) \} : \langle \Psi_{e k_n'/n', a_n', a_0'}(t) | \psi_{ea}(0^+) \rangle | \Psi_{e k_n a_n, a_0}(t) \rangle : = \sum_{\sigma, \sigma' \in \text{Sym}(n)} \sum_{(\sigma') = n} \left( \text{sgn} \sigma \right) \left( \text{sgn} \sigma' \right) \frac{\partial}{\partial t} Q_n(t; k_{\sigma n} - k_{\sigma' n})
\]

\[
\times \Xi_{n-1}[a_{\sigma' o(n/n)}; a_{\sigma o(n/n)}] \mathcal{M}_{a_{\sigma n} b_{\sigma n}}^{a_{\sigma n} b_{\sigma n}}
\]

(A.25a)

\[
= \xi : \langle \Psi_{e k_n'/n', a_n', a_0'}(t) | c_{n} a_{n}(t) | \Psi_{e k_n a_n, a_0}(t) \rangle : \quad \text{[see Eq. (4.110)]}.
\]

(A.25b)

Thus, we see that \( Re[-(ii)\mid_{x=0^+}] \) agrees exactly with the right-hand side of Eq. (4.58) (the contribution of term \( (ii) \) to the current in the \(-\frac{d}{dt} \langle \hat{N}_1 \rangle \) calculation). This confirms that

\[
\langle \psi_{1a}(0^-) \psi_{1a}(0^-) - \psi_{1a}(0^+) \psi_{1a}(0^+) \rangle = -\frac{d}{dt} \langle \hat{N}_1 \rangle.
\]

The calculation with \( x = t^\pm \) instead of \( x = 0^\pm \) should be similar, again yielding \( I(t) \) (up to a sign) so that (4.52) in the main text sums to zero. (Note that is already implied by the equality \( I(t) = (\tilde{I}_t, \text{which we verified above and in the main text.})\)

### A.3 Proof of spin sum identity

We prove the identity (4.135) that is used in the main text for showing convergence of the current in time to all orders. We repeat the identity here for reference:

\[
\Xi_n[a_n; a_{\text{vec}}]^{\sigma c}_{a_0 a_0} = 0 \quad [n \geq 1, \sigma \in \text{Sym}(n)],
\]

(A.26)
with implied summation over any repeated spin indices. We recall that $S = \xi (Z_I + Z_P P)$; only even powers of $\xi$ appear in the tensor $\Xi_n$, so $\xi = \pm 1$ drops out of all calculations in this section. Rather than use the explicit forms of the coefficients $Z_I$ and $Z_P$, we only use the fact that they are constrained by the unitarity of the bare $S$-matrix $(S_{\alpha_0\alpha_1}^{\beta_0\beta_1} S_{\beta_0\beta_1}^{\alpha_0\alpha_1} = r_{\alpha_1\alpha_0})$:

$$|Z_I|^2 + |Z_P|^2 = 1,$$
(A.27a)

$$Z_I Z_P^* + Z_P Z_I^* = 0.$$  
(A.27b)

Recall the “update rule” for generating $\Xi_{n+1}$ from $\Xi_n$ and the $n = 2$ base [Eqs. (4.123) and (4.124) from the main text, reproduced here for reference]:

$$\Xi_{n+1}[a_n'; a_{n+1}'; a_n, a_{n+1}]_{\alpha'_0\alpha_0} = -|Z_P|^2 \Xi_n[a_n'; a_n]_{\alpha'_0\alpha_0} \delta_{\alpha_0+1} + Z_I Z_P^* (\Xi_n[a_n'; a_0]_{\alpha'_0\alpha_0} \delta_{\alpha_0+1} - \Xi_n[a_n'; a_0]_{\alpha'_0\alpha_0} \delta_{\alpha_0+1})$$
(A.28)

and:

$$\Xi_1[a_1'; a_1]_{\alpha'_0\alpha_0} = |Z_P|^2 \left( 2I_{a'_1c}^{a_1'c} - I_{a'_1c}^{a_1'c} \right).$$
(A.29)

To give a sense of the pattern, we present the $n = 2$ case, as well:

$$\Xi_2[a_1', a_2'; a_1, a_2]_{\alpha'_0\alpha_0} = |Z_P|^2 \left[ |Z_P|^2 \left( I_{a_1a_2c}^{a_1'a_2'c} - 2I_{a_2a_1'c}^{a_1'a_2'c} \right) + 2Z_I Z_P^* \left( I_{a_2a_1'c}^{a_1'a_2'c} - I_{a_1a_2'c}^{a_1'a_2'c} \right) \right].$$
(A.30)

From the base case and the update rule (A.28), the pattern is the following: a sum of identity tensors multiplied by some function of $Z_I$ and $Z_P$. In each identity tensor, we can either have 1) $c'$ contracts with $c$ and each $a'_j$ contracts with $a_j$, or 2) $c'$ contracts with some $a'_j$, $c$ contracts with some $a_j$, and the remaining $a_m$ and $a'_m$ indices contract in some way (always pairing a primed with an unprimed index). To be precise, we will show by induction the following general form:

$$\Xi[a_n'; a_n]_{\alpha'_0\alpha_0} = X_n I_{\alpha_0\alpha_c}^{a_0'} + \sum_{\sigma' \in \text{Sym}(n-1)} \sum_{j,j'=1}^n Y_{n,j,j'}^{(\sigma')} I_{a_{(n/j)}(j')\sigma}^{a_{(n/j')}j'} I_{a_0}^{a_0'c} c,$$
(A.31)

where the coefficients $X_n$ and $Y_{n,j,j'}^{(\sigma')}$ depend on $Z_I$ and $Z_P$. The base case is of this form, with $-X_1 = \frac{1}{2} Y_{1,1,1}^{(1)} = |Z_P|^2$. For the induction step, we assume this general form for some
setting $n \geq 1$ and use the update rule to obtain:

$$
\Xi_{n+1}[a'_n, a_{n+1}; a_n, a_{n+1}]_c^{c'} = -|Z_P|^2 X_n I_{a_{n+1}c}^{a'_n a_0} - \sum_{\sigma' \in \text{Sym}(n-1)} \sum_{j,j'=1}^n Y^{(\sigma')}_{n,j,j'} I_{a_{n+1}j}^{a'_n j'} n_{a_0 a_{n+1}}^c \delta_{a_0}^{a_0} \delta_{a_{n+1}}^{a_{n+1}} \delta_{a_j}^{a_j} \delta_{a_{j'}}^{a_{j'}} + Z_1 Z_2 \left( \delta_{a_0}^{a_0} \delta_{a_{n+1}}^{a_{n+1}} \delta_{a_j}^{a_j} \delta_{a_{j'}}^{a_{j'}} + \delta_{a_0}^{a_0} \delta_{a_{n+1}}^{a_{n+1}} \delta_{a_{j'}}^{a_{j'}} \delta_{a_{j}}^{a_{j}} \right). \tag{A.32}
$$

As claimed, this expression is of the general form (A.31). We can read off $X_{n+1} = -|Z_P|^2 X_n$. While extracting $Y^{(\sigma')}_{n+1,j,j'}$ would be messy, we can see that the remaining terms all include $I_{a_{j'}a_j}^{c'c}$ with $j,j' \in \{1, \ldots, n+1\}$, with remaining $a_m$ indices contracted with the remaining $a_m'$ indices in some order. [Note that we have written some contractions as Kronecker deltas for typographical clarity. Also, we can put the unprimed indices in the canonical order $a_{n/j'}$ that appears in (A.31) simply by rearranging the corresponding unprimed indices below, which is just some choice of the permutation $\sigma' \in \text{Sym}(n)$].

We proceed to the prove the main result by induction. For the base case, we note that setting $c' = c$ yields zero in Eq. (A.29). Next, we assume that (A.26) holds for some $n \geq 1$ [and for any $\sigma \in \text{Sym}(n)$], and we let $w \in \text{Sym}(n+1)$. Then the update rule (A.28) yields:

$$
\Xi_{n+1}[a_n, a_{n+1}; a_{\text{wom}}, a_{w_{n+1}}]_c^{c'} = -|Z_P|^2 \Xi_n[a_n; a_{\text{wom}}]_c^{c'} a_{w_{n+1}} \delta_{a_0}^{a_0} \delta_{a_{n+1}}^{a_{n+1}} + Z_1 Z_2 \left( \Xi_n[a_n; a_{\text{wom}}]_c^{c'} a_{w_{n+1}} \delta_{a_0}^{a_0} \delta_{a_{n+1}}^{a_{n+1}} - \Xi_n[a_n; a_{\text{wom}}]_c^{c'} a_{w_{n+1}} \delta_{a_0}^{a_0} \delta_{a_{n+1}}^{a_{n+1}} \right). \tag{A.33}
$$

The first term on the right hand side vanishes due to the induction assumption. This is particularly clear if $w_{n+1} = n$; but even if $w_{n+1} \leq n$, we are free to relabel the summation indices to obtain the same form (A.26) that vanishes by assumption. To deal with the second term on the right-hand side, we use the general form (A.31) to find:

$$
\text{coeff. of } Z_1 Z_2 = X_n I_{a_{\text{wom}}}^{a_{w_{n+1}}} \left( \delta_{a_{n+1}}^{a_{n+1}} \delta_{a_{w_{n+1}}}^{a_{w_{n+1}}} - \delta_{a_{n+1}}^{a_{n+1}} \delta_{a_{w_{n+1}}}^{a_{w_{n+1}}} \right) + \sum_{\sigma' \in \text{Sym}(n-1)} \sum_{j,j'=1}^n Y^{(\sigma')}_{n,j,j'} I_{a_{\text{wom}}(n/j)}^{a_{n/j'}} \left( \delta_{a_j}^{a_j} \delta_{a_{j'}}^{a_{j'}} - \delta_{a_j}^{a_j} \delta_{a_{j'}}^{a_{j'}} \right). \tag{A.34}
$$

In the $X_n$ term, we get zero immediately if $w_{n+1} = n+1$; if instead $w_{n+1} \leq n$, then $I_{a_{\text{wom}}} = (\text{const}) a_{w_{n+1}}$ (where the constant is some number obtained from summing all the other spin indices), yielding zero once we sum over $a_{n+1}$ and $a_m$.

Similarly, in each $Y^{(\sigma')}_{n,j,j'}$,
term, we will have to contract either (1) $a_{w_j}$ with $a_{j'}$ and $a_{w_{n+1}}$ with $a_{n+1}$, or (2) $a_{w_j}$ with $a_{n+1}$ and $a_{w_{n+1}}$ with $a_{j'}$, and either way, the two terms in parentheses cancel once the spin indices are summed. For instance, if $w_j = j'$ and $w_{n+1} = n + 1$, then we are in case (1) immediately; if instead $w_j = j'$ but $w_{n+1} \leq n$, then the identity tensor in front yields $(\text{const})\delta_{a_{n+1}}$, and we are again in case (1); and so on.\footnote{If $w_j \neq j'$ and $w_{n+1} \leq n$, then the identity tensor in front becomes either (const)$\delta_{a_{w_{n+1}}}^{'\delta}$ and (1) [yielding case (1) or (const)$\delta_{a_{n+1}}^{'\delta}$ and (2) [yielding case (2)], depending on how the remaining spin indices are contracted.} Thus, we have shown that Eq. (A.26) holds for $n + 1$, completing the induction proof.

**A.4 RG improvement**

This section reviews some material that is standard, but not (as far as I know) collected in any one place in as much detail. See Refs. [5], [30], [59], and [40].

We consider an observable $O(D, g; E)$ that depends on a single external energy scale $E$ (in addition to the cutoff $D$ and dimensionless coupling constant $g$ of the model). From renormalizability, we expect that in the regime $E \ll D$, the observable becomes a “scaling form,” $O(D, g; E) \xrightarrow{D \to \infty} O_{\text{scaling form}}(D, g; E) + O(1/D)$, meaning that it satisfies the Callan-Symanzik equation:

$$
\left[ D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g} + \gamma(g) \right] O_{\text{scaling form}}(D, g; E) = 0. \tag{A.35}
$$

In practice, one calculates $O(D, g; E)$ as a power series (in $g$ for now, though we later consider a series in $1/g$) and identifies the scaling form by keeping only the terms that are divergent or constant as $D \to \infty$. The divergences in this case can only be logarithmic [5], i.e. powers of $\ln \frac{D}{E}$, and the coefficients of the logarithms determine the functions $\beta(g)$ and $\gamma(g)$ (usually up to a certain order in an expansion). Due to the large logarithms, one does not really have an expansion in $g$, but instead an expansion in some parameter that depends on $g$ and $D/E$. RG improvement can be viewed as a resummation technique for turning the series in $g$ into a series in the correct expansion parameter.
The well-known solution to the Callan-Symanzik equation is:

\[ O_{\text{scaling form}}(D, g; E) = O_{\text{scaling form}}(D, g_M; E) \exp \left[ \int_g^{g_M} dg' \frac{\gamma(g')}{\beta(g')} \right], \quad (A.36) \]

where \( M \) is an energy scale that can be chosen arbitrarily, and where \( g_M \equiv g_R(D, g; M) \) is the “running” coupling at the scale \( M \), determined by:

\[ \left[ D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g} + \gamma(g) \right] g_R(D, g; M) = 0, \quad g_R(D, g; M = D) = g. \quad (A.37) \]

A convenient way to calculate the running coupling is to first identify a scaling invariant via \( T_K \equiv D e^{-\int^g dg' 1/\beta(g')} \), which satisfies \( \left[ D \frac{\partial}{\partial D} + \beta(g) \frac{\partial}{\partial g} \right] T_K = 0 \) by construction. (We write the invariant in the notation of the Kondo model, though so far the discussion is more general.) This invariant – which is only defined up to an overall rescaling by a pure number – is thus a function of \((D, g)\). We can then calculate \( g_M \) as a function of \( M/T_K \) by requiring that \((M, g)\) corresponds to the same \( T_K \) as the original \((D, g)\).

Setting the arbitrary scale to \( M = E \) is a particularly convenient choice, since it eliminates the large logarithm terms in \( O_{\text{scaling form}} \). If \( \gamma(g) \) is identically zero, then the full answer is found by deleting the logarithm terms and replacing \( g \rightarrow g_E \) in the constant terms (which only involve powers of \( g \) and pure numbers). The quantity \( g_E \), which only depends on \( E/T_K \), is then the correct expansion parameter, and typically we must restrict \( E/T_K \) to some particular regime in order for this parameter to be small (even though \( g \) is small). Non-zero \( \gamma(g) \) introduces some extra complication, as we discuss below.

Let us consider a more particular case, which we need for the Kondo model, in which the beta function starts at second order:

\[ \beta(g) = \beta_2 g^2 + \beta_3 g^3 + O(g^4). \quad (A.38) \]

The corresponding invariant \( T_K \) is:

\[ T_K = \alpha^{-1} D \exp \left[ \frac{1}{\beta_2 g} + \frac{\beta_3}{\beta_2^2} \ln |g| + O(g) \right], \quad (A.39) \]

where \( \alpha > 0 \) is an arbitrary constant. The interesting case is \( T_K \ll D \), which occurs for \( \text{sgn}(\beta_2 g) = -1 \). In the Kondo model, \( \beta_2 \) is negative and the antiferromagnetic regime
(g > 0) is universal, since we can send \( g \to 0^+ \) and \( D \to \infty \) with \( T_K \ll D \) fixed. RG improvement turns \( \mathcal{O}_{\text{scaling}} \) form into a function \( \mathcal{O}_{\text{universal}}(gE) \) [we again assume \( \gamma(g) \) is identically zero for the moment], or equivalently, a function \( \mathcal{O}_{\text{universal}}(E/T_K) \), which should be the same function even if we make convenient simplifications in the high energy part of the Hamiltonian (e.g. linearized band structure).

Setting \( \epsilon = 1/\ln \frac{M}{\alpha T_K} \), \( a_1 = 1/\beta_2 \), and \( a_2 = \beta_3/\beta_2^2 \), we see that the running coupling \( g_M \) must satisfy:

\[
-a_1 \frac{1}{g_M} - a_2 \ln |g_M| = \frac{1}{\epsilon} + O(g_M),
\]

which has the following solution for small \( \epsilon \):

\[
g_M = -a_1 \epsilon \left[ 1 - a_2 \epsilon \ln \epsilon - a_2 \ln |a_1| \epsilon + a_2^2 \epsilon^2 \ln^2 \epsilon + a_2^2 (1 + 2 \ln |a_1|) \epsilon^2 \ln \epsilon \right] + O(\epsilon^3). \tag{A.40}
\]

Expanding \( 1/\ln \frac{M}{\alpha T_K} = (1/\ln \frac{M}{T_K})(1 + n \ln \alpha / \ln \frac{M}{T_K}) + O(1/\ln^{n+2} \frac{M}{T_K}) \), we obtain:

\[
g_M = -\frac{1}{\beta_2 \ln \frac{M}{T_K}} \left[ 1 + \frac{\beta_3 \ln \frac{M}{T_K}}{\beta_2^2 \ln \frac{M}{T_K}} + \left( \frac{\beta_3 \ln |\beta_2| + \ln \alpha}{\beta_2^2} \right) \frac{1}{\ln \frac{M}{T_K}} + \left( \frac{\beta_3}{\beta_2^2} \right)^2 \frac{\ln^2 \ln \frac{M}{T_K}}{\ln^2 \frac{M}{T_K}} \right. \\
+ \left. 2 \frac{\beta_3}{\beta_2^2} \left( \frac{\beta_3 \ln |\beta_2| + \ln \alpha - \frac{\beta_3}{2 \beta_2^2}}{\ln \frac{M}{T_K}} \right) \frac{\ln \ln \frac{M}{T_K}}{\ln^2 \frac{M}{T_K}} \right] + O \left( \frac{1}{\ln^3 \frac{M}{T_K}} \right). \tag{A.41}
\]

The standard two loop result in the Kondo model is \( T_K = De^{-\frac{1}{2} + \frac{1}{2}g} \) \[9, 51\], which corresponds to \( \beta_2 = -2 \) and \( \beta_3 = 2 \); in this case, Eq. (A.42) agrees with Eq. (112) of Ref. [30] [note from their unnumbered equation before Eq. (113) that \( \ln \alpha = -(1/2) \ln 2 + a \)]. With \( \beta_2 < 0 \), the universal regime is \( g > 0 \) (antiferromagnetic). Setting \( \beta_2 = -2 \) with \( \beta_3 \) arbitrary yields Eq. (4.151) in the main text.

To see the effect of \( \gamma(g) \), it is convenient to write the exponential scale factor in Eq. (A.36) as:

\[
\exp \left[ \int_g^{g_M} \frac{dg'}{\beta(g')} \right] = \exp \left[ \int_0^{g_M} dg' \frac{\gamma(g')}{\beta(g')} \right] \exp \left[ -\int_0^{g} dg' \frac{\gamma(g')}{\beta(g')} \right]. \tag{A.43}
\]

With \( M = E \), we have a product of a term that depends only on \( gE \) (and hence can be absorbed into \( \mathcal{O}_{\text{universal}} \)) and a term that depends on the bare coupling \( g \). In other words,
we can write:

\[ O_{\text{scaling form}}(E/T_K) = O_{\text{universal}}(E/T_K) \exp \left[ - \int_0^g dg' \frac{\gamma(g')}{\beta(g')} \right], \]

(A.44)

where \( O_{\text{universal}}(E/T_K) \) is obtained by deleting all log terms in \( O_{\text{scaling form}} \) and multiplying by the \( g_E \)-dependent exponential factor. If \( \gamma(g) \) starts at the same order as \( \beta(g) \) (\( g^2 \) in the present case), then the \( g \)-dependent exponential factor is \( 1 + O(g) \), and can be dropped in the scaling limit \( (g \to 0^+ \text{ with fixed } T_K) \). In this limit, \( g \) vanishes like \( 1/\ln D \), as opposed to \( 1/D \) (the latter being what we have neglected in replacing \( O \to O_{\text{scaling form}} \)); it may be important to distinguish between the scaling limit (small \( 1/D \)) and the “extreme scaling limit” \([76]\) (small \( 1/\ln D \)).

In the main text, we obtain a beta function of the form \( \beta(g) = 1 + \beta_1 \frac{1}{g} + \ldots \) in the regime of large \( |g| \). The above calculations carry through straightforwardly with the change of variables \( \tilde{g} = 1/g \), which leads to a beta function starting at second order in the small parameter \( \tilde{g} \).

## A.5 Cutoff artifact in the time-dependent magnetization

Formally, the evaluation of the Kondo spin \( S_z \) following a quench in the one lead model is one of the simplest applications of our formalism in an interacting model. Unfortunately, the results seem to suffer from infrared pathologies. However, the calculation is still useful as a way of testing the unconventional cutoff scheme we have used throughout.

Consider three different cutoffs: a cutoff \( D_H \) on the Hamiltonian, a cutoff \( D_\rho \) on the initial density matrix prior to the quench, and a cutoff \( D_{\text{proj}} \) on the time-evolving density matrix. This last cutoff is implemented by calculating expectation values with respect to \( P_{D_{\text{proj}}} e^{-iHt} \rho e^{iHt} P_{D_{\text{proj}}} \), where \( P_{D_{\text{proj}}} \) is the projection operator onto the modes in \([-D_{\text{proj}}, D_{\text{proj}}]\). The conventional scheme is \( D_H = D_\rho = D_{\text{proj}} \); indeed, once \( D_H \) is finite, the other two cutoffs make no difference as long as neither is less than \( D_H \). Our calculation has so far used \( D_H = D_{\text{proj}} = \infty \) with \( D_\rho \) finite. It seems that we have to set \( D_H = \infty \) in
order to solve for the wavefunction; however, it seems based on the following example that we need to set $D_{\text{proj}} = D_\rho$ in order to get the right answer (see Fig. (A.1). In particular,

![Projection scheme](image)

Figure A.1: Projection scheme. We represent the initial state prior to the quench as a flat line, indicating that the modes from $-D$ to 0 are occupied (a zero temperature Fermi sea). The conventional scheme would be to evolve this state by the Hamiltonian that also is cut off by $D$; however, our approach in this thesis has been to evolve with the Hamiltonian with no cutoff. Since the modes in the Hamiltonian are in $(-\infty, \infty)$, the wavefunction “leaks out” from the bandwidth region $[-D, D]$, no matter how large $D$ is. In the toy example of the time-dependent magnetization, we can see that this leakage leads to an extra term $J^2 \ln(Dt)$ relative to the conventional scheme: a “cutoff artifact.” Projecting the time-dependent wavefunction back onto the bandwidth region (and rescaling to unit norm) eliminates the artifact, recovering the same answer in the conventional scheme. We suspect that this projection procedure would fix the higher-order discrepancies we find in the Kondo current.

the time-dependent magnetization up to second order, starting from an initial state with impurity spin $a_0$ and working at zero temperature, is found to be:

$$\langle S^z \rangle_t = S^z_{a_0a_0} \left[ 1 - (2\rho J_\perp)^2 X(Dt) + \ldots \right], \quad (A.45)$$

where $X(Dt)$ is given in the different schemes by (for large bandwidth):

$$X(Dt) = \begin{cases} 
\ln(Dt) + 1 + \gamma - \ln 2 & \text{for } D_H = D_\rho = D_{\text{proj}} \equiv D \text{ (conventional scheme)} \\
2[\ln(Dt) + 1 + \gamma] & \text{for } D_H = D_{\text{proj}} = \infty, \ D_\rho \equiv D \text{ (our scheme)} \\
\ln(Dt) + 1 + \gamma - \ln 2 & \text{for } D_H = \infty, \ D_{\text{proj}} = D_\rho \equiv D \text{ (projection scheme)}
\end{cases} \quad (A.46)$$

Note in particular that in our scheme, the log term has an extra factor of 2. This is carefully checked by referring to a calculation in the literature. Most likely, we should identify the
conventional scheme as the correct answer, and conclude that our scheme would break down at sufficiently high order in $J$ (though it may appear at low orders as if the theory has been regulated).

We proceed with the setup of the calculation. We consider the anisotropic Kondo Hamiltonian with cutoff $D_H$:

$$
H = \sum_{|k|<D_H} kc_{ka}^\dagger c_{ka} + \frac{1}{L} \sum_{|k|<D_H,|k'|<D_H} c_{ka}^\dagger \left[J_\perp (\sigma_{aa'}^x S^x + \sigma_{aa'}^y S^y) + J_z \sigma_{aa'}^z S^z\right] c_{k'a'}^\dagger. \quad (A.47)
$$

The anisotropy is not essential, but is included to ensure a precise match with a calculation in the literature. We take as the initial density matrix for the quench to be a thermal distribution with cutoff $D$, which then evolves with $H$ from $t = 0$ onward:

$$
\rho = e^{-\frac{i}{\hbar} \int_0^t \sum_{|k|<D} kc_{k}\dagger c_k}, \quad \rho(t) = e^{-iHt} \rho e^{iHt}. \quad (A.48)
$$

We define a projection operator $P_{D_{\text{proj}}}$ that projects onto the modes bounded by $D_{\text{proj}}$:

$$
P_{D_{\text{proj}}} = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{q_1,\ldots,q_n} \sum_{b_0,b_1,\ldots,b_n} |q_1 b_1 \ldots q_n b_n, b_0\rangle \langle q_1 b_1 \ldots q_n b_n, b_0|, \quad (A.49)
$$

where the states $|q_1 b_1 \ldots q_n b_n, b_0\rangle \equiv c_{q_1}^\dagger b_n \ldots c_{q_1}^\dagger b_0|b_0\rangle$ form a complete basis if all are included (the limit $D_{\text{proj}} = \infty$).

We are interested in calculating the time-dependent expectation value of $S^z$ projected time-evolving density matrix:

$$
(S^z)_t \equiv \text{Tr} \left(P_{D_{\text{proj}}} \rho(t) P_{D_{\text{proj}}} S^z\right) / \text{Tr} \left(P_{D_{\text{proj}}} \rho(t) P_{D_{\text{proj}}}\right). \quad (A.50)
$$

Formally, with $D_H = D_{\rho} = D_{\text{proj}} = \infty$, the Hamiltonian takes the usual field-theoretic form, the initial density matrix becomes $\rho = e^{-\frac{i}{\hbar} H^{(0)}}$, and $P_{D_{\text{proj}}} = 1$. In the conventional cutoff scheme, the time evolution keeps the modes in the initial density matrix within the bandwidth region; then we can replace $\rho(t) \rightarrow \rho$ in the denominator (since the partition function is time-independent) and set $P_{D_{\text{proj}}} = 1$ everywhere. However, if $D_H < D_{\text{proj}}$, then the normalization factor is, in general, time-dependent. This is simplest to see at zero
temperature, in which case \( \rho = |\Psi\rangle\langle\Psi| \) and 
\[
\text{Tr}(P_{D_{\text{proj}}}\rho(t)P_{D_{\text{proj}}}) = |\langle\Psi(t)|P_{D_{\text{proj}}}\Psi(t)\rangle|^2.
\]
If \( D_H > D_{\text{proj}} \), then some part \( |\Psi(t)\rangle \) is projected out, and so we will obtain a time-dependent factor instead of the full norm \( \langle\Psi(t)|\Psi(t)\rangle = 1 \).

### A.5.1 A calculation from the literature

In the case \( D_{\text{proj}} = D_H \geq D_{\rho} \), we can read off the magnetization to second order from a calculation in the literature (Anders and Schiller [77], hereafter “AS”). They do the calculation by iterated commutators of \( H \) with \( S^z \). It is straightforward to convert their notation to ours: their \( \rho_F J_\perp \) is our \( \rho J_\perp \), with \( \rho = 1/(2\pi) \) being the density of states per unit length in our setup. Their density of states (per spin) in the Hamiltonian is given by \( \rho(\epsilon) = \rho_F \Theta(D - |\epsilon|) \) in the wide-band limit; thus, their \( \rho \) is our \( D_H \). They do not explicitly include \( D_{\rho} \), but we can include it by replacing their Fermi functions via 
\[
f(k) \rightarrow \Theta(D_{\rho} - |k|)f(k).
\]
Implicitly, they have set \( D_{\text{proj}} = D_H \) (or indeed, any \( D_{\text{proj}} \geq D_H \) is equivalent.) Converting their Eq. (71) to our notation yields:

\[
\langle S^z \rangle_t = S^z_{a_0a_0} - S^z_{a_0a_0}(2\rho J_\perp)^2 \int_{-D_H}^{D_H} dk_1dk_2 \left[ 1 - \Theta(D_\rho - |k_1|)\Theta(D_\rho - |k_2|) \right] f(k_1) f(k_2) \times \text{Re} \left( \frac{1 - e^{-i(k_1-k_2)t}}{(k_1-k_2)^2} - \frac{it}{k_1-k_2} \right) + O(J^3). 
\tag{A.51}
\]

The \( \frac{it}{k_1-k_2} \) term is pure imaginary and can hence be dropped. For later reference, we note:

\[
\text{Re} \left( \frac{1 - e^{-i(k_1-k_2)t}}{(k_1-k_2)^2} - \frac{it}{k_1-k_2} \right) = 2 \left[ \sin \left( \frac{k_1-k_2}{2} t \right) \right]^2. \tag{A.52}
\]

Let us first consider the conventional scheme, \( D_H = D_\rho \equiv D \) (and recall that \( D_{\text{proj}} = D_H \) by assumption). Then Eq. (A.51) becomes:

\[
\langle S^z \rangle_t = S^z_{a_0a_0} - S^z_{a_0a_0}(2\rho J_\perp)^2 \int_{-D}^{D} dk_1dk_2 \left[ 1 - f(k_1) \right] f(k_2)2 \left[ \sin \left( \frac{k_1-k_2}{2} t \right) \right]^2. \tag{A.53}
\]

---

2Repeating the calculation of AS, I find that they have used the convention \( J\sigma \cdot S \) rather than the alternatives \( \sigma \cdot \sigma_0 \) or \( S \cdot S \) that rescale \( J \) by a factor of 2 one way or the other. Thus, in the anisotropic case, their spin-flipping term, \( J_\perp \left( \sigma^+ S^- + \sigma^- S^+ \right) \), is correct as written, but their spin-preserving term should be \( J_x \sigma^z S^z \) and appears to be written as \( J_x \sigma^z S^z \); instead. Also, AS say in a footnote that they use the same convention as Ref. [2], which would be \( \sigma \cdot \sigma_0 \). The spin-preserving term has no effect on the calculation at the order considered here.
This is the case considered by AS. At zero temperature, their result is:

$$\langle S^z \rangle_t = S^z_{a_0 a_0} - S^z_{a_0 a_0} (2 \rho J_\perp)^2 \left[ G(2Dt) - 2G(Dt) \right],$$  \hspace{1cm} (A.54a)

where:  

$$G(x) = \sum_{l=1}^\infty \frac{(-1)^{l+1}}{(2l)!2l(2l-1)} x^{2l}.$$  \hspace{1cm} (A.54b)

They show that this agrees well with their numerics at short times, but they do not pursue further evaluation. However, it is straightforward to show the asymptotic relation $G(x) \xrightarrow{x \to \infty} \frac{\pi}{2} x - \ln x - 1 - \gamma$, from which we obtain the first case in the result stated earlier [Eq. (A.46)].

To verify this directly, and to highlight the difference with the next case, let us separate the terms $[1 - f(k_1)] f(k_2) = f(k_2) - f(k_1) f(k_2)$ in Eq. (A.53) to find:

$$\langle S^z \rangle_t = S^z_{a_0 a_0} - S^z_{a_0 a_0} (2 \rho J_\perp)^2 \left\{ \int_{-D}^D dk_1 dk_2 f(k_2) \left[ \sin \left( \frac{k_1-k_2 t}{2} \right) \right]^2 \right. $$

$$- \left. \int_{-D}^D dk_1 dk_2 n(k_1) f(k_2) \left[ \sin \left( \frac{k_1-k_2 t}{2} \right) \right]^2 \right\}. \hspace{1cm} (A.55)

Evaluation of the two terms in curly braces at zero temperature yields the following results in the large bandwidth limit:

$$1st \ term = \int_{-D}^D dk_1 \int_{-D}^0 dk_2 2 \left[ \sin \left( \frac{k_1-k_2 t}{2} \right) \right]^2 \rightarrow \pi Dt - [\ln(Dt) + 1 + \gamma + \ln 2] + \ldots, \hspace{1cm} (A.56a)$$

$$2nd \ term = - \int_{-D}^0 dk_1 dk_2 2 \left[ \sin \left( \frac{k_1-k_2 t}{2} \right) \right]^2 \rightarrow -\pi Dt + 2 [\ln(Dt) + 1 + \gamma] + \ldots \hspace{1cm} (A.56b)$$

Adding these together, we confirm the first case in Eq. (A.46).

We now show that in the cutoff scheme used throughout this thesis, only the linear term $(\pi Dt)$ is present in (A.56a), thus leading to the second case in Eq. (A.46). With $D_H = \infty$
(which sets $D_{\text{proj}} = \infty$ as well, by assumption) and $D_{\rho} \equiv D$, Eq. (A.51) becomes:

$$\langle S_z \rangle_t = S_{z_{a_0a_0}} - S_{z_{a_0a_0}}(2\rho J_\perp)^2 \left\{ \int_{-\infty}^{\infty} dk_1 \int_{-D}^{D} dk_2 \ f(k_2)2 \left[ \frac{\sin \left( \frac{k_1-k_2}{2} t \right)}{k_1-k_2} \right]^2 \right. \left. - \int_{-D}^{D} dk_1dk_2 \ f(k_1)f(k_2)2 \left[ \frac{\sin \left( \frac{k_1-k_2}{2} t \right)}{k_1-k_2} \right]^2 \right\}. \quad (A.57)$$

Comparing to the form (A.53), we see that the second term in curly braces, with $f(k_1)f(k_2)$, matches exactly. However, the first term is different, because in this term the $k_1$ integration is unrestricted (since $D_H = \infty$ now, and since there is no Fermi function in $k_1$ in that term).

We can carry out the $k_1$ integration explicitly to find:

$$\text{first term} = \int_{-D}^{D} dk_2 \ f(k_2) \int_{-\infty}^{\infty} dk_1 2 \left[ \frac{\sin \left( \frac{k_1-k_2}{2} t \right)}{k_1-k_2} \right]^2 = \int_{-D}^{D} dk_2 \ f(k_2) \pi t = \pi Dt. \quad (A.58)$$

Note that this holds for arbitrary temperature $T$. At zero temperature, we see that only the linear term in the corresponding contribution from case 1 [Eq. (A.56a)] is the same; the log term and constants are not there. Combining with Eq. (A.56b), we obtain the second case in Eq. (A.46).

### A.5.2 Wavefunction calculation

We now set up the calculation in the wavefunction formalism, with no cutoff on the Hamiltonian ($D_H = \infty$). We consider $D_{\text{proj}} \geq D_{\rho} \equiv D$ at first, then specialize first to $D_{\text{proj}} = \infty$ (the scheme used in the main text) and then to $D_{\text{proj}} = D_{\rho}$ (the projection scheme).

We are interested in the time-evolving expectation value of $S^z$ in the projected density matrix [i.e. Eq. (A.50) with $\mathcal{O} = S^z$ and the temperature set to zero; later we generalize to include temperature]:

$$\langle S_z \rangle_t = \frac{\langle \Psi(t) | S^z P_{D_{\text{proj}}} | \Psi(t) \rangle}{\langle \Psi(t) | P_{D_{\text{proj}}} | \Psi(t) \rangle}, \quad (A.59)$$

where $|\Psi(t)\rangle = e^{-iHt} |\Psi\rangle$ and $|\Psi\rangle \equiv c_{N a_0 N}^\dagger |a_0\rangle$, with the quantum numbers $k_N a_N$ later chosen to describe a filled Fermi sea (cut off by $D_{\rho} \equiv D$) and the initial impurity spin $a_0$ arbitrary. When we generalize to include temperature, we assume a thermal distribution
only in the lead (i.e. the initial spin of the impurity is $a_0$ regardless of temperature), as would occur if the impurity is in a strong magnetic field prior to the quench.

We thus consider the expectation value $\langle \Psi(t)|\mathcal{O}|\Psi(t)\rangle$, where $\mathcal{O}$ is either $S^z P_{\text{proj}}$ or $S^z$. The calculation is significantly simpler if we consider $D_{\text{proj}} \geq D_\rho$ and work in the $J = 0$ basis, for then $\mathcal{O}$ commutes with any of the $c_{k}^\dagger(t)$ operators that appear in $|\Psi(t)\rangle$; this commutation property then we can treat $\mathcal{O}$ as a $\mathcal{O}_{\text{imp}}$ operator and use normal ordered formula 2 from Chapter 2. The reason for the commutation property is that the field operators in the $J = 0$ basis evolve by phases $(c_{k}^\dagger(t) = e^{-ikt}c_{k}^\dagger)$, which means that they commute with the projector $P_{D_{\text{proj}}}$ as long as $D_{\text{proj}} \geq D$.

From normal ordered formula 2 (2.76), we obtain the time-evolving expectation value of $\mathcal{O}$ in terms of normal ordered matrix elements:

$$
\langle \Psi(t)|\mathcal{O}|\Psi(t)\rangle = \langle a_0(t)|\mathcal{O}|a_0(t)\rangle + \sum_{n=1}^{N} \frac{1}{n!} L^n \sum_{m_1, \ldots, m_n=1}^{N} \Omega_{n,a_0}(t; k_0 a_n),
$$

where:

$$
\Omega_{n,a_0}(t; k_0 a_n) = L^n : \langle \Psi_{k_0 a_n,a_0}(t) | \mathcal{O} | \Psi_{k_0 a_n,a_0}(t) \rangle :.
$$

As in the calculation of the current, it is useful to consider the “off-diagonal” case defined via:

$$
\Omega^{(\text{off-diag})}_{n,a_0}(t; k'_0 a'_n; k_0 a_n) = L^n : \langle \Psi_{k'_0 a'_n,a_0}(t) | \mathcal{O} | \Psi_{k_0 a_n,a_0}(t) \rangle :.
$$

By the symmetry properties of normal ordered overlaps (Sec. 2.3.4), we know that $\Omega^{(\text{off-diag})}_{n,a_0}$ inherits the fermionic symmetry properties of the wavefunctions on either side; thus, we must be able to write it as the antisymmetrization of some “reduced” function $\Omega^{(\text{red})}_{n,a_0}$:

$$
\Omega^{(\text{off-diag})}_{n,a_0}(t; k'_0 a'_n; k_0 a_n) = \sum_{\sigma, \sigma' \in \text{Sym}(n)} (\text{sgn} \sigma)(\text{sgn} \sigma') \Omega^{(\text{red})}_{n,a_0}(t; k'_0 a'_n; k_0 a_n; \sigma; k_0 a_n; \sigma').
$$

This step breaks down if we use the $|J| = \infty$ basis, for then the time-evolving operators $c_{k}^\dagger(t)$ include all modes and thus do not commute with $P_{D_{\text{proj}}}$ unless $D_{\text{proj}} = \infty$. 
Relabeling summation indices, we then obtain:

\[
\langle \Psi(t)|O|\Psi(t)\rangle = \langle a_0(t)|O|a_0(t)\rangle \\
+ \sum_{n=1}^{N} \frac{1}{L^n} \sum_{m_1,...,m_n=1}^{N} \sum_{\sigma \in \text{Sym}(n)} (\text{sgn } \sigma) \Omega^{(\text{red})}_{n,a_0}(t; k_m a_m; k_m \sigma a_m \sigma).
\]  

(A.64)

Our scheme from the main text.

In the \(D_{\text{proj}} = \infty\) case, the projector \(P_{D_{\text{proj}}}\) is the identity, and so has no effect; the general expectation value (A.50) becomes (at zero temperature for now):

\[
\langle S^z \rangle_t = \langle \Psi(t)|S^z|\Psi(t)\rangle,
\]  

(A.65)

where there is no denominator because \(\langle \Psi(t)|\Psi(t)\rangle = 1\). Thus, we only need to calculate (A.64) with \(O = S^z\). From Eq. (4.109) in the main text, we can read off:

\[
\Omega^{(\text{red})}_{n,a_0}(t; k'_n a'_n; k_n a_n) = Q_n(t; k_n - k'_n) \Xi_n[a'_n; a_n] b'_0 b_0 S^z b_0 b_0.
\]  

(A.66)

Thus, Eq. (A.64) yields:

\[
\langle S^z \rangle_t \xrightarrow{\text{therm. limit}} S^z_{a_0 a_0} + \sum_{n=1}^{\infty} \int_{-D}^{D} \frac{dk_n}{2(2\pi)^n} \left[ \prod_{j=1}^{n} f(k_j) \right] \sum_{\sigma \in \text{Sym}(n)} W^{(\sigma)}_{a_0} Q_n(t; k_{\sigma n} - k_n),
\]  

(A.67)

where the spins sums are given in this case by:

\[
W^{(\sigma)}_{a_0} = (\text{sgn } \sigma) \sum_{a_1,...,a_n} \Xi_n[a_n; a_{n\sigma}] b'_0 b_0 S^z b'_0 b_0.
\]  

(A.68)

For the anisotropic Kondo model, the \(S\)-matrix is \(S = I + \mathcal{M}\), with \(\mathcal{M}\) given in Eq. (A.8) (with the potential scattering \(J'\) set to zero). Then the first few spin sums are:

\[
W^{(1)}_{a_0} = -2S^z_{a_0 a_0} J^2_{\perp} + O(J^4),
\]  

(A.69a)

\[
W^{(1,2)}_{a_0} = O(J^4),
\]  

(A.69b)

\[
W^{(2,1)}_{a_0} = 4S^z_{a_0 a_0} J^2_{\perp} + O(J^4),
\]  

(A.69c)

where \(a_0\) is not summed, and where we have taken \(J_{\perp}\) and \(J_z\) to each be of the same order \((J)\) with fourth order and higher terms neglected. The remaining spin sums are order \(J^3\)
or higher. The only $Q_n$ integrals we need to this order are:

$$Q_1(t; 0) = t,$$

$$Q_2(t; k_2 - k_1, k_1 - k_2) = \frac{1 - e^{-i(k_1-k_2)t}}{(k_1 - k_2)^2} - \frac{it}{k_1 - k_2}.$$  

(A.70a)

(A.70b)

Up to second order, the answer is therefore:

$$\langle S^z \rangle_t = S^z_{a_0a_0} + W^{(1)}_{a_0} \int_{-D}^{D} \frac{dk_1}{2\pi} f(k_1) Q_1(t; 0)$$

$$+ W^{(2,1)}_{a_0} \int_{-D}^{D} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} f(k_1) f(k_2) Q_2(t; k_2 - k_1, k_1 - k_2) + O(J^3)$$

(A.71a)

$$= S^z_{a_0a_0} - S^z_{a_0a_0} (2\rho J_\perp)^2 \left[ \pi D t - \int_{-D}^{D} dk_1 dk_2 f(k_1) f(k_2) \text{Re} \left( \frac{1 - e^{-i(k_1-k_2)t}}{(k_1 - k_2)^2} \right) \right] + O(J^3).$$

(A.71b)

The imaginary part of $Q_2$ makes no contribution (due to the symmetry of the integration).

We have also used $\int_{-D}^{D} dk f(k) = D$, which holds independent of temperature. Comparing with Eq. (A.57) and Eq. (A.58), we see that we have reached the same answer (A.57) as before, culminating in the second case of Eq. (A.46).

**Projection scheme.**

We now consider the new cutoff scheme, in which $D_\rho = D_{\text{proj}} = D$ is finite (with $D_H = \infty$ still, so that we can use our solution for the wavefunction). Then the regulated expectation value (A.50) becomes (at zero temperature for now):

$$\langle S^z \rangle_t = \frac{\langle \Psi(t) | S^z P_D | \Psi(t) \rangle}{\langle \Psi(t) | P_D | \Psi(t) \rangle}.$$  

(A.72)

We evaluate the numerator and denominator separately up to the second order.\(^4\) To cover both cases at once, we calculate $\langle \Psi(t) | \hat{A} P_D | \Psi(t) \rangle$, where $\hat{A}$ is an arbitrary ($J$-independent) 2-by-2 matrix that acts only the impurity spin, with matrix elements written as:

$$\langle b_0^\dagger | \hat{A} | b_0 \rangle = A_{b_0 b_0} = \begin{cases} 
S_{b_0 b_0}^z & \hat{A} = S^z \\
\delta_{b_0 b_0} & \hat{A} = 1
\end{cases}.$$  

(A.73)

\(^4\text{It would be nicer if we could combine these into a single calculation, e.g. by some rule analogous to "vacuum bubbles" for taking care of the denominator automatically.}\)
Working to second order amounts to keeping up to \( n = 2 \) in the sum in Eq. (A.64), yielding:

\[
\langle \Psi(t) | \hat{A} P_D | \Psi(t) \rangle = \langle a_0 | \hat{A} | a_0 \rangle + \frac{1}{L} \sum_{m_1=1}^{N} \Omega_{1, a_0}^{(\text{red})} (t; k_1 a_1; k_1 a_1) \\
+ \frac{1}{L^2} \sum_{m_1, m_2 = 1}^{N} \sum_{\sigma \in \text{Sym}(2)} (\text{sgn } \sigma) \Omega_{2, a_0}^{(\text{red})} (t; k_1 a_1, k_2 a_2; k_\sigma a_\sigma_1, k_{\sigma_2} a_{\sigma_2}) + \ldots \\
= A_{a_0 a_0} + \frac{1}{L} \sum_{D<k_1<0} \sum_{a_1} \Omega_{1, a_0}^{(\text{red})} (t; k_1 a_1; k_1 a_1) \\
+ \frac{1}{L^2} \sum_{-D<k_1<0} \sum_{a_1} \sum_{a_2} (\text{sgn } \sigma) \Omega_{2, a_0}^{(\text{red})} (t; k_1 a_1, k_2 a_2; k_\sigma a_\sigma_1, k_{\sigma_2} a_{\sigma_2}) + \ldots, \quad (A.74)
\]

where \( \Omega_{1, a_0}^{(\text{red})} \) is defined via Eqs. (A.62) and (A.63) with \( O = \hat{A} P_D \). All of the \( n \geq 3 \) terms are third order or higher due to the normal ordering. We will find that up to the second order, the projection operator only makes a difference in the \( n = 1 \) term.

For the \( n = 1 \) term, we need to calculate the following normal ordered overlap:

\[
: \langle \Psi_{k_1 a_1, a_0} (t) | \hat{A} P_D | \Psi_{k_1 a_1, a_0} (t) \rangle : = : \langle \Psi_{k_1 a_1, a_0}^0 (t) | \hat{A} P_D | \Psi_{k_1 a_1, a_0}^1 (t) \rangle :
+ : \langle \Psi_{k_1 a_1, a_0}^1 (t) | \hat{A} P_D | \Psi_{k_1 a_1, a_0}^0 (t) \rangle :
+ : \langle \Psi_{k_1 a_1, a_0}^0 (t) | \hat{A} P_D | \Psi_{k_1 a_1, a_0}^1 (t) \rangle :, \quad (A.75)
\]

where:

\[
| \Psi_{k_1 a_1, a_0}^0 (t) \rangle = c_{k_1 a_1}^\dagger (t) | a_0 \rangle, \quad (A.76a) \\
| \Psi_{k_1 a_1, a_0}^1 (t) \rangle = | \chi_{k_1 a_1, a_0} (t) \rangle. \quad (A.76b)
\]

The momentum \( k_1 \) is in the initial state, so it is in the bandwidth region (\( |k_1| < D \)); thus, the projection operator has no effect in the \((0, 1)\) and \((1, 0)\) terms:

\[
: \langle \Psi_{k_1 a_1, a_0}^0 (t) | \hat{A} P_D | \Psi_{k_1 a_1, a_0}^1 (t) \rangle : = \langle a_0 | c_{k_1 a_1} (t) | \hat{A} | \chi_{k_1 a_1, a_0} (t) \rangle \\
= \sum_{b_0} \frac{1}{L} \int dx \ A_{a_0 b_0} (x) \Theta(0 < x < t) = \sum_{b_0} \frac{1}{L} A_{a_0 b_0} \left( -i T_{a_1 a_0}^{a_1 b_0} \right) t \\
= \left( : \langle \Psi_{k_1 a_1, a_0}^0 (t) | \hat{A} P_D | \Psi_{k_1 a_1, a_0}^1 (t) \rangle : \right)^*. \quad (A.77)
\]

In other words, taking the overlap of a crossing state with a momentum operator (with momentum in the bandwidth region) already projects onto the bandwidth region, so the
projector has no effect.\footnote{This would not be so simple in the $|J| = \infty$ basis, for then $c^\dagger_k(t)$ would not project onto the bandwidth region.}

In the $(1,1)$ term, with a crossing state on both sides, the presence of the projection operator changes the answer. The projection introduces another variable $q_1 \in [-D, D]$ which represents the modes of the crossing state that fall within the bandwidth region. We find:

\[
: \langle \Psi_{k_1 a_1 a_0}^1(t)|\hat{A}P_D|\Psi_{k_1 a_1 a_0}^1(t) : = \langle \chi_{k_1 a_1 a_0}(t)|\hat{A}P_D|\chi_{k_1 a_1 a_0}(t) \rangle
\]

\[
= \frac{1}{L} \sum_{|q_1|<D} \sum_{b_0, b_1} \int dx' \text{e}^{ik_1(t-x')} \text{e}^{iq_1 x'} \text{i} D_{a_1 a_0}^{b_1 b_0} A_{b_0 b_1} \int dx \text{e}^{-ik_1(t-x)} \text{e}^{-iq_1 x} \\
\times (-i T_{a_1 a_0}^{b_1 b_0}) \Theta(0<x<t)
\]

\[
= \frac{1}{L^2} \sum_{|q_1|<D} \sum_{b_0, b_1} T_{a_1 a_0}^{b_1 b_0} A_{b_0 b_1} T_{a_1 a_0}^{b_1 b_0} Q_1(t;k_1 - q_1) Q_1(t;k_1 - q_1)
\]

\[
= \frac{1}{L^2} \sum_{|q_1|<D} \sum_{b_0, b_1} T_{a_1 a_0}^{b_1 b_0} A_{b_0 b_1} T_{a_1 a_0}^{b_1 b_0} (Q_2(t;k_1 - q_1, q_1 - k_1) + Q_2(t;q_1 - k_1, k_1 - q_1)) \] \hspace{1cm} (A.78)

where we have used a simple Heaviside function to separate the product of $Q_1$ integrals into a sum of two $Q_2$ integrals. All together, we obtain the following for the $n = 1$ contribution to the matrix element:

\[
\frac{1}{L} \sum_{-D<k_1<0} \sum_{a_1} \Omega^{(\text{red})}_{a_0 a_1}(t;k_1 a_1; k_1 a_1) = \frac{1}{L} \sum_{-D<k_1<0} \left[ \sum_{b_0, a_1} A_{a_0 b_0} \left( -i T_{a_1 a_0}^{a_1 b_0} \right) + \text{c.c.} \right] t \\
+ \frac{1}{L^2} \sum_{-D<k_1<0} \sum_{|q_1|<D} \sum_{b_0, b_1, a_1} T_{a_1 a_0}^{b_1 b_0} A_{b_0 b_1} T_{a_1 a_0}^{b_1 b_0} \times [Q_2(t;k_1 - q_1, q_1 - k_1) + Q_2(t;q_1 - k_1, k_1 - q_1)] \] \hspace{1cm} (A.79)

The spin sums appearing here are given to second order by:

\[
\sum_{b_0, a_1} A_{a_0 b_0} \left( -i T_{a_1 a_0}^{a_1 b_0} \right) = \begin{cases} 
-\frac{1}{2} S_{a_0 a_0} (J^2_\perp + \frac{1}{2} J^2_\parallel) + \ldots & \hat{A} = S^z \\
-\frac{1}{2} (J^2_\perp + \frac{1}{2} J^2_\parallel) + \ldots & \hat{A} = 1 
\end{cases} \] \hspace{1cm} (A.80)
and:

$$
\sum_{b_0',b_0,a_0,k_1,a_1} T_{a_1a_0}^{b_1b_0} A_{b_0' b_0} T_{a_1a_0}^{b_1b_0} = \begin{cases} 
-S_{a_0a_0}^z (J_{\perp}^2 - \frac{1}{2} J_z^2) + \ldots & \hat{A} = S^z \\
J_{\perp}^2 + \frac{1}{2} J_z^2 + \ldots & \hat{A} = 1
\end{cases}
$$

(A.81)

In the $n = 2$ contribution, it turns out that we can get the right answer up to second order by setting $P_D = 1$ (which allows us to use the calculation of the previous section). To show this, we begin by recalling the two particle wavefunction:

$$
|\Psi_{k_1a_1k_2a_2,a_0}(t)\rangle = |\Psi_{k_1a_1k_2a_2,a_0}^0(t)\rangle + |\Psi_{k_1a_1k_2a_2,a_0}^1(t)\rangle + |\Psi_{k_1a_1k_2a_2,a_0}^2(t)\rangle,
$$

(A.82a)

$$
|\Psi_{k_1a_1k_2a_2,a_0}^0(t)\rangle = c_{k_2a_2}^{\dagger}(t) c_{k_1a_1}^{\dagger}(t) |a_0\rangle,
$$

(A.82b)

$$
|\Psi_{k_1a_1k_2a_2,a_0}^1(t)\rangle = c_{k_2a_2}^{\dagger}(t) |\chi_{k_1a_1,a_0}(t)\rangle - c_{k_1a_1}^{\dagger}(t) |\chi_{k_2a_2,a_0}(t)\rangle
$$

(A.82c)

$$
|\Psi_{k_1a_1k_2a_2,a_0}^2(t)\rangle = |\chi_{k_1a_1,k_2a_2,a_0}(t)\rangle - |\chi_{k_2a_2,k_1a_1,a_0}(t)\rangle.
$$

(A.82d)

Since $\chi_{k_1a_1,a_0}(t)$ is $O(J)$ and $\chi_{k_2a_2,k_1a_1,a_0}(t)$ is $O(J^2)$, we obtain:

$$
\langle \Psi_{k_1' a_1' k_2' a_2' a_0'}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle = \langle \Psi_{k_1' a_1' k_2' a_2' a_0'}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle
$$

$$
\langle \Psi_{k_1a_1k_2a_2,a_0}(t) | S^z P_D | \Psi_{k_1' a_1' k_2' a_2' a_0'}(t) \rangle = \langle \Psi_{k_1a_1k_2a_2,a_0}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle
$$

$$
\langle \Psi_{k_1a_1k_2a_2,a_0}(t) | S^z P_D | \Psi_{k_1' a_1' k_2' a_2' a_0'}(t) \rangle = \langle \Psi_{k_1a_1k_2a_2,a_0}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle
$$

$$
+ O(J^3). \quad (A.83)
$$

The momenta $k_1, k_2, k_1'$, and $k_2'$ are all in the bandwidth region. Carrying out the normal ordering, we find:

$$
\langle \Psi_{k_1' a_1' k_2' a_2', a_0}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle = \langle a_0'| c_{k_1'a_1'}^{\dagger}(t) c_{k_2'a_2'}^{\dagger}(t) S^z P_D (|\chi_{k_1a_1k_2a_2,a_0}(t)\rangle - |\chi_{k_2a_2,k_1a_1,a_0}(t)\rangle)
$$

(A.84)

$$
\langle \Psi_{k_1'a_1' k_2'a_2', a_0}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle = - \left[ \langle \chi_{k_1'a_1', a_0'}(t) | c_{k_2'a_2'}^{\dagger}(t) S^z P_D c_{k_2'a_2'}(t) | \chi_{k_1a_1,a_0}(t) \rangle 

- (k_1 \leftrightarrow k_2, a_1 \leftrightarrow a_2) - (k_1' \leftrightarrow k_2', a_1' \leftrightarrow a_2') + (k_1 \leftrightarrow k_2, a_1 \leftrightarrow a_2, k_1' \leftrightarrow k_2', a_1' \leftrightarrow a_2') \right]
$$

(A.85)

$$
\langle \Psi_{k_1'a_1' k_2'a_2', a_0}(t) | S^z P_D | \Psi_{k_1a_1k_2a_2,a_0}(t) \rangle = \left( \langle \chi_{k_1'a_1' k_2'a_2', a_0}(t) \rangle - \langle \chi_{k_2'a_2' k_1'a_1', a_0}(t) \rangle \right) S^z P_D c_{k_2'a_2'}^{\dagger}(t) c_{k_1'a_1'}(t) |a_0\rangle.
$$

(A.86)
In each of these terms, the projection operator $P_D$ can be replaced by 1. The point is that the momenta in the freely-evolving field operators are in the bandwidth region, and the only terms that occur here are contractions between freely-evolving field operators and crossing states. These contractions already project onto the bandwidth region. At the next order, we would encounter terms like: $\langle \Psi^1(t)|S_z P_D|\Psi^2(t) \rangle$: in which crossing states would contract directly with each other, in which case the projection operator does make a difference.

Thus, to the second order, we can read off the answer using the previous calculation (which had $D_{\text{proj}} = \infty$):

$$
\Omega_{2,0}^{(\text{red})}(t; k'_1 k'_2; k_1 k_2) = \sum_{b_0, b'_0} Q_0(t; k_1 - k'_1, k_2 - k'_2) \Xi_2[a'_1, a'_2|a_1, a_2, b'_0, b_0, A_{b'_0 b_0}] + O(J^3).
$$

(A.87)

The contribution to the matrix element is therefore:

$$
\frac{1}{L^2} \sum_{-D<k_1<0} \sum_{-D<k_2<0} (\text{sgn} \sigma) \sum_{b_0, b'_0, a_1, a_2} \Xi_2[a_1, a_2; a_{\sigma_1}, a_{\sigma_2}, b_0, b'_0, A_{b'_0 b_0}] Q_2(t; k_{\sigma_1} - k_1, k_{\sigma_2} - k_2) + O(J^3)
$$

(A.88)

We need the following spin sums:

$$
\sum_{b_0, b'_0, a_1, a_2} (\text{sgn} \sigma) \Xi_2[a_1, a_2; a_{\sigma_1}, a_{\sigma_2}] b'_0 b_0 A_{b'_0 b_0} = \begin{cases} 
O(J^4) & \hat{A} = S^z \text{ and } \sigma = (1, 2) \\
4S^z_{a_0 a_0} J^2_\perp + O(J^4) & \hat{A} = S^z \text{ and } \sigma = (2, 1) \\
0 & \hat{A} = 1 
\end{cases}
$$

(A.89)

All together, we have shown the following to second order:

$$
\langle \Psi(t)|S_z P_D|\Psi(t) \rangle = S^z_{a_0 a_0} - S^z_{a_0 a_0} (J^2_\perp + \frac{1}{2} J^2_z) \sum_{-D<k_1<0} t
$$

$$
- S^z_{a_0 a_0} (J^2_\perp - \frac{1}{2} J^2_z) \frac{1}{L^2} \sum_{-D<k_1<0, |q_1|<D} [Q_2(t; k_1 - q_1, q_1 - k_1) + Q_2(t; q_1 - k_1, k_1 - q_1)]
$$

$$
+ \frac{1}{L^2} \sum_{-D<k_1<0, -D<k_2<0} 4S^z_{a_0 a_0} J^2_\perp Q_2(t; k_2 - k_1, k_1 - k_2) + O(J^3),
$$

(A.90)
\[\langle \Psi(t)|P_D|\Psi(t)\rangle = 1 - (J_\perp^2 + \frac{1}{2}J_z^2) \sum_{-D<k_1<0} t + \left(J_\perp^2 + \frac{1}{2}J_z^2\right) \frac{1}{L^2} \sum_{-D<k_1<0, |q_1|<D} [Q_2(t; k_1 - q_1, q_1 - k_1) + Q_2(t; q_1 - k_1, k_1 - q_1)] + O(J^3)\]

Taking the ratio, some terms cancel, leaving the following expression for the regulated expectation value:

\[
\frac{\langle \Psi(t)|S^z P_D|\Psi(t)\rangle}{\langle \Psi(t)|P_D|\Psi(t)\rangle} = S_{a_0a_0}^z - S_{a_0a_0}^z J_z + \frac{1}{L^2} \sum_{-D<k_1<0, |q_1|<D} [Q_2(t; k_1 - q_1, q_1 - k_1) + Q_2(t; q_1 - k_1, k_1 - q_1)] + 4S_{a_0a_0}^z J_\perp \frac{1}{L^2} \sum_{-D<k_1<0} Q_2(t; k_2 - k_1, k_1 - k_2) + O(J^3). \quad (A.92)
\]

The \(J_z\) dependence of the numerator has cancelled with that of the denominator. Had we only done the projection in the numerator and used the full norm \(\langle \Psi(t)|\Psi(t)\rangle = 1\) as the denominator, we would have obtained \(\langle S^z \rangle_t\) changing with time even in the case \(J_\perp = 0\) (in which no spin flips are possible and we should have \(\langle S^z \rangle_t = S_{a_0a_0}^z\)).

We note that the symmetric part of \(Q_2\) is the same as the real part (at least in the case we need, when the momenta in the argument add to zero):

\[Q_2(t; q_1', -q_1') + Q_2(t; -q_1', q_1') = 2\text{Re} \left[ \frac{1 - e^{-iq_1't}}{(q_1')^2} \right]. \quad (A.93)\]

Then the thermodynamic limit yields:

\[
\frac{\langle \Psi(t)|S^z P_D|\Psi(t)\rangle}{\langle \Psi(t)|P_D|\Psi(t)\rangle} \xrightarrow{\text{therm. limit}} S_{a_0a_0}^z - S_{a_0a_0}^z (2J_\perp)^2 \int_{-D}^{0} \frac{dk_1}{2\pi} \int_{-D}^{D} \frac{dq}{2\pi} \text{Re} \left[ \frac{1 - e^{-i(q_1-k_1)t}}{(q_1-k_1)^2} \right] + S_{a_0a_0}^z (2J_\perp)^2 \int_{-D}^{0} \frac{dk_1}{2\pi} \int_{-D}^{D} \frac{dk_2}{2\pi} \text{Re} \left[ \frac{1 - e^{-i(k_1-k_2)t}}{(k_1-k_2)^2} \right] + O(J^3), \quad (A.94)
\]

where we have used the symmetry of the integration in the second term. Generalizing to include temperature replaces each \(\int_{-D}^{0} dk \to \int_{-D}^{D} dk \ f(k)\), while leaving the \(q_1\) integral
una

ected. Then, relabelling \((q_1, k_1) \rightarrow (k_1, k_2)\) in the first term, we obtain:

\[
\frac{\langle \Psi(t) | S^z P_D | \Psi(t) \rangle \text{ therm. limit}}{\langle \Psi(t) | P_D | \Psi(t) \rangle} \rightarrow S^z_{a_0 a_0} - S^z_{a_0 a_0} (2J_z) \left( \int_{-D}^{D} \frac{dk_1 dk_2}{2\pi} f(k_2) \text{Re} \left[ \frac{1 - e^{-i(k_1-k_2)t}}{(k_1-k_2)^2} \right] \right)
\]

\[
+ S^z_{a_0 a_0} (2J_z) \left( \int_{-D}^{D} \frac{dk_1 dk_2}{2\pi} f(k_1) f(k_2) \text{Re} \left[ \frac{1 - e^{-i(k_1-k_2)t}}{(k_1-k_2)^2} \right] \right) + O(J^3), \quad (A.95)
\]

which is the same answer as in the conventional scheme [i.e. Eq. (A.51) with \(D_H = D_\rho = D\)], leading to the third case of Eq. (A.46).
Appendix B

Asymptotic evaluation of integrals

B.1 Main evaluation

We study the asymptotic behavior as $\lambda \to \infty$ of the general form (4.144b), written again here for reference:

$$R^{(\sigma)}[f,h,\lambda] \equiv \int_0^\infty du_1 \ldots du_{n-1} \left[ \prod_{j=1}^{n-1} \frac{e^{i\lambda v_j^{(\sigma)}} - f(v_j^{(\sigma)})}{v_j^{(\sigma)}} \right] h(v_n^{(\sigma)}), \quad (B.1)$$

where $\sigma \in \text{Sym}(n)$ and the $v_j^{(\sigma)}$ variables are linear combinations of the integration variables:

$$v_j^{(\sigma)} = \sum_{m=j}^{n-1} u_m - \sum_{m=\sigma^{-1}(j)}^{n-1} u_m \quad (1 \leq j \leq n). \quad (B.2)$$

These linear combinations are listed in Table B.1 for all of the eleven permutations $\sigma$ that we need in order to evaluate the current up to and including the $J^5$ or $1/J^5$ term. We

<table>
<thead>
<tr>
<th>$\sigma \equiv (\sigma_1, \ldots, \sigma_n)$</th>
<th>$v_1^{(\sigma)}$</th>
<th>$v_2^{(\sigma)}$</th>
<th>$v_3^{(\sigma)}$</th>
<th>$v_4^{(\sigma)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>(2, 1)</td>
<td>$u_1$</td>
<td>$-u_1$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>(3, 1, 2)</td>
<td>$u_1$</td>
<td>$u_2$</td>
<td>$-u_1 - u_2$</td>
<td>-</td>
</tr>
<tr>
<td>(2, 3, 1)</td>
<td>$u_1 + u_2$</td>
<td>$-u_1$</td>
<td>$-u_2$</td>
<td>-</td>
</tr>
<tr>
<td>(3, 2, 1)</td>
<td>$u_1 + u_2$</td>
<td>0</td>
<td>$-u_1 - u_2$</td>
<td>-</td>
</tr>
<tr>
<td>(2, 3, 4, 1)</td>
<td>$u_1 + u_2 + u_3$</td>
<td>$-u_1$</td>
<td>$-u_2$</td>
<td>$-u_3$</td>
</tr>
<tr>
<td>(2, 4, 1, 3)</td>
<td>$u_1 + u_2$</td>
<td>$-u_1$</td>
<td>$u_3$</td>
<td>$-u_2 - u_3$</td>
</tr>
<tr>
<td>(3, 1, 4, 2)</td>
<td>$u_1$</td>
<td>$u_2 + u_3$</td>
<td>$-u_1 - u_2$</td>
<td>$-u_3$</td>
</tr>
<tr>
<td>(3, 4, 1, 2)</td>
<td>$u_1 + u_2$</td>
<td>$u_2 + u_3$</td>
<td>$-u_1 - u_2$</td>
<td>$-u_2 - u_3$</td>
</tr>
<tr>
<td>(4, 1, 2, 3)</td>
<td>$u_1$</td>
<td>$u_2$</td>
<td>$u_3$</td>
<td>$-u_1 - u_2 - u_3$</td>
</tr>
<tr>
<td>(4, 3, 2, 1)</td>
<td>$u_1 + u_2 + u_3$</td>
<td>$u_2$</td>
<td>$-u_2$</td>
<td>$-u_1 - u_2 - u_3$</td>
</tr>
</tbody>
</table>

Table B.1: Linear combinations $v_1^{(\sigma)}, \ldots, v_n^{(\sigma)}$. See Eq. (B.2)
use braces to indicate that $R^{(\sigma)}[\{f,h\}, \lambda]$ is a functional of $f$ and $h$, as well as a function of the real parameter $\lambda$. As discussed in the main text, $\lambda$ is essentially the dimensionless bandwidth (i.e. $\lambda = 2D/M + \ldots$). The functions $f$ and $h$ of interest are given by Eqs. (4.143a)-(4.143b) in the main text (their dependence on the spectator variables $\theta$ and $\phi$ is suppressed); we find it advantageous to keep $f$ and $h$ unspecified, appealing instead to general properties like the location of poles. This dimensionless $f$ is not to be confused with the Fermi functions $f_1$ and $f_2$ of the leads.

We have found the asymptotic form as $\lambda \to \infty$ of $R^{(\sigma)}[\{f,h\}, \lambda]$ for all eleven of the necessary permutations. We will not attempt to characterize exactly what properties of $f$ and $h$ are necessary for our calculations below to be valid. At the very least, we assume that $f$ and $h$ are both analytic with poles only along the imaginary axis (but no pole at the origin), that $f(0) = 1$ (otherwise $R^{(\sigma)}[\{f,h\}, \lambda]$ would be ill-defined due to the denominators), and that $h(v)$ decays like $1/v$ or faster as $v \to \infty$; we also assume that $f'(0) = 0$ and that $h(0)$ is real, although these last two conditions could easily be relaxed. All of these assumptions hold for the particular $f$ and $h$ functions that we need for the Kondo model.

Before presenting the full results, we show one more example. We have already given the simplest non-trivial example in (4.146) in the main text, which is the asymptotic expansion of $R^{(2,1)}[\{f,h\}, \lambda]$. An example result from the next order ($n = 3$) is:

$$R^{(2,3,1)}[\{f,h\}, \lambda] \equiv \int_0^\infty du_1 du_2 \frac{e^{i\lambda(u_1+u_2)} - f(u_1 + u_2) e^{-i\lambda u_1} - f(-u_1) h(-u_2)}{u_1 + u_2 - u_1},$$

and

$$\lambda \to \infty \quad -\frac{1}{2} h(0) \ln^2 \lambda + \left[-h(0) \left(\gamma + i \frac{\pi}{2}\right) + \int_0^\infty du \ln u \frac{d}{du} (f(u)h(-u))\right] \ln \lambda$$

$$- \left(\frac{7\pi^2}{24} + \frac{1}{2} \gamma^2 + i \frac{1}{2} \pi \gamma\right) h(0) + \left(\gamma + i \frac{\pi}{2}\right) \int_0^\infty du \ln u \frac{d}{du} [f(u)h(-u)]$$

$$+ \frac{1}{2} \int_0^\infty du \ln^2 u \frac{d}{du} [f(u)h(-u)]$$

$$- \int_0^\infty du_1 du_2 \frac{1}{u_2} \ln \frac{u_1 + u_2}{u_1} \frac{\partial}{\partial u_1} [f(u_1 + u_2) f(-u_1) h(-u_2)],$$

where $\gamma$ is the Euler constant. Notice that here and in the simpler example (4.146), the
asymptotic expansion consists of powers of $\ln \lambda$ with coefficients that are functionals of $f$ and $h$; higher powers of $\ln \lambda$ are multiplied by simpler functionals, and the highest power is $\ln^{n-1} \lambda$.

We have shown analytically that for all of the eleven necessary permutations, the asymptotic form of $R^{(\sigma)}[\{f, h\}, \lambda]$ is a sum of logarithmic terms (including a constant term, i.e. $\ln^0 \lambda$) and a linear term:

$$R^{(\sigma)}[\{f, h\}, \lambda] \xrightarrow{\lambda \to \infty} z^{(\sigma)}_{\text{linear}}[\{f, h\}] \lambda + \sum_{j=0}^{n-1} z^{(\sigma)}_j[\{f, h\}] \ln^j \lambda,$$  \hspace{1cm} (B.3)

where $z^{(\sigma)}_{\text{linear}}[\{f, h\}]$ and $z^{(\sigma)}_j[\{f, h\}]$ are complex numbers (functionals of $f$ and $h$). Let us first discuss the coefficient $z^{(\sigma)}_{\text{linear}}[\{f, h\}]$ of the linear term. This coefficient vanishes for all of the eleven permutations except for $(3, 2, 1)$ and $(4, 3, 2, 1)$; for these two permutations, we find:

$$z^{(3, 2, 1)}_{\text{linear}}[\{f, h\}] = \frac{i}{\pi} z^{(4, 3, 2, 1)}_{\text{linear}}[\{f, h\}] = -i \int_0^\infty du f(u)h(u).$$  \hspace{1cm} (B.4)

In the current, these linear terms cancel at the order we are working to ($J^5$ or $1/J^5$), so we can ignore them.

We proceed to the logarithmic terms. It turns out that for all eleven permutations, the coefficients $z^{(\sigma)}_j[\{f, h\}]$ can be expressed entirely in terms of the following three functionals:

$$\rho_1[\{f, h\}] = \left(-\gamma + i \frac{\pi}{2}\right) h(0) + \int_0^\infty du \ln u \frac{d}{du} [f(u)h(-u)],$$  \hspace{1cm} (B.5a)

$$\rho_2[\{f, h\}] = -\left(7\frac{\pi^2}{24} + \frac{1}{2} \gamma^2 + i \frac{1}{2} \pi \gamma\right) h(0) + \left(\gamma + i \frac{\pi}{2}\right) \int_0^\infty du \ln u \frac{d}{du} [f(u)h(-u)]
+ \frac{1}{2} \int_0^\infty du \ln^2 u \frac{d^2}{du^2} [f(u)h(-u)]
- \int_0^\infty du_1 du_2 \frac{1}{u_2} \ln \frac{u_1 + u_2}{u_1 + u_2} \frac{\partial}{\partial u_1} [f(u_1 + u_2)f(-u_1)h(-u_2)],$$  \hspace{1cm} (B.5b)

$$\rho_3[\{f, h\}] = \left(\gamma - i \frac{\pi}{2}\right)^2 h(0) - 2 \left(\gamma - i \frac{\pi}{2}\right) \int_0^\infty du \ln u \frac{d}{du} [f(u)h(-u)]
+ \int_0^\infty du_1 du_2 \ln u_1 \ln u_2 \frac{\partial}{\partial u_1} \frac{\partial}{\partial u_2} [f(u_1)f(u_2)h(-u_1 - u_2)],$$  \hspace{1cm} (B.5c)
Table B.2 contains our results for the coefficients $z_j^{(\sigma)}\{\{f, h\}\}$ of the asymptotic expansion.

These results completely specify the integrals we need for $n = 1, 2, 3$, while for $n = 4$, they provide the complete expansion except for the coefficient $z_0^{(\sigma)}\{\{f, h\}\}$ of the smallest term (the $\lambda$-independent constant); these remaining coefficients can also be written as lengthy functionals of $f$ and $h$ (including triple integrals), and we list their approximate numerical values in Table B.3 for the two special cases corresponding to $G(T)$ and $I(T_1 = 0, T_2 = 0, V)$.

<table>
<thead>
<tr>
<th>$\sigma \equiv (\sigma_1, \ldots, \sigma_n)$</th>
<th>$z_{n-1}^{(\sigma)}{{f, h}}$</th>
<th>$z_{n-2}^{(\sigma)}{{f, h}}$</th>
<th>$z_{n-3}^{(\sigma)}{{f, h}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>$h(0)$</td>
<td>$\rho_1$</td>
<td>$\rho_2$</td>
</tr>
<tr>
<td>(2, 1)</td>
<td>$-h(0)$</td>
<td>$\rho_1$</td>
<td></td>
</tr>
<tr>
<td>(2, 3, 1)</td>
<td>$-\frac{1}{2}h(0)$</td>
<td>$-i\pi h(0) + \rho_1$</td>
<td>$\rho_2$</td>
</tr>
<tr>
<td>(3, 1, 2)</td>
<td>$h(0)$</td>
<td>$-2\rho_1$</td>
<td>$\rho_3$</td>
</tr>
<tr>
<td>(3, 2, 1)</td>
<td>0</td>
<td>0</td>
<td>$-h(0)$</td>
</tr>
<tr>
<td>(2, 3, 4, 1)</td>
<td>$-\frac{1}{3}h(0)$</td>
<td>$-i\pi h(0) + \rho_1$</td>
<td>$\frac{2}{7}\pi^2 h(0) + 2\rho_2$</td>
</tr>
<tr>
<td>(2, 4, 1, 3)</td>
<td>$\frac{1}{7}h(0)$</td>
<td>$i\pi h(0) - \frac{3}{7}\rho_1$</td>
<td>$-i\pi \rho_1 - \rho_2 + \rho_3$</td>
</tr>
<tr>
<td>(3, 1, 4, 2)</td>
<td>$\frac{1}{6}h(0)$</td>
<td>$-\frac{1}{2}\rho_1$</td>
<td>$\frac{2}{7}\pi^2 h(0) + i\pi \rho_1 - \rho_2$</td>
</tr>
<tr>
<td>(3, 4, 1, 2)</td>
<td>0</td>
<td>$h(0)$</td>
<td>$(2 + i\pi) h(0) - 2\rho_1$</td>
</tr>
<tr>
<td>(4, 1, 2, 3)</td>
<td>$-h(0)$</td>
<td>$3\rho_1$</td>
<td>$-3\rho_3$</td>
</tr>
<tr>
<td>(4, 3, 2, 1)</td>
<td>0</td>
<td>$-h(0)$</td>
<td>$-(2 + i\pi) h(0) + 2\rho_1$</td>
</tr>
</tbody>
</table>

Table B.2: Leading log, sub-leading log, and sub-sub-leading log terms in $R^{(\sigma)}\{\{f, h\}, \lambda\}$. See Eq. (B.3) for explanation of the notation.

<table>
<thead>
<tr>
<th>$\sigma \equiv (\sigma_1, \ldots, \sigma_n)$</th>
<th>$z_0^{(\sigma)}{{f, h}}$ for $f(v) = h(v) = v/sinh v$</th>
<th>$z_0^{(\sigma)}{{f, h}}$ for $f(v) = sinh v, h(v) = cosh v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2, 3, 4, 1)</td>
<td>$2.24 + 1.06i$</td>
<td>$1.14 + 3.51i$</td>
</tr>
<tr>
<td>(2, 4, 1, 3)</td>
<td>$4.50 - 3.12i$</td>
<td>$1.35 - 1.76i$</td>
</tr>
<tr>
<td>(3, 1, 4, 2)</td>
<td>$1.48 - 7.24i$</td>
<td>$0.97 - 6.02i$</td>
</tr>
<tr>
<td>(3, 4, 1, 2)</td>
<td>$3.51 - 3.14i$</td>
<td>$0.37 - 3.14i$</td>
</tr>
<tr>
<td>(4, 1, 2, 3)</td>
<td>$6.76 - 3.20i$</td>
<td>$1.90 - 2.62i$</td>
</tr>
<tr>
<td>(4, 3, 2, 1)</td>
<td>$-3.95$</td>
<td>$-1.49$</td>
</tr>
</tbody>
</table>

Table B.3: Constant terms $z_0^{(\sigma)}\{\{f, h\}\}$ for $n = 4$ integrals in two special cases.
Our asymptotic results are in good agreement with Monte Carlo evaluation. An example of this agreement is shown in Fig. B.1

![Graph showing the comparison between asymptotic and Monte Carlo evaluations](image)

Figure B.1: Sample numerical checks of our asymptotic result for $R^{(3,1,4,2)}[\{f, h\}, \lambda]$. Case 1 is $f(v) = h(v) = v / \sinh v$, which is used in the calculation of $G(T)$; case 2 is $f(v) = \cos v$ and $h(v) = \text{sinc} v$, which is used in the calculation of $I(T_1 = 0, T_2 = 0, V)$ (and hence, $G(V)$). Only the real part of $R^{(3,1,4,2)}[\{f, h\}, \lambda]$ appears in the answer to the order we consider ($J^3$ or $1/J^5$), but the agreement for the imaginary part is similar.

The calculations that produce Table B.2 are lengthy; to illustrate the method used, we derive the asymptotic expansion (4.146) in the main text. The integral to be studied is:

$$R^{(2,1)}[\{f, h\}, \lambda] = \int_0^{\infty} du_1 \frac{e^{i\lambda u_1} - f(u_1)}{u_1} h(-u_1).$$

We would like to separate the $\lambda$-dependent term of (B.6), but cannot do so because $e^{i\lambda u_1}/u_1$ by itself diverges too strongly at $u_1 = 0$. We therefore integrate by parts, finding (note that $h$ falls off sufficiently rapidly at infinity so that the boundary contribution is zero):

$$R^{(2,1)}[\{f, h\}, \lambda] = R_1^{(2,1)}[\{f, h\}, \lambda] + R_2^{(2,1)}[\{f, h\}],$$

where:

$$R_1^{(2,1)}[\{f, h\}, \lambda] = -\int_0^{\infty} du_1 \ln u_1 \frac{d}{du_1} \left[ e^{i\lambda u_1} h(-u_1) \right],$$

$$R_2^{(2,1)}[\{f, h\}] = \int_0^{\infty} du_1 \ln u_1 \frac{d}{du_1} \left[ f(u_1) h(-u_1) \right].$$

I acknowledge the Office of Advanced Research Computing (OARC) at Rutgers, The State University of New Jersey for providing access to the Amarel cluster. URL: [http://oarc.rutgers.edu](http://oarc.rutgers.edu)
We evaluate $R^{(2,1)}\{\{f, h\}, \lambda\}$ for large $\lambda$ by shifting the contour so that the rapidly oscillating phase becomes a decaying exponential. This is a textbook method – see example 1 in section 6.6 of Ref [78].

Recall that any poles of $h$ are on the imaginary axis. Write $C$ for the contour that starts at 0 and extends to $i\infty$ going slightly to the right ($\text{Re} \ u_1 > 0$) around each of the poles. This contour $C$ taken in reverse, the original integration contour from 0 to $\infty$, and a semicircular arc from $\infty$ to $i\infty$ form a closed contour that contains no poles. Furthermore, it can be verified that the semicircular arc makes no contribution.$^2$ Therefore, the original contour can be replaced by $C$:

$$R^{(2,1)}_1\{\{f, h\}, \lambda\} = - \int_C du_1 \ln u_1 \frac{d}{du_1} \left[ e^{i\lambda u_1} h(-u_1) \right]. \quad \text{(B.9)}$$

For large $\lambda$, the function $h$ can be replaced by its value at zero; the reason for this is that the difference $h(-u_1) - h(0)$ starts at linear order, which permits integration by parts:

$$- \int_C du_1 \ln u_1 \frac{d}{du_1} \left[ e^{i\lambda u_1} (h(-u_1) - h(0)) \right] = \int_C du_1 \frac{1}{u_1} (h(-u_1) - h(0)) e^{i\lambda u_1} \quad \text{(B.10a)}$$

$$= \int_C du_1 \frac{d}{du_1} \left[ \frac{1}{u_1} (h(-u_1) - h(0)) \frac{1}{i\lambda} e^{i\lambda u_1} \right]$$

$$- \int_C du_1 \frac{d}{du_1} \left[ \frac{1}{u_1} (h(-u_1) - h(0)) \right] \frac{1}{i\lambda} e^{i\lambda u_1} \quad \text{(B.10b)}$$

$$= O \left( \frac{1}{\lambda} \right). \quad \text{(B.10c)}$$

We have therefore shown:

$$R^{(2,1)}_1\{\{f, h\}, \lambda\} = - \int_C du_1 \ln u_1 \frac{d}{du_1} \left[ e^{i\lambda u_1} h(0) \right] + O \left( \frac{1}{\lambda} \right). \quad \text{(B.11)}$$

Since there are no longer any poles, we can shift the contour $C$ to be exactly the positive imaginary axis; then the remaining integrals are elementary after the change of variables $s_1 = \lambda u_1$:

$$R^{(2,1)}_1\{\{f, h\}, \lambda\} = - \int_0^\infty du_1 \ln(iu_1) \frac{d}{du_1} \left[ e^{-\lambda u_1} h(0) \right] + O \left( \frac{1}{\lambda} \right) \quad \text{(B.12a)}$$

$$= h(0) \left( - \ln \lambda - \gamma + \frac{1}{2\pi} \right) + O \left( \frac{1}{\lambda} \right). \quad \text{(B.12b)}$$

$^2$This is true for the particular $f$ and $h$ of interest, and more generally we need to require that $f$ and $h$ decay sufficiently rapidly so that the semicircular arc does not contribute.
Adding this to Eq. (B.8b), we obtain the second row of Table B.2.

For the higher order integrals, the basic strategy is the same: use integration by parts to rewrite the integral in a form that can be separated into a sum of simpler terms, shift integration contours to turn oscillating phases into decaying exponentials, and replace functions by their values at zero via integration by parts. In the case of \( \sigma = (4, 3, 2, 1) \), this last step has to be done more carefully due to the linear divergence.

### B.2 Alternate regulation of the Fermi function

It is interesting to view the sharp cutoff on the left-hand side of Eq. (4.130) as just one possible regularization scheme. It turns out that the upper limit of integration can be extended to infinity up to extremely small error terms (of order \( e^{-\left|D - |\mu|\right|/T} \)), so we can think of the cutoff we have chosen as multiplying the Fermi function by a step function \( \Theta(D + k) \). It is natural, then, to try using a smooth approximation to this step function, instead.

For one example of an alternate cutoff scheme, we replace the step function by a Fermi function of negative energies with chemical potential \(-D'\); that is, the Fourier transform (4.130) is replaced by:

\[
\int_{-\infty}^{\infty} dk \ f(k) \frac{1}{e^{-\frac{1}{T}(D'+k)} + 1} e^{-iky} = \frac{\pi}{i} T \frac{e^{iD'y} - e^{-i\mu y}}{\sinh(\pi Ty)} + O \left( e^{-\left(D' + \mu\right)/T} \right). \tag{B.13}
\]

We write the new cutoff as \( D' \) as a reminder that, while it plays the same role, it is not identical to the sharp cutoff \( D \) (except in the case \( T = 0 \)). Notice that we have taken the temperature \( T \) to be the scale over which the step function drops to zero; in principle any energy scale much smaller than the bandwidth could have been used here, but we wish to avoid introducing another scale into the problem. As before, we will ignore the exponentially small error term from now on.
To get this Fourier transform, we note the following exact integral and its large $p$ asymptotics:

\[
\int_{-\infty}^{\infty} du \frac{1}{e^u + 1} e^{-iu} \frac{1}{e^{-s/p} + 1} = \frac{1}{1 - 1/p} \left[ p^{iv} \left( e^{\pi v} B(-1/p; 1 + iv, 0) \right. \right.
\]
\[
- e^{-\pi v} B(-p; 1 - iv, 0) \left. \right) + \frac{1}{i} \left( \frac{1}{v} - \frac{\pi}{\sinh(\pi v)} \right) \right] \quad (v \in \mathbb{R}, p \geq 0) \quad (B.14a)
\]
\[
= \frac{\pi}{i} \frac{p^{iv} - 1}{\sinh \pi v} + O \left( \frac{1}{p} \right) \quad (p \to \infty). \quad (B.14b)
\]

In this section, we focus on the zero bias conductance $G(T)$, which requires us to finding the large $\lambda$ behavior of:

\[
R^{(\sigma)}(\lambda) \equiv R^{(\sigma)}\{f, h\}, \lambda] = \int_{0}^{\infty} du_1 \ldots du_{n-1} \left( \prod_{j=1}^{n-1} e^{i\lambda v_j^{(\sigma)} / \sinh(v_j^{(\sigma)})} - 1 \right) \frac{v_n^{(\sigma)}}{\sinh(v_n^{(\sigma)})}, \quad (B.15)
\]

where $f(v) = h(v) = v / \sinh v$, and $f$ and $h$ will be omitted from the remainder of this section. While it is possible to use the same strategies of integration by parts and shifting contours, this approach is laborious. We pursue a different strategy: we take the Laplace transform with respect to $\lambda$ in order to get rid of the oscillating phase, arriving at integrals that are easier to evaluate numerically.

Recall that the Laplace transform of a function $F(\lambda)$ is defined as:

\[
\tilde{F}(s) = \int_{0}^{\infty} d\lambda \ e^{-s\lambda} F(\lambda). \quad (B.16)
\]

There is a correspondence between the large $\lambda$ behavior of the original function $F(\lambda)$ (which is what we are interested in) and the small $s$ behavior of the transform $\tilde{F}(s)$ (which we find easier to evaluate numerically). The correspondences we need are listed in Table B.4. The basic picture is that any non-singular (as $s \to 0^+$) terms in $\tilde{F}(s)$ can be ignored (as they correspond to terms in $F(\lambda)$ that vanish as $\lambda \to \infty$), and singularities of the form $\frac{\ln^a s}{s}$ lead to powers of $\ln \lambda$ in the original function. Most likely, the above statements have to be restricted to sufficiently “nice” functions $F(\lambda)$; for a more rigorous discussion of this approach (which is standard), see Ref. [79].
Table B.4: Useful Laplace transforms. The Laplace transform of $F(\lambda)$ is $\tilde{F}(s) \equiv \int_0^\infty d\lambda \ e^{-s\lambda} F(\lambda)$, $\gamma$ is the Euler constant (included to make the equations simpler), and $\zeta$ is the Riemann-Zeta function.

Our strategy is to evaluate the transform $s\tilde{R}^{(\sigma)}(s)$ numerically for several small values of $s$ (logarithmically spaced), curve fit the result to a polynomial in $\ln(e^s)$, then transfer the results to a polynomial in $\ln \lambda$. Based on our more detailed analysis of the integrals in the case of the sharp cutoff, we expect the order of the polynomial to be $n - 1$, where $\sigma \in \text{Sym}(n)$. For the two special permutations $(3, 2, 1)$ and $(4, 3, 2, 1)$, we expect (and will find) a linearly divergent (in $\lambda$) part that must be separated before doing the curve fit to find the logarithmic terms.

Multiplying out the product in Eq. (B.15) using:

$$
\prod_{j=1}^{n-1} \left( e^{i\lambda v_j^{(\sigma)}} - 1 \right) = (-1)^{n-1} \sum_{m_1, \ldots, m_{n-1} = 0, 1} (-1)^{m_1 + \cdots + m_{n-1}} \exp \left[ i \lambda \sum_{\ell=1}^{n-1} m_\ell v_\ell^{(\sigma)} \right], \quad (B.17)
$$

and using $\int_0^\infty d\lambda \ e^{i\lambda \nu - s\lambda} = \frac{i}{\nu + is}$, we obtain the following useful formula for the Laplace transform of $R^{(\sigma)}(\lambda)$:

$$
\tilde{R}^{(\sigma)}(s) = (-1)^{n-1} \int_0^\infty du_1 \cdots du_{n-1} \left( \sum_{m_1, \ldots, m_{n-1} = 0, 1} (-1)^{m_1 + \cdots + m_{n-1}} \frac{i}{\sum_{\ell=1}^{n-1} m_\ell v_\ell^{(\sigma)} + is} \right) v_n^{(\sigma)} \prod_{j=1}^n \frac{1}{\sinh(v_j^{(\sigma)})}. \quad (B.18)
$$

We find that for each $R^{(\sigma)}(\lambda)$, the leading log and sub-leading log terms (i.e. the final answers for the coefficients of $\ln^{n-1} \lambda$ and $\ln^{n-2} \lambda$ agree within a few percent with the corresponding terms obtained in the sharp cutoff scheme. This means that the leading log and sub-leading logs of $G(T)$ are the same in both cutoff schemes, which in turn implies
that the first two orders of the beta function are the same in both schemes, as expected. The $g^3$ term differs from the conventional one by a factor of 8.

B.3 Alternate evaluation of integrals at zero temperature.

In the special case of zero temperature, we can evaluate the full asymptotics of the integrals (for the same 11 permutations considered in Sec. B.1). This provides a check on our earlier results. Also, this evaluation yields analytical answers for the constant coefficients in the last column of Table B.3 (there calculated numerically). Working at zero temperature allows us to calculate the necessary integrals exactly (or to be precise, their Laplace transforms in time) in Mathematica; the exact answers are then expanded in the regime $D/V \gg 1$ to find the logarithmic terms.

Recall that the basic integral we need for the current is the following:

$$
\varphi_n(T_1, \mu_1; T_2, \mu_2; \epsilon) = \left(\frac{i}{2}\right)^{n-1} \frac{\partial}{\partial t} \int_0^t dx_n \Theta(x_n < \cdots < x_1) \int_{-D}^D dk_n \left[\prod_{j=1}^{n-1} (f_1(k_j) + f_2(k_j))\right] [f_1(k_n) - f_2(k_n)] \prod_{\ell=1}^n e^{i(k_{\sigma_\ell} - k_\ell)x_\ell}. \quad (B.19)
$$

Taking the Laplace transform allows us to do the position integrals in a compact fashion, yielding:

$$
\epsilon \varphi_n(T_1, \mu_1; T_2, \mu_2; \epsilon) = \left(\frac{i}{2}\right)^{n-1} \int_{-D}^D dk_n \left[\prod_{j=1}^{n-1} (f_1(k_j) + f_2(k_j))\right] [f_1(k_n) - f_2(k_n)] \prod_{\ell=1}^n \frac{i}{k_{\sigma_\ell} + \cdots + k_{\sigma_\ell} - k_1 - \cdots - k_\ell + i\epsilon}. \quad (B.20)
$$

The large time behavior of the original function is equivalent to the $\epsilon \to 0^+$ behavior of $\epsilon \varphi$ (see Table B.4). At zero temperature, the Fermi functions reduce to $f_1(k) + f_2(k) = 2\Theta(-D < k < -V) + \Theta(-V < k < 0)$ and $f_1(k) - f_2(k) = \Theta(-V < k < 0)$. Performing
some relabeling of coordinates, we obtain:

\[
\epsilon \varphi_n^{(\sigma)}(0, 0; 0, -V; \epsilon) = i^{n-1} \sum_{m=0}^{n-1} \left( \frac{1}{2} \right)^m \binom{n-1}{m} \int_{-D}^{V} dk_1 \ldots dk_{n-m+1} \int_{-V}^0 dk_{n-m} \ldots dk_n \, S_{k_1 \ldots k_{n-1}} \prod_{\ell=1}^{n-1} \frac{i}{k_{\sigma_1} + \ldots + k_{\sigma_{\ell}} - k_1 - \ldots - k_{\ell} + i\epsilon},
\]

(B.21)

where the symmetrizer \( S_{k_1 \ldots k_{n-1}} \) acts on the first \( n-1 \) momenta via:

\[
S_{k_1 \ldots k_{n-1}} F(k_1, \ldots, k_{n-1}) = \frac{1}{(n-1)!} \sum_{\sigma' \in \text{Sym}(n-1)} F(k_{\sigma'_1}, \ldots, k_{\sigma'_{n-1}}).
\]

We then rescale the momenta by \( V \), which yields a prefactor of \( V \) times an integral that depends on the dimensionless quantities \( D/V \) and \( \epsilon/V \).

The necessary integrals were done exactly, with considerable labor, in Mathematica. Each term of the sum over \( m \) and each term in the summation implicit in the symmetrizer was treated separately (noting that many terms are related to each other by complex conjugation and/or relabeling variables). While some of these individual terms were found to have \( \ln \frac{V}{\epsilon} \) singularities (indicating growth without bound in the time domain as \( Vt \to \infty \)), these singularities always cancelled in the final answer for \( \epsilon \varphi_n^{(\sigma)} \). The limit as \( \epsilon \to 0^+ \) of \( \epsilon \varphi_n^{(\sigma)} \) (which is same as the limit \( t \to \infty \) of \( \varphi_n^{(\sigma)} \)) was then expanded for large \( D/V \), yielding logarithms – and in the case of the special permutations \( (3, 2, 1) \) and \( (4, 3, 2, 1) \), a term linear in \( D/V \), as well.

We write the final asymptotic results in the following form (note that since \( T_1 = T_2 = 0 \), we have \( \lambda = 2 \frac{D}{V} - 1, f(v) = \cos v, \) and \( h(v) = \sin v \)):

\[
\lim_{t \to \infty} \varphi_n^{(\sigma)}(0, 0; 0, -V; t) = \lim_{\epsilon \to 0^+} \epsilon \varphi_n^{(\sigma)}(0, 0; 0, -V; \epsilon) = VR^{(\sigma)} \left\{ f, h \right\}, \frac{2D}{V} - 1 \right],
\]

(B.23a)

\[
R^{(\sigma)}[\{f, h\}, \lambda] = a_0 + a_1 \left( \ln \frac{\lambda}{2} + 1 \right) + a_2 \left( \frac{1}{2} \ln^2 \frac{\lambda}{2} + \ln \frac{\lambda}{2} + 1 \right) + a_3 \left( \frac{1}{6} \ln^3 \frac{\lambda}{2} + \frac{1}{2} \ln^2 \frac{\lambda}{2} + \ln \frac{\lambda}{2} + 1 \right) + b \frac{\lambda}{2} \quad (\lambda \to \infty),
\]

(B.23b)

with the coefficients \( a_0, a_1, a_2, a_3 \) and \( b \) given in Table B.5. The results are in good agreement with the more general calculations of Sec. B.1.
Table B.5: Full asymptotics for $R^{(\sigma)}\{\{f, h\}, \lambda\}$ in the zero temperature case ($T_1 = T_2 = 0$, hence $f(v) = \cos v$ and $h(v) = \text{sinc} v$).
Appendix C

Equilibrium occupancy of the IRL from the literature

From Bethe Ansatz, a series form is known for the occupancy \( \langle n_d \rangle_{\text{equilibrium}} \) at zero temperature as a function of \( \epsilon_d \) in the multi-lead IRL. It turns out that the number of leads does not appear in the answer. The calculation was first done by Ponomarenko [80]. In the one lead case, Rylands and Andrei [81] calculated the occupancy including a Luttinger interaction, and Camacho et al. [64] have verified that setting the Luttinger interaction to zero (which recovers the one lead IRL) results in exact agreement between the answers of Ponomarenko and of Rylands and Andrei. I transcribe the result from Camacho et al. with some minor changes in notation:

\[
\langle n_d \rangle_{\text{equilibrium}} = n_d(x_d) = \begin{cases} 
\frac{1}{2} - \sum_{n=0}^{\infty} h_n^< (\alpha) \left( \frac{x_d}{\pi h_{n=0}^< (\alpha)} \right)^{2n+1} & 0 \leq x_d < 1 \\
\sum_{n=1}^{\infty} h_n^> (\alpha) \left( \frac{x_d}{\pi h_{n=0}^> (\alpha)} \right)^{-2n} & x_d \geq 1 \\
1 - n_d(-x_d) & x_d \leq -1
\end{cases}
\]  

(C.1)

where \( x_d = \epsilon_d/T_K \) (note that \( \epsilon_0 \) in Ref. [64] is our \( \epsilon_d \)) and:

\[
h_n^< (\alpha) = \frac{1}{\sqrt{\pi}} \frac{(-1)^n}{n!} \frac{\Gamma(1 + \frac{\alpha}{2}(2n + 1))}{\Gamma(1 + \frac{\alpha^2}{4}(2n + 1))},
\]

(C.2a)

\[
h_n^> (\alpha) = \frac{1}{2\sqrt{\pi}} \frac{(-1)^{n+1}}{n!} \frac{\Gamma(1/2 + n/\alpha)}{\Gamma(1 - \frac{\alpha^2}{4}n)}.
\]

(C.2b)

The quantity \( \alpha \) is an RG invariant, with \( \alpha = 2 \) in the non-interacting case (\( U = 0 \)). In principle the Bethe Ansatz \( \alpha \) could differ from our formula (5.79b) for \( \alpha \) in the main text, but we find that they are the same (at least to leading order in \( U \)). To compare with our answer for the occupancy in the main text, we expand to linear order about \( \alpha = 2 \). For
\[ |x_d| < 1, \text{ we obtain:} \]
\[
n_d(x_d) = \frac{1}{2} - \sum_{n=0}^{\infty} \left\{ \frac{(-1)^n}{n(1 + 2n)} + \frac{(\alpha - 2)}{2\pi} \left[ 1 - 2\ln 2 + \psi(2 + 2n) - \psi(3/2 + n) \right] \right. \]
\[
+ O\left( (\alpha - 2)^2 \right) \right\} x_d^{2n+1}, \quad (C.3) \]

where \( \psi = \Gamma' \) is the digamma. This sum yields (5.85) in the main text once we identify \( \alpha - 2 = -\frac{2U}{\pi} \) at leading order [in agreement with Eq. (5.79b)]. For \( x_d > 1 \), we obtain:

\[
n_d(x_d) = \sum_{n=1,3,\ldots} \left\{ \frac{(-1)^{(n-1)/2}}{\pi n} \right. \]
\[
+ (\alpha - 2) \frac{(-1)^{(n-1)/2}}{2\pi} \left[ 1 - \ln 2 - \ln x_d + \psi(1/2 + n/2) - \psi(1 + n/2) \right] + O\left( (\alpha - 2)^2 \right) \right\} x_d^{-n} \]
\[
+ \sum_{n=2,4,\ldots} \left\{ \frac{(\alpha - 2)(-1)^{(n/2-1)}}{4} + O\left( (\alpha - 2)^2 \right) \right\} x_d^{-n}. \quad (C.4) \]

The sum over the \( \alpha = 2 \) part yields the standard non-interacting result \( 1/2 - (1/\pi) \arctan x_d \).

Numerical evaluation of the \( \alpha - 2 \) correction term again agrees with Eq. (5.85) in the main text.
Appendix D

Perturbative check: the current in the Anderson model

We calculate the steady state current in the Anderson model to leading order in $U$ using Keldysh perturbation theory. We obtain exact agreement with the result (6.92) from the main text. Rather than evaluate the current operator directly, we find it more convenient to use the Meir-Wingreen formula [56], which relates the steady state current to an impurity-impurity Green’s function.\footnote{I thank Yashar Komijani and Yigal Meir for assistance in this calculation.}

For this calculation, we allow a magnetic field on the dot; that is, the dot energy can be spin-dependent:

\begin{align}
H^{(0)} &= -i \int_{-L/2}^{L/2} dx \sum_{\gamma=1,2} \psi_{\gamma a}^{\dagger}(x) \frac{d}{dx} \psi_{\gamma a}(x) + \sum_a \epsilon_a d_a^\dagger d_a \\
&+ \left[ \frac{v}{\sqrt{2}} \sum_{\gamma=1,2} \psi_{\gamma a}^{\dagger}(0) d_a + \text{h.c.} \right], \\
H^{(1)} &= U n^\uparrow n^\downarrow, \\
H &= H^{(0)} + H^{(1)}.
\end{align}

Our conventions in this Appendix depart in two ways from the rest of the thesis. First, all time-dependent operators are in either the Heisenberg picture (subscript $H$) or the interaction picture (no subscript), with the usual sign (i.e. $e^{iHt}$ or $e^{iH(0)t}$ on the left, respectively). Second, repeated spin indices are \textit{not} summed in the absence of a summation sign.
Let $\rho$ be the density matrix describing the two leads each separately in thermal equilibrium, with no tunneling:

$$\rho = \exp \left[ -\frac{1}{T_1} \sum_{|k|<D} (k - \mu_1) c_{1ka}^\dagger c_{1ka} \right] \otimes \exp \left[ -\frac{1}{T_2} \sum_{|k|<D} (k - \mu_2) c_{2ka}^\dagger c_{2ka} \right]. \quad (D.2)$$

The Fermi functions of the leads are $f_\gamma (k) = \left[ e^{(k - \mu_\gamma)/T_\gamma} + 1 \right]^{-1} (\gamma = 1, 2)$.

The retarded Green’s function with respect to the time-evolving density matrix $\rho(t) \equiv e^{iHt} \rho e^{-iHt}$ is given by:

$$\mathcal{G}_{a,a}^R(t_1, t_2) \equiv -i\Theta(t_1 - t_2) \text{Tr} \left[ \rho(t) \{ d_a H(t_1), d_a^\dagger H(t_2) \} \right] / \text{Tr} \rho. \quad (D.3)$$

In the steady state, we get a function of the time difference only:

$$\lim_{t \to \infty} \mathcal{G}_{a,a}^R(t_1, t_2) \equiv \mathcal{G}_{a,a}^R(t_1 - t_2). \quad (D.4)$$

The Meir-Wingreen formula, specialized to the Hamiltonian we consider here, is the following expression for the steady state current:

$$\lim_{t \to \infty} I_{\text{Sym}}(t) = -\Delta \sum_a \int_{-D}^{D} \frac{dw}{2\pi} \left[ f_1 (w) - f_2 (w) \right] \text{Im} \left[ \mathcal{G}_{a,a}^R (w) \right], \quad (D.5)$$

where $I_{\text{Sym}}(t) = \text{Tr} \left[ \rho(t) \tilde{I}_{\text{Sym}} \right] / \text{Tr} \rho$, $\tilde{I}_{\text{Sym}} = -\frac{i}{2\sqrt{2}} v \left( \psi_{1a}^\dagger (0) - \psi_{2a}^\dagger (0) \right) d_a + \text{h.c.}$, and $\mathcal{G}_{a,a}^R (w) \equiv \int dt' e^{iwt'} \mathcal{G}_{a,a}^R (t')$. The derivation [56] proceeds by applying Keldysh identities to Dyson equations for Green’s functions.3

Eq. (D.3) is more conveniently written as:

$$\mathcal{G}_{a,a}^R (t; t_1, t_2) = \mathcal{G}_{a,a}^R (t + t_1, t + t_2), \quad (D.6)$$

where $\mathcal{G}_{a,a}^R (t_1, t_2) = -i\Theta(t_1 - t_2) \text{Tr} \left[ \rho \{ d_a H(t_1), d_a^\dagger H(t_2) \} \right] / \text{Tr} \rho$ is the retarded Green’s function defined relative to the initial density matrix $\rho$ (rather than the time-evolving density matrix). For perturbative evaluation of $\mathcal{G}_{a,a}^R (t_1, t_2)$ (with $0 < t_2 < t_1$ and with $t_1$ and $t_2$ later to be shifted by $t$), we introduce a Keldysh contour that runs from 0 to $t_1$ (the + branch) and back (the − branch) – see Fig. D.1a. The Keldysh Green’s functions with

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2This is actually a nontrivial assumption—that a time-independent steady state is reached.

3There are some slight differences between our setup and that of MW (Meir and Wingreen, Ref. [56]); we turn on the couplings at $t = 0$ (suddenly), while MW turn on the couplings at $t = -\infty$ (gradually, it seems). However, repeating the calculation of MW directly in our case confirms Eq. (D.5).
respect to \( \rho \) are defined by:

\[
G^{\alpha_1\alpha_2}_{a,a}(t_1, t_2) = -i \text{Tr} \left[ \rho \ T_C \ d_{aH}(t_1^{(\alpha_1)})d_{aH}^\dagger(t_2^{(\alpha_2)}) \right] / \text{Tr}\rho, \tag{D.7}
\]

where \( \alpha_1 \) and \( \alpha_2 \) are branch indices (\( \pm \)) and \( T_C \) is the path-ordering symbol. The retarded Green’s function is given by \( G^R_{a,a} = G^T_{a,a} - G^<_a \), where \( G^T_{a,a} = G^{++}_{a,a} \) and \( G^<_a = G^{+-}_{a,a} \).

By some standard manipulations, we obtain another form more suitable for perturbation theory:

\[
G^{\alpha_1\alpha_2}_{a,a}(t_1, t_2) = -i \text{Tr} \left[ \rho \ T_C \ U_C d_{a}(t_1^{(\alpha_1)})d_{a}^\dagger(t_2^{(\alpha_2)}) \right] / \text{Tr}\rho, \tag{D.8}
\]

where the impurity operators evolve in the interaction picture and \( U_C \) is the interaction picture propagator:

\[
U_C = T_C \exp \left[ -i \int_C dt' \ H^{(1)}(t') \right]. \tag{D.9}
\]

Our first task is to expand \( G_{a,a} \) to first order in \( U \) in terms of the Keldysh Green’s functions of the two lead RLM, which are defined as follows:

\[
G^{(0)\alpha_1\alpha_2}_{a,a}(t_1, t_2) = -i \text{Tr} \left[ \rho \ T_C \ d_{a}(t_1^{(\alpha_1)})d_{a}^\dagger(t_2^{(\alpha_2)}) \right] / \text{Tr}\rho. \tag{D.10}
\]

We write the interaction term in the Hamiltonian as \( H^{(1)} = Ud_{a}^\dagger d_{\pi}d_{a}d_{\pi} \), where \( \pi \) is the opposite spin to \( a \) (\( \pi = \downarrow \) if \( a = \uparrow \) and vice-versa). In the first order correction to the Green’s function, the \( \pi \) impurity operators contract with each other, yielding a factor of \(-iG^{(0)\alpha}_a(t', t')\). We find (see Fig D.1b):

\[
G_{a,a}(t_1, t_2) = G^{(0)}_{a,a}(t_1, t_2) - iU \int_C dt' \ G^{(0)\alpha}_{\pi,a}(t', t')G^{(0)\alpha}_{a,a}(t_1, t')G^{(0)}_{a,a}(t', t_2) + O(U^2), \tag{D.11}
\]
where Keldysh branch indices have been suppressed. We specialize the left-hand side to the retarded Green’s function, then use a Langreth rule to obtain:

$$G^{R}_{a,a}(t_1, t_2) = G^{(0)R}_{a,a}(t_1, t_2) - iU \int dt' G^{(0)<}_{a,a}(t', t') G^{(0)R}_{a,a}(t + t_1, t') G^{(0)R}_{a,a}(t' + t_2). \quad (D.12)$$

Note that we have replaced $\int_0^1 dt' \rightarrow \int_{-\infty}^\infty dt'$, since the retarded Green’s functions restrict $t'$ to the interval $0 < t_2 < t' < t_1$. The retarded Green’s function of the RLM depends only on the difference of times (see below), so we find:

$$G^{R}_{a,a}(t_1 - t_2) =$$

$$\lim_{t \rightarrow \infty} \left[ G^{(0)R}_{a,a}(t + t_1, t + t_2) - iU \int dt' G^{(0)<}_{a,a}(t', t') G^{(0)R}_{a,a}(t + t_1, t') G^{(0)R}_{a,a}(t' + t_2) \right] \quad (D.13a)$$

$$= G^{(0)R}_{a,a}(t_1 - t_2) - iU \left[ \lim_{t \rightarrow \infty} G^{(0)<}_{a,a}(t, t) \right] \int dt' G^{(0)R}_{a,a}(t_1 - t') G^{(0)R}_{a,a}(t' - t_2). \quad (D.13b)$$

The time integral is a convolution, so the Fourier transform yields:

$$\tilde{G}^{R}_{a,a}(w) = \tilde{G}^{(0)R}_{a,a} - iU \left[ \lim_{t \rightarrow \infty} G^{(0)<}_{a,a}(t, t) \right] \left[ \tilde{G}^{(0)R}_{a,a}(w) \right]^2. \quad (D.14)$$

Thus, the only Green’s functions that we need from the two lead RLM are the following:

$$G^{(0)R}_{a,a}(t_1, t_2) = -i \Theta(t_1 - t_2) e^{-iz_a(t_1 - t_2)} \equiv G^{(0)R}_{a,a}(t_1 - t_2), \quad (D.15a)$$

$$\tilde{G}^{(0)R}_{a,a}(w) = \frac{1}{w - z_a} = \frac{T_a(w)}{2\Delta}, \quad (D.15b)$$

$$-i \left[ \lim_{t \rightarrow \infty} G^{(0)<}_{a,a}(t, t) \right] = \lim_{t \rightarrow \infty} \text{Tr} \left[ \rho e^{iH^{(0)}t} \hat{d}_a \hat{d}_a^\dagger e^{-iH^{(0)}t} \right] / \text{Tr} \rho$$

$$= \frac{1}{2} \int_{-D}^D \frac{dk}{2\pi} \left| f_1(k) + f_2(k) \right| \frac{|T_a(k)|^2}{2\Delta}, \quad (D.15c)$$

$$- \frac{1}{2} \int_{-D}^D \frac{dk}{2\pi} \left| f_1(k) - f_2(k) \right| |T_a(k)| \frac{|T_a(w)|^2}{2\Delta} \quad (D.15d)$$

where $z_a = \epsilon_a - i\Delta$ and $T_a(k) = 2\Delta/(k - z_a)$. These Green’s functions can be found by conventional means, or by using the time-dependent operators of Sec. 3.3. Eq. (D.15d) is the two lead case of the more general Eq. (3.102a) from the main text.

Using the “optical” identity (3.80), we then obtain:

$$\text{Im} \left[ \tilde{G}^{R}_{a,a}(w) \right] = - \frac{|T_a(w)|^2}{4\Delta} - \frac{U}{16\Delta^3} \int_{-D}^D \frac{dk}{2\pi} \left| f_1(k) - f_2(k) \right| |T_a(k)| \frac{|T_a(w)|^2}{|T_a(w)|^2 \text{Re} [T_a(w)]}, \quad (D.16)$$
Then we find steady state current from (D.5):

\[
\lim_{t \to \infty} I_{Sym}(t) = \int_{-D}^{D} \frac{dw}{2\pi} \left[ f_1(w) - f_2(w) \right] \sum_a \frac{1}{4} |T_a(w)|^2 \\
+ \frac{U}{16\Delta^2} \int_{-D}^{D} \frac{dk}{2\pi} \int_{-D}^{D} \frac{dw}{2\pi} \left[ f_1(k) + f_2(k) \right] \left[ f_1(w) - f_2(w) \right] \sum_a |T_a(k)|^2 |T_a(w)|^2 \text{Re} \left[ T_a(w) \right]. \tag{D.17}
\]

This agrees with Eq. (6.92) from the main text once we take the dot energy to be spin-independent \([\epsilon_a = \epsilon, \text{ hence } T_a(k) = T(k)]\). As stated in the main text, we can also obtain the answer with spin dependence using the wavefunction method.
Appendix E

Beyond the wide-band limit

The main purpose of this Appendix is to provide a more careful justification of the averaging prescription for the delta function (Sec. 3.4) that is used throughout this thesis. Recall that this prescription becomes necessary because we take the Hamiltonian to have no cut off. We therefore put in a cutoff and examine the limit as it is sent to infinity. Note that the most reliable setup would be to calculate an observable in the time-evolving state $|\Psi(t)\rangle = e^{-iHt}|\Psi\rangle$, with both the modes in the initial state and the modes in $H$ cutoff by the same $D$; here, we starting with a cutoff on $H$, but still sending it to infinity before the cutoff on $|\Psi\rangle$. (See Sec. A.5 for more discussion.)

A secondary purpose is to introduce a Laplace transform approach to solving the “inverse problems” that determine the crossing states. While our results in the interacting case are very preliminary, this technique could be of interest as a way of solving for the crossing states without needing to make an ansatz.

E.1 Potential scattering model

We consider a more general version of the potential scattering model:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{kk'} c_k^\dagger V_{kk'} c_{k'},$$

(E.1)

in which all sums over momenta are cut off by $|\epsilon_k| < D$. The number of spatial dimensions is arbitrary for the moment, though we will write the system size as $L$. The model previously considered is obtained by specializing to the wideband case, which has one spatial dimension, $\epsilon_k = k, V_{kk'} = J' / L$, and $D = \infty$. To get the same answer as obtained previously using
the averaging prescription, we will find it necessary to take the limit of infinite system size (with \( J' \) fixed), as well.

We write:

\[
c_k(t) \equiv e^{-iHt}c_k e^{iHt} = e^{-i\epsilon_k t} c_k + \frac{1}{L} \sum_q F_k(t, q) c_q^+, \tag{E.2}
\]

where a factor of \( L \) is included for the convenience of later taking the system size to infinity.

The equation of motion \([H, c_k(t)] - i\frac{\partial}{\partial t} c_k^+(t) = 0\) yields:

\[
\left( \epsilon_q - i \frac{\partial}{\partial t} \right) F_k(t, q) + LV_{qk} e^{-i\epsilon_k t} + \sum_{q'} V_{qq'} F_k(t, q') = 0, \tag{E.3}
\]

which we are to solve with the initial condition \( F_k(t = 0, q) = 0 \). The equation can be solved iteratively to yield a series solution \( F_k(t, q) = F_k^{(1)}(t, q) + F_k^{(2)}(t, q) + \ldots \); this is conveniently done by taking the Laplace transform of both sides:

\[
(\epsilon_q - is) F_k(s, q) + \frac{iLV_{qk}}{is - \epsilon_k} + \sum_{q'} V_{qq'} F_k(s, q') = 0, \tag{E.4a}
\]

i.e.,

\[
F_k(s, q) = \frac{1}{is - \epsilon_q} \left( \frac{iLV_{qk}}{is - \epsilon_k} + \sum_{q'} V_{qq'} F_k(s, q') \right), \tag{E.4b}
\]

where \( \text{Re} \ s > 0 \) and \( F_k(s, q) = \int_0^\infty dt \ e^{-st} F_k(t, q) \) (we use the same symbol for the original function \( F_k \) and its transform). Iterating this equation, one is lead to the following ansatz:

\[
F_k(s, q) = \frac{i}{is - \epsilon_q} \frac{i}{is - \epsilon_k} \mathcal{M}_{qk}(s), \tag{E.5}
\]

where \( \mathcal{M}_{qk}(s) \), one finds, must satisfy an equation that can be solved by iterating, yielding a (possibly formal) series answer:

\[
\mathcal{M}_{qk}(s) = -iLV_{qk} + \sum_{q'} V_{qq'} \frac{1}{is - \epsilon_{q'}} \mathcal{M}_{q'k}(s) \tag{E.6a}
\]

\[
= -iL \left( V_{qk} + \sum_{n=1}^{\infty} \sum_{q_1 \ldots q_n} V_{q_1q_2} \frac{1}{is - \epsilon_{q_1}} V_{q_3q_2} \frac{1}{is - \epsilon_{q_2}} \ldots \frac{1}{is - \epsilon_{q_n}} V_{q_kq_n} \right). \tag{E.6b}
\]

Let us assume that the potential scattering term is separable: \( V_{kk'} = (J'/L)v_kv_{k'}^* \). Then the series is geometric, yielding:

\[
\mathcal{M}_{qk}(s) = -iJ'v_qv_k^* \sum_{n=0}^{\infty} \left( \sum_{q'} \frac{J'|q'_q|^2}{is - \epsilon_{q'}} \right)^n = -iJ'v_qv_k^* \frac{1}{1 + iJ'\alpha(s)}, \tag{E.7}
\]
where we have defined a quantity that will appear again in the Kondo and resonant level calculations:

\[
\alpha(s) = \frac{1}{L} \sum_{q'} |v_{q'}|^2 \frac{i}{is - \epsilon_{q'}}.
\] (E.8)

Direct substitution into Eq. (E.6a) verifies this answer, regardless of whether or not the geometric series converges. It is straightforward, if not very illuminating, to return to the time domain:

\[
F_k(t, q) = \frac{i}{\epsilon_q - \epsilon_k} \int_0^t dt' \left( e^{-i\epsilon_q(t-t')} - e^{-i\epsilon_k(t-t')} \right) \mathcal{M}_{qk}(t') \quad (t \geq 0).
\] (E.9)

We now wish to examine the simplest limit: one spatial dimension (the usual size \(L\) with periodic boundary conditions), linear spectrum \(\epsilon_k = k\), and constant scattering \(v_k = 1\). Then we have:

\[
\alpha(s) = \frac{1}{L} \sum_{q'} \frac{i}{is - q'} \int_0^\infty \frac{dq'}{2\pi} \frac{i}{is - q'} \int_0^\infty \frac{dD}{2\pi} \frac{i}{is - q} \frac{D}{1/2},
\] (E.10a)

thus, \(\mathcal{M}_{qk}(s) \rightarrow \frac{-iJ'}{1 + i\frac{1}{2}J'} = \mathcal{M}\), (E.10b)

where we have identified the same constant \(\mathcal{M}\) as appeared in the real space solution [Eq. (3.7)]. We have thus shown that the solution in the limit of infinite volume and bandwidth is (in the Laplace domain):

\[
c_k^\dagger(s) = \frac{i}{is - k} c_k^\dagger + \int \frac{dq}{2\pi} F_k(s, q) c_q^\dagger = \frac{i}{is - k} c_k^\dagger + \int \frac{dq}{2\pi} \frac{i}{is - q} \mathcal{M} c_q^\dagger,
\] (E.11)

where the momentum operators are now Dirac normalized. We can then transform back to the time and real space domain:

\[
c_k^\dagger(t) = e^{-ikt} c_k^\dagger + \mathcal{M} \int \frac{dq}{2\pi} \frac{i}{q - k} \left( e^{-iqt} - e^{-ikt} \right) c_q^\dagger \quad (t \geq 0)
\] (E.12a)

\[
= e^{-ikt} c_k^\dagger + \int dx e^{-ik(t-x)} \mathcal{M} \Theta(0 < x < t) \psi^\dagger(x) \quad (t \geq 0),
\] (E.12b)

which agrees exactly (in the infinite size limit) with the solution found in Sec. 3.1 using the averaging prescription. It is not surprising that the \(L \rightarrow \infty\) limit was necessary, for the following reason: the solution for arbitrary \(t\) and \(L\) is more complicated since it includes the
times $t > L/2$ during which the effect of the quench passes the boundary and goes around again any number of times. The Laplace transform probes arbitrarily large times and not only the time interval $0 \leq t \leq L/2$ which is of interest. Taking $L \to \infty$ sends the time of the first crossing to infinity, so that we are effectively in the regime $0 \leq t \leq L/2$.

### E.2 Kondo model

Following the same steps as in the potential scattering model, we can show that the real space solution from the main text is the large bandwidth limit of the solution of the model with the Hamiltonian (including both the kinetic term and the interaction term) cut off by the bandwidth. Unlike the potential scattering model, it does not seem possible to solve for the wavefunction at finite bandwidth, except for the one particle case (which is essentially non-interacting). The Kondo Hamiltonian is:

$$H = \sum_k \epsilon_k c^\dagger_k a_k + \sum_{k,k'} c^\dagger_{k} J_{kk'} \sigma_{a0} c^\dagger_{k'} \cdot S,$$

(E.13)

where all sums over momenta are cut off by $|\epsilon_k| < D$. We take the single-particle operators to evolve via the non-interacting part of the Hamiltonian: $c^\dagger_k(t) = e^{-i\epsilon_k t} c^\dagger_k$. We find:

$$A_{ka}(t) \equiv [H, c^\dagger_k(t)] - i \frac{\partial}{\partial t} c^\dagger_k(t) = e^{-i\epsilon_k t} \sum_q J_{qk} c^\dagger_q \sigma_{ba} \cdot S$$

(E.14)

**One particle.**

To solve the single-particle problem, we must find $|\chi_{ka,a_0}(t)\rangle$ satisfying:

$$\left(H - i \frac{d}{dt}\right) |\chi_{k_{1a1},a_0}(t)\rangle = -A_{k_{1a1}}(t) |a_0\rangle$$

(E.15a)

$$|\chi_{k_{1a1},a_0}(t = 0)\rangle = 0$$

(E.15b)

The Laplace transform yields:

$$(H - is) |\chi_{k_{1a1},a_0}(s)\rangle = -A_{k_{1a1}}(s) |a_0\rangle = -\sum_{q_1} J_{q_1 k_{1}} \frac{i}{i\lambda - \epsilon_{k_{1}}} \sigma_{b_{1}a_{1}} \cdot S_{a_{0}b_{0}} c^\dagger_{q_{1}b_{1}} |b_0\rangle.$$

(E.16)
We write the (Laplace-transformed) crossing state as:

$$\chi_{k_{1a_1},a_0}(s) = \frac{1}{L} \sum_{q_1} F_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1) c_{q_1 b_1}^\dagger |b_0\rangle,$$  \hspace{1cm} (E.17)

which yields the following requirement for the function $F$:

$$(\epsilon_{q_1} - i s) F_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1) + \sum_{q'} J_{q_1 q'} \sigma_{b_1 d_1} \cdot S_{b_0 d_0} F_{k_{1a_1},a_0}^{d_1,d_0}(s,q') = -L J_{q_1 k_1} \frac{i}{i s - \epsilon_{k_1}} \sigma_{b_1 a_1} \cdot S_{a_0 b_0},$$

that is,

$$F_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1) = \frac{1}{i s - \epsilon_{q_1}} \left( \frac{i L J_{q_1 k_1}}{i s - \epsilon_{k_1}} \sigma_{b_1 a_1} \cdot S_{b_0 a_0} + \sum_{q'} J_{q_1 q'} \sigma_{b_1 d_1} \cdot S_{b_0 d_0} F_{k_{1a_1},a_0}^{d_1,d_0}(s,q') \right).$$  \hspace{1cm} (E.18)

Writing $F_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1) = \frac{i}{i s - \epsilon_{q_1}} \sigma_{b_1 a_1} \cdot S_{b_0 a_0} C_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1)$, we find that $G$ must satisfy:

$$C_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1) = -i \left( L J_{q_1 k_1} \sigma_{b_1 a_1} \cdot S_{b_0 a_0} + \sum_{q'} J_{q_1 q'} \sigma_{b_1 d_1} \cdot S_{b_0 d_0} G_{k_{1a_1},a_0}^{d_1,d_0}(s,q') \right).$$  \hspace{1cm} (E.19)

While it may be possible to write a series expression for $G$ by iterating the above equation, we will not pursue this. Let us take the interaction term to separable: $J_{kk'} = (J/L) v_k v_{k'}$. Then, writing $G_{k_{1a_1},a_0}^{b_1,b_0}(s,q_1) = v_{q_1} v_{k_1}^* M_{a_1 a_0}^{b_1 b_0}(s)$, we obtain:

$$M_{a_1 a_0}^{b_1 b_0}(s) = -i J \left[ \sigma_{b_1 a_1} \cdot S_{b_0 a_0} + \alpha(s) \sigma_{b_1 d_1} \cdot S_{b_0 d_0} M_{a_1 a_0}^{d_1 d_0}(s) \right]$$

$$= \frac{i \frac{1}{2} J}{1 - i \alpha(s) J + \frac{3}{4} \alpha(s)^2 J^2} \left[ \left( 1 + i \frac{3}{2} J \right) I - 2 P \right]^{b_1 b_0}_{a_1 a_0},$$  \hspace{1cm} (E.21a)

where $\alpha(s)$ is given in Eq. (E.8) and we have solved for $M(s)$ via matrix inversion (a very similar calculation to the main text). In the one-dimensional problem with linear spectrum and momentum-independent interaction ($v_k = 1$), we have:

$$\alpha(s) \xrightarrow{L \to \infty, D \to \infty} 1/2 \text{ [see Eq. (E.10a)]}, \text{ hence: } M_{a_1 a_0}^{b_1 b_0}(s) \xrightarrow{L \to \infty, D \to \infty} M_{a_1 a_0}^{b_1 b_0},$$  \hspace{1cm} (E.22)

where $M_{a_1 a_0}^{b_1 b_0}$ is the $s$-independent matrix found in the main text [Eq. (4.24)]. We have thus found, in this simple limit:

$$\chi_{k_{1a_1},a_0}(s) = \int \frac{dq_1}{2\pi} \frac{i}{i s - k_1} \frac{i}{i s - q_1} M_{a_1 a_0}^{b_1 b_0} c_{q_1 b_1}^\dagger |b_0\rangle,$$  \hspace{1cm} (E.23)
where the momentum operators are now Dirac normalized. In the time and real space domain, this answer is:

\[ |\chi_{k_{1a_1},a_0}(t)\rangle = \int dx_1 \, e^{-ik_1(t-x_1)} \mathcal{M}_{a_1a_0}^b \Theta(0 < x_1 < t) \psi_{b_1}^\dagger(x)|b_0\rangle \quad (t \geq 0), \tag{E.24} \]

in agreement with the main text.

**Two particles.**

We will show that the answer in the main text is obtained in the limit of infinite system size and bandwidth, though we will not be able to solve the problem for arbitrary bandwidth. The goal is to find a state \( |\chi_{k_{1a_1}k_{2a_2},a_0}(t)\rangle \) that satisfies:

\[
\left( H - i\frac{d}{dt} \right) |\chi_{k_{1a_1}k_{2a_2},a_0}(t)\rangle = -A_{k_{2a_2}}(t)|\chi_{k_{1a_1},a_0}(t)\rangle, \tag{E.25a} \]

\[
|\chi_{k_{1a_1}k_{2a_2},a_0}(t = 0)\rangle = 0. \tag{E.25b} \]

Taking the Laplace transform converts these to:

\[
(H - is) |\chi_{k_{1a_1}k_{2a_2},a_0}(s)\rangle = -\int_0^\infty dt \, e^{-st} A_{k_{2a_2}}(t)|\chi_{k_{1a_1},a_0}(t)\rangle \\
= -\frac{1}{L} \sum_{q_1,q_2} J_{q_2k_2} \sigma_{b_2a_2} \cdot S_{b_0d_0} \, F_{k_{1a_1},a_0}^{b_1d_0} (s + i\epsilon_{k_2}, q_1) c_{q_2b_2}^\dagger c_{q_1b_1}^\dagger |b_0\rangle \tag{E.26a} \]

\[
= -\frac{i}{is - \epsilon_{k_1} - \epsilon_{k_2}} \frac{1}{L} \sum_{q_1,q_2} i\frac{J_{q_2k_2}}{is - \epsilon_{k_1} - \epsilon_{k_2}} \sigma_{b_2a_2} \cdot S_{b_0d_0} G_{k_{1a_1},a_0}^{b_1d_0} (s + i\epsilon_{k_2}, q_1) c_{q_2b_2}^\dagger c_{q_1b_1}^\dagger |b_0\rangle. \tag{E.26b} \]

We write:

\[
|\chi_{k_{1a_1}k_{2a_2},a_0}(s)\rangle = \frac{1}{L^2} \sum_{q_1,q_2} F_{k_{1a_1}k_{2a_2},a_0}^{b_1b_2} (s) c_{q_2b_2}^\dagger c_{q_1b_1}^\dagger |b_0\rangle, \tag{E.27} \]

which leads to:

\[
(H - is) |\chi_{k_{1a_1}k_{2a_2},a_0}(s)\rangle = \frac{1}{L^2} \sum_{q_1,q_2} \left[ (\epsilon_{q_1} + \epsilon_{q_2} - is) F_{k_{1a_1}k_{2a_2},a_0}^{b_1b_2} (s,q_1,q_2) \right. \\
+ \sum_{q'} J_{q_2q'} \sigma_{b_2a_2} \cdot S_{b_0d_0} F_{k_{1a_1}k_{2a_2},a_0}^{b_1d_0} (s,q_1,q') + \sum_{q'} J_{q_1q'} \sigma_{b_1a_1} \cdot S_{b_0d_0} F_{k_{1a_1}k_{2a_2},a_0}^{d_1b_2} (s,q',q_2) \left. \right] c_{q_2b_2}^\dagger c_{q_1b_1}^\dagger |b_0\rangle. \tag{E.28} \]
The simplest way to proceed is to require equality of the coefficients of \( c_{q_2}^\dagger c_{q_1}^\dagger |b_0\rangle \) in this equation and in the right-hand side of Eq. (E.26b). (Only the antisymmetric parts need to be equal, but this requirement is sufficient and parallels what was done in the main text.) After some rearrangement of terms, this requirement becomes:

\[
F_{b_1 b_2, b_0}^{k_1, k_2, a_2, a_0}(t, q_1, q_2) = \frac{1}{i\delta - \epsilon_{q_1} - \epsilon_{q_2}} \left[ iL \mathcal{J}_{q_2 k_2} \frac{i}{i\delta - \epsilon_{k_2}} \mathbf{\sigma}_{b_2 a_2} \cdot \mathbf{S}_{b_0 d_0} G_{b_1, d_0}^{b_1, d_0} (s + i\epsilon_{k_2}, q_1) + \sum_{q'} \mathcal{J}_{q_2 q'} \mathbf{\sigma}_{b_2 a_2} \cdot \mathbf{S}_{b_0 d_0} F_{b_1 d_2, d_0}^{b_1, d_2, d_0} (s, q_1, q') + \sum_{q'} \mathcal{J}_{q_1 q'} \mathbf{\sigma}_{b_1 d_1} \cdot \mathbf{S}_{b_0 d_0} F_{b_1 d_2, d_0}^{b_1, d_2, d_0} (s, q', q_2) \right]. \tag{E.29}
\]

Proceeding as in the single-particle case, we write:

\[
F_{b_1 b_2, b_0}^{k_1, k_2, a_2, a_0}(t, q_1, q_2) = \frac{i}{i\delta - \epsilon_{q_1} - \epsilon_{q_2}} \frac{i}{i\delta - \epsilon_{k_2}} \frac{i}{i\delta - \epsilon_{q_2}} \frac{i}{i\delta - \epsilon_{k_2}} G_{b_1 b_2, b_0}^{k_1, k_2, a_2, a_0} (s, q_1, q_2), \tag{E.30}
\]

which leads to the requirement:

\[
G_{b_1 b_2, b_0}^{k_1, k_2, a_2, a_0} (s, q_1, q_2) = -i \left[ L \mathcal{J}_{q_2 k_2} \mathbf{\sigma}_{b_2 a_2} \cdot \mathbf{S}_{b_0 d_0} G_{b_1, d_0}^{b_1, d_0} (s + i\epsilon_{k_2}, q_1) + \sum_{q'} \mathcal{J}_{q_2 q'} \mathbf{\sigma}_{b_2 a_2} \cdot \mathbf{S}_{b_0 d_0} G_{b_1 d_2, d_0}^{b_1, d_2, d_0} (s, q_1, q') + \left( \frac{i}{i\delta - \epsilon_{q_1} - \epsilon_{k_2}} \right)^{-1} \sum_{q'} i\mathcal{J}_{q_1 q'} \mathbf{\sigma}_{b_1 d_1} \cdot \mathbf{S}_{b_0 d_0} G_{b_1 d_2, d_0}^{b_1, d_2, d_0} (s, q', q_2) \right]. \tag{E.31}
\]

In principle, this could be solved by iteration. However, the third term on the right-hand side (hereafter called “third term”) seems to prevent any neat re-summation, even in the separable case \( \mathcal{J}_{kk'} = (J/L)v_k v_{k'}^* \). We can show, though, that the trial solution \( G_{k_1, k_2, a_2, a_0}^{b_1, c_1} (s, q_1, q_2) = G_{k_1, a_1, a_0}^{b_1, c_1} (s + i\epsilon_{k_2}, q_1) G_{k_2 a_2, c_1}^{b_2, b_0} (s + i\epsilon_{q_1}, q_2) \) works in the limit of large system size and bandwidth (with linear spectrum and \( v_k = 1 \)). To see this, we plug in the
trial solution to find:

\[
\text{right-hand side of Eq. (E.31)} = -i e^{b_{1c_1}}(s + i \epsilon_{k_2}, q) \left[ L^b_{s} J_{q_2} \sigma_{s} \cdot S_{b_0c_1} \right] + \sum_{q'} J_{q_2} q' \frac{i}{i s - \epsilon_{q_1} - \epsilon_{q'}} \sigma_{k_2} d_2 \cdot S_{b_0 d_0} G_{b_0 d_0}^{c_2 d_0}(s + i \epsilon_{q_1}, q_2) + \text{(third term)} \quad (E.32a)
\]

\[
= G_{b_1 b_2, b_0}^{b_{1c_1}}(s, q_1, q_2) + \text{(third term)}, \quad (E.32b)
\]

where we used Eq. (E.20). Thus, the trial solution is correct whenever the third term vanishes. Let us now show that the third term vanishes in the simplest limit. We note that

\[
\frac{i}{i s - \epsilon_{q_1} - \epsilon_{q_2}} = \frac{i}{i s - \epsilon_{q_1} - \epsilon_{q_2}} \left( \frac{i}{i s - \epsilon_{q_2} - \epsilon_{q_2}} \right), \quad \text{then set } \epsilon_{k} = k \text{ and } v_{k} = 1 \text{ to find:}
\]

third term \( \lim_{D \to \infty} \) (prefactor) \( \int_{-D}^{D} dq' \frac{i}{i s - q' - q_2} \frac{i}{i s - q' - k_2} \mathcal{M}_{b_{2c_1}}^{b_{2b_0}}(s + q') \quad (E.33a) \)

\[
\lim_{D \to \infty} 0. \quad (E.33b)
\]

The point is that \( \mathcal{M}_{a_{2c_1}}^{b_{2b_0}}(s + q') \) goes to the \( s \)-independent \( \mathcal{M}_{a_{2c_1}}^{b_{2b_0}} \), and the two integrals cancel against each other in the large bandwidth limit. Thus, the trial solution is confirmed in this simple limiting case. The final result for the crossing state can be written as:

\[
|\chi_{k_1 a_1, k_2 a_2, a_0}(s)\rangle = \int \frac{dq_1 dq_2}{2 \pi} \frac{i}{i s - q_1 - q_2} \frac{i}{i s - k_1 - k_2} \frac{i}{i s - q_1 - k_2} \mathcal{M}_{a_{1c_0}}^{b_{1c_1}} \mathcal{M}_{a_{2c_1}}^{b_{2b_0}} c_2 c_{b_2}^{\dagger} |b_0\rangle, \quad (E.34)
\]

which becomes, in the time and real space domain:

\[
|\chi_{k_1 a_1, k_2 a_2, a_0}(t)\rangle = \int dx_1 dx_2 e^{-i k_1(t-x_1)} e^{-i k_2(t-x_2)} \mathcal{M}_{a_{1c_0}}^{b_{1c_1}} \mathcal{M}_{a_{2c_1}}^{b_{2b_0}} \Theta(0 < x_2 < x_1 < t) \times \psi_{b_2}^{\dagger}(x_2) \psi_{b_1}^{\dagger}(x_1) |b_0\rangle \quad (t \geq 0), \quad (E.35)
\]

in agreement with the main text.

**Further comments.**

The above calculations can probably be extended to an arbitrary number of particles. Also, it is interesting to note that the long time limit of the single particle solution is exactly
the same as the single particle solution in Bethe Ansatz. It is probable, then, that the same approach as taken here can show that the Bethe Ansatz solution, with two or more particles and with the averaging prescription, is reached as the limit of sending the cutoff on the Hamiltonian to infinity.

From the above calculations, we can immediately read off what happens if we solve the potential scattering model with the potential considered as an interaction term. One simply replaces \( J_{kk'} \sigma \cdot S \to V_{kk'} \) and deletes all spin indices. It may be surprising, then, that the difficulty in solving the two particle problem at finite bandwidth does not appear to come from the spin structure of the problem. Indeed, the “third term” referenced above still poses a difficulty even if the spin indices are deleted. This seems to contradict the fact that we can construct a two particle solution to the potential scattering model, even at finite bandwidth, by taking a product of the single-particle operators found above.

The resolution is the following. The two particle solution to the potential scattering model can be written as:

\[
|\Psi_{k_1k_2}(t)\rangle = c^\dagger_{k_2}(t) c^\dagger_{k_1}(t)|0\rangle + c^\dagger_{k_2}(t)|\Phi_{k_1}(t)\rangle - c^\dagger_{k_2}(t)|\Phi_{k_1k_2}(t)\rangle + |\Psi_{k_1k_2}(t)\rangle,
\]

(E.36)

where the \( c^\dagger_k(t) \) operators evolve with the potential scattering term and \( c^\dagger_k(t) = e^{-i\epsilon_k t} c^\dagger_k \).

Using the previously-calculated results for \( c^\dagger_k(t) \), we can read off the crossing states \( |\Phi_{k_1}(t)\rangle = |\chi_{k_1}(t)\rangle \) and \( |\Phi_{k_1k_2}(t)\rangle \). However, there may not be a convenient separation of \( |\Phi_{k_1k_2}(t)\rangle = |\chi_{k_1k_2}(t)\rangle - |\chi_{k_1k_2}(t)\rangle \). This separation is of no significance in the potential scattering model. In the Kondo model, however, the two terms that the \( n=2 \) crossing state needs to cancel \( A_{k_2a_2}(t)|\chi_{k_1a_1a_0}(t)\rangle \) and \( A_{k_1a_1}(t)|\chi_{k_2a_2a_0}(t)\rangle \) have different spin structure, so it does not seem as straightforward to find a single state \( |\Phi_{k_1a_1k_2a_2, a_0}(t)\rangle \) that cancels both.
E.3 Resonant level model

This calculation follows along the same lines as the potential scattering case (Sec. E.1); in the same limit, we find agreement with the averaging prescription results from the main text. We start with the more general version of the model:

\[ H^{(0)} = \sum_k \epsilon_k c_k^\dagger c_k + \epsilon_d d^\dagger d + \left( \sum_k V_k c_k^\dagger d + \text{h.c.} \right), \]

where the sums over momenta are again cutoff by \( |\epsilon_k| < D \). The time-evolving single particle operators are found as follows:

\[
\begin{align*}
    c_k^\dagger(t) &\equiv e^{-iH^{(0)}t}c_k^\dagger e^{iH^{(0)}t} = e^{-i\epsilon_k t} c_k^\dagger + \frac{1}{L} \sum_q F_k(t, q) c_q^\dagger + \frac{1}{\sqrt{L}} G_k(t) d^\dagger, \\
    d^\dagger(t) &\equiv e^{-iH^{(0)}t}d^\dagger e^{iH^{(0)}t} = e^{-i\epsilon_d t} d^\dagger + \frac{1}{\sqrt{L}} \sum_q F(t, q) c_q^\dagger + G(t) d^\dagger.
\end{align*}
\]

The equations of motion are:

\[
\begin{align*}
    \left( \epsilon_q - i \frac{\partial}{\partial t} \right) F_k(t, q) + \sqrt{L} V_q G_k(t) &= 0, \\
    \left( \epsilon_d - i \frac{\partial}{\partial t} \right) G_k(t) + \sqrt{L} V_k^* e^{-ikt} + \frac{1}{\sqrt{L}} \sum_{q'} V_{q'}^* F_k(t, q') &= 0.
\end{align*}
\]

with initial conditions \( F_k(t = 0, q) = G_k(t = 0) = 0 \); the equations for \( F \) and \( G \) are similar.

The Laplace transform yields:

\[
\begin{align*}
    F_k(s, q) &= \frac{\sqrt{L} V_q G_k(s)}{is - \epsilon_q}, \\
    G_k(s) &= \frac{1}{is - \epsilon} \left( \frac{i\sqrt{L} V_k^*}{is - \epsilon} + \frac{1}{\sqrt{L}} \sum_{q'} V_{q'}^* F_k(s, q') \right),
\end{align*}
\]

from which we obtain:

\[
\begin{align*}
    F_k(s, q) &= \frac{i}{(is - \epsilon_q)(is - \epsilon)} \frac{LV_k^* V_q}{is - \epsilon + i \sum_{q'} |V_{q'}|^2 \frac{i}{is - \epsilon_q}}, \\
    G_k(s) &= \frac{i}{is - \epsilon_k} \frac{\sqrt{L} V_k^*}{is - \epsilon + i \sum_q |V_q|^2 \frac{i}{is - \epsilon_q}}.
\end{align*}
\]
We specialize to the wideband case: $\epsilon_k = k$, $V_k = \frac{1}{\sqrt{L}} v$. In the limit $L \to \infty, D \to \infty$, we obtain:

\[
F_k(s, q) \to \frac{2i\Delta}{(is - q)(is - k)(is - z)}, \quad (E.42a)
\]
\[
G_k(s, q) \to \frac{iv}{(is - k)(is - z)}, \quad (E.42b)
\]

where we have again used (E.10a) (recall also that $\Delta = \frac{1}{2} |v|^2$ and $z = \epsilon - i\Delta$). Thus, we have shown:

\[
c_k^\dagger(s) \to \frac{i}{is - k} c_k^\dagger + \int \frac{dq}{2\pi} \frac{2i\Delta}{(is - q)(is - k)(is - z)} c_q^\dagger + \frac{iv}{(is - k)(is - z)} d^\dagger \quad (E.43a)
\]
\[
= \frac{i}{is - k} c_k^\dagger + \int dx \frac{2\Delta}{(is - k)(is - z)} e^{-sx} \Theta(0 < x) \psi(x) + \frac{iv}{(is - k)(is - z)} d^\dagger. \quad (E.43b)
\]

Returning to the time domain then recovers the same answer as in the main text (with $L \to \infty$).