TWO PROBLEMS IN MATHEMATICAL PHYSICS

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ABSTRACT OF THE DISSERTATION

Two Problems in Mathematical Physics

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In chapter 1, a rigorous proof is presented of the existence of the static, spherically symmetric spacetime that is the solution of the Einstein field equations coupled with an electric field obeying the equations of electromagnetism of Bopp-Landé-Thomas-Podolsky for a static point charge. It is shown that the electric field energy is finite, just as the case is for this theory on a background flat spacetime. The argument proves the existence of a 2-parameter family of solutions in the regime of large radial variable and of a 1-parameter family when this variable is small, by means of a new technique for estimating the radius of convergence of a power series whose coefficients are defined by a polynomial recursion. The existence of the intersection of the families of solutions from these two regimes is established through carefully restricting the allowable ranges of their parameters so that the Poincaré-Miranda theorem can be applied.

In chapter 2, a generalization of the system of so-called Jacobi coordinate transformations for classical and quantum many-body problems is developed, suitable for the study of questions involving the center-of-mass of the system when the interaction between the bodies enjoys symmetry properties. It is applied to the study of asymptotic ground-state properties of a quantum Hamiltonian that models an atom with N bosonic electrons without the Born-Oppenheimer approximation. The conjectured Hartree limit $N \to \infty$ is shown to supply a rigorous upper bound to the ground state energy.

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Dedication

To my Math and Physics teachers from many years ago: Cássia, Dona Dirce, Jefferson, Norma, Pião and Alexandre "Piãozinho", Seu Rizzo, Tecão, Valdir, and especially Tia Sílvia. Today I live happily in the world of numbers only because I had the best people show me around when I first discovered it.

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Chapter 1

Maxwell-Bopp-Landé-Thomas-Podolsky-Einstein system with static point source

(Supervised by Michael Kiessling and Shadi Tahvildar-Zadeh)

1.1 Overview

This work fits in the much wider scope of investigating the claim, originally made by Einstein, Infeld and Hoffmann [EIH38], that the equations of General Relativity alone imply the equations of motion of the point sources of gravity (viewed as singularities in spacetime) - see [KT19] for details.

The problem of the *self-force* in electrodynamics consists of finding an expression for the force that the electromagnetic field generated by a charged point particle exerts on the particle itself. The possibility to write well-posed classical systems of equations for the joint evolution of electromagnetic (EM) fields and their sources, without resorting to *ad hoc* field averaging or bare mass renormalization at point charges, requires working with laws of electromagnetism such that the energy-momentum density of the electromagnetic field generated by charged particles is locally integrable, which is not the case for the usual Maxwell equations. There are generalized EM theories that were proposed specifically to address this problem, one of them being the so-called *Bopp-Podolsky* theory (which we will call *Bopp-Landé-Thomas-Podolsky*, or BLTP, theory).

Using this theory, Kiessling [Kie19] has recently shown how to formulate a well-posed system for the joint evolution of point particles and their EM fields in **flat-space** (that is, the Minkowski spacetime of Special Relativity). Local integrability of the field energy-momentum at the location of the particles is essential in his work, hence why it is important to work with generalizations of the usual Maxwell equations. But the nonlinearities in the Einstein field equations pose serious obstacles to generalizing this study to the theory of General Relativity.

The present work is a small first step towards extending Kiessling's framework to General Relativity: we rigorously show the existence of a finite-energy solution to the Einstein equations for the spacetime of a single, static point charge whose electric field obeys the equations in Bopp-Podolsky theory. The natural next step going forward, after completing the proof, will be to study our spacetime in the framework of [BKT19], which defines a *weak second Bianchi identity* for spacetimes with point singularities and studies its implications for physical conservation laws, and then to start investigating the case of two particles.

1.1.1 Problem description

The usual Maxwell equations for the EM fields $\boldsymbol{E}, \boldsymbol{B}, \boldsymbol{D}, \boldsymbol{H}$ of a point particle in flat-space, which we call the **Maxwell-Maxwell** system, consists of the **pre-metric Maxwell equations** (see [HO03])

$$\begin{cases} \nabla \cdot \boldsymbol{B} = 0 \quad , \quad \nabla \cdot \boldsymbol{D} = 4\pi Q \delta_{q(t)} \\ \nabla \times \boldsymbol{E} + c^{-1}\partial_t \boldsymbol{B} = 0 \quad , \quad \nabla \times \boldsymbol{H} - c^{-1}\partial_t \boldsymbol{D} = 4\pi c^{-1} Q \dot{q}(t) \delta_{q(t)} \end{cases} \tag{1.1.1}$$

together with the **Maxwell vacuum law**

$$\begin{cases} \boldsymbol{D} = \boldsymbol{E} \\ \boldsymbol{H} = \boldsymbol{B} \end{cases} . \tag{1.1.2}$$

Here, $q(t)$ is the position of the point particle at time t, considered to be given a priori, with $\dot{q}$ being its velocity and Q its charge (we work in Gaussian units). Upon solving this system, one finds that the field energy density $\varepsilon_{\text{MM}} := (8\pi)^{-1}(|\boldsymbol{E}|^2 + |\boldsymbol{B}|^2)$ is not integrable in space over any neighborhood of the particle. In the 1940's, a modification of the above system was proposed. It is often called the system of *Bopp-Podolsky* field equations, but we are going to call it the **Maxwell-BLTP** system, in honor of its original proponents Bopp [Bop40], Landé and Thomas [LT41], and Podolsky [Pod42]. The pre-metric equations (1.1.1) remain the same (hence the name "Maxwell"), but the vacuum law that relates $\boldsymbol{D}$ and $\boldsymbol{H}$ to $\boldsymbol{E}$ and $\boldsymbol{B}$ becomes the **BLTP vacuum law**

$$\begin{cases} \boldsymbol{D} = \boldsymbol{E} - \varkappa^{-2} \square \boldsymbol{E} \\ \boldsymbol{H} = \boldsymbol{B} - \varkappa^{-2} \square \boldsymbol{B} \end{cases} \tag{1.1.3}$$

where $\square = -c^{-2}\partial_t + \Delta$ is the wave operator and $\varkappa > 0$ is a parameter with dimension of inverse length. Note that $\varkappa = \infty$ recovers the Maxwell-Maxwell system. The solution, assuming that the particle is static and located at $q(t) \equiv 0$ for all t, has zero magnetic fields $\boldsymbol{B}, \boldsymbol{H}$ and

$$\boldsymbol{D}(\boldsymbol{r}) = \frac{Q}{4\pi r^2}\boldsymbol{e_r} \quad , \quad \boldsymbol{E}(\boldsymbol{r}) = \varphi'(r)\boldsymbol{e_r} \;\text{ where }\; \varphi(r) = \frac{Q(1-e^{-\varkappa r})}{r} \;, \tag{1.1.4}$$

for $r = \|(x,y,z)\| = \|\boldsymbol{r}\|$ and $\boldsymbol{e_r} = r^{-1}\boldsymbol{r}$. We remark that the electric potential φ is continuous at $r = 0$ and everywhere bounded. The exponential term in it is a small correction to the *Coulomb potential* Q/r for large values of r, while also ensuring that $\varphi(r)$ be bounded for small r. The field energy density, which in this static case works out to be $\varepsilon_{\text{BLTP}} = (8\pi)^{-1}(\boldsymbol{E}\cdot\boldsymbol{D} - \frac{1}{2}(|\boldsymbol{E}|^2 - \varkappa^{-2}(\nabla\cdot\boldsymbol{E})^2))$, gives a finite value for the total field energy $\mathcal{E}$:

$$\mathcal{E} := \int_{\mathbb{R}^3} \varepsilon_{\text{BLTP}}\ \mathrm{d}V = \frac{\varphi(0)}{2} = \frac{Q\varkappa^2}{2}\ . \tag{1.1.5}$$

Now suppose we "switch on gravity," that is, we consider the Einstein field equations of General Relativity for a static, spherically symmetric spacetime with a naked timelike singularity representing a single point charge at rest. This universe is devoid of matter away from this particle, but the latter generates electromagnetic fields that can be calculated at any point of spacetime (they depend on the EM theory assumed) and contribute to $T_{\mu\nu}$ (the source term in the Einstein equations). The underlying manifold is $\mathbb{R}^4$ minus a line, with a spherical coordinate system (ct, r, θ, ϕ) and a metric

$$\mathrm{d}s^2 = -c^2 e^{2\lambda(r)}\mathrm{d}t^2 + e^{2\nu(r)}\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\phi^2) \tag{1.1.6}$$

where r is the area-radius coordinate and $\lambda(r), \nu(r)$ are unknown. A globally defined electric potential $\varphi(r)$ is the third unknown of the problem. For $T_{\mu\nu}$ obtained from the Maxwell-Maxwell system, one obtains the **Reissner-Weyl-Nordström (RWN) solution**:

$$e^{2\lambda(r)} = 1 - \frac{2GM}{c^2 r} + \frac{GQ^2}{c^4 r^2} \quad , \quad \nu(r) = -\lambda(r) \quad , \quad \varphi(r) = \frac{Q}{r}\ , \tag{1.1.7}$$

with G being the gravitational constant and M a free parameter that can be identified as the total mass content of the spacetime (the *ADM mass*). However, it can be calculated that the electric field energy density on any constant-time hypersurface is not integrable around the singularity, meaning that the electric field energy of the particle is infinite. To understand how the ADM mass could be finite while the field energy is infinite, one has to assume that the RWN singularity carries a negative infinite bare mass.

Our goal will be to couple the Maxwell-BLTP system to the Einstein field equations. We call the system obtained the **Maxwell-BLTP-Einstein equations**, and the goal is to prove the existence of a solution $(\lambda(r), \nu(r), \varphi(r))$ that

1. has a finite value for $\mathcal{E}$;

2. has a finite value for $\lim_{r\to 0}\varphi(r)$;

3. is defined for all $r > 0$;

4. far away from the singularity, is asymptotic to the RWN solution;

5. pointwise in r, converges to the flat-space space solution of the Maxwell-BLTP equations when the gravitational constant G converges to 0.

The justification for items 1 and 2 was described in the context paragraph above. Item 3 says that there are no horizons, that is, the particle is modelled as a naked singularity of spacetime. Item 4 is desirable from a physical point of view, because it implies that the laws of electromagnetism that would be observed far away from the particle if BLTP theory were to be true would not differ from what we actually observe in nature far away from a charged spacetime singularity. Item 5 is to be expected given that gravitational effects in nature tend to be much weaker compared to electromagnetic effects, so the coupling of gravity to the flat-space equations should not perturb the solutions by too much.

Remark 1.1.1. There is another well-known formulation of the vacuum law which also deals with the problem of infinite field energy-momentum of a point particle in flat-space. Originally proposed by Born [Bor33], it is part of what nowadays is commonly called *Born-Infeld electrodynamics.* It was then first observed by Hoffmann [Hof35] that, under this formulation of EM, the singularity of the static, spherically symmetric spacetime of a resting point charge is milder than that of the RWN spacetime, in the sense that the blowup of certain curvature scalars is less severe. In [Tah11], a class of electrostatic, spherically symmetric spacetimes that generalize that of Hoffmann is studied with regard to the presence of horizons, the blowup of curvature scalars at the singularity, and finiteness of the electric field energy and its relation to the ADM mass. But the properties that define this class quickly allow for their metric coefficients to be explicitly solved by quadrature, partly due to the helpful fact that their metric coefficients satisfy $g_{tt}g_{rr} = -1$. This is however not the case for our metric in this thesis, a fact that will become evident once we write down the equations of the Maxwell-BLTP-Einstein system. This turns even the question of existence of a solution into a completely different and more challenging task for us than for the systems considered in that paper.

Remark 1.1.2. Regarding the Maxwell-BLTP-Einstein system, Cuzinatto et al. [Cuz+18] have proved that, if it is assumed that an event horizon exists at some $r = r_* > 0$, then finiteness of the field energy outside of this horizon implies a no-hair theorem - the solution outside of the horizon coincides with the RWN solution. But in our framework we would like to assume that there are no horizons: the particle is modelled as a naked singularity and the coordinate chart is assumed global. This situation happens also in the RWN spacetime when the parameters are such that $GM^2 < Q^2$, which is the case for example for the mass and charge of a proton or electron (Q^2 is more than 36 orders of magnitude larger than GM^2).

Remark 1.1.3. It is known that, for any solution of the Maxwell-BLTP-Einstein equations, φ will be the difference between usual Coulomb potential and a Proca potential (arising in the solution to the *Einstein-Proca* equations, with $\varkappa$ thought of as its mass parameter). There are numerical investigations of some properties of static, spherically symmetric spacetimes satisfying the Einstein-Proca or the Einstein-BLTP system ([VIG02], [OV99]), but a rigorous proof of existence of the solution cannot be found in the literature.

1.1.2 Summary of results

The value of the constant $1/\varkappa$ is unknown, but there are reasons to believe that it would be small if Maxwell-BLTP theory were the "true" classical theory of electromagnetism in nature. We will mostly work with units in which $Q = \varkappa = c = 1$, which then turns G into an exceptionally small dimensionless constant that we call ε. The Maxwell-BLTP-Einstein system can then be considered an ε-perturbation (or G-perturbation) of the flat-space Maxwell-BLTP equations. After obtaining the Einstein Field Equations from a Lagrangian for BLTP theory, we will recast everything in terms of the variables

$$\psi(r) = e^{\lambda(r)+\nu(r)} \quad , \quad \zeta(r) = e^{2\nu(r)} \quad , \quad w(r) = r^2 e^{-(\lambda(r)+\nu(r))}\varphi'(r) + 1 \ , \tag{1.1.8}$$

with the corresponding flat-space variables (solution of the system with $\varepsilon = 0$) being

$$\psi_0 \equiv \zeta_0 \equiv 1 \quad , \quad w_0(r) = (1+r)e^{-r} \ . \tag{1.1.9}$$

We will show that the equations reduce to a second-order ODE system for ψ, ζ, w (see (1.1.13) ahead). The asymptotic conditions far away from the singularity that we want to be satisfied can be written as

$$\lim_{r\to\infty} \psi(r) = \lim_{r\to\infty} \zeta(r) = 1 \quad , \quad \lim_{r\to\infty} w(r) = 0 \; . \tag{1.1.10}$$

Another one that will come for free in the solution is

$$\lim_{r\to\infty} w'(r) = 0 \; . \tag{1.1.11}$$

We will also identify sufficient conditions for the electromagnetic energy to be finite and for $\lim_{r\to 0} \varphi(r)$ to exist and be finite. They are

$$\left| \int_0^\infty \frac{\psi(r)(w(r)-1)}{r^2} \mathrm{d}r \right| < \infty \quad , \quad \left| \int_0^\infty \frac{\psi(r)(w(r)')^2}{\zeta(r) r^2} \mathrm{d}r \right| < \infty \; . \tag{1.1.12}$$

Once (1.1.10) and (1.1.11) are established, we see that finiteness of these integrals is not a problem around the $r = \infty$ endpoint, so we think of (1.1.12) as a condition for small r.

The main result to be proved is:

Theorem 1.1.4. *There exists $\varepsilon_* > 0$ such that, for all $\varepsilon \in [0, \varepsilon_*]$, the Maxwell-BLTP-Einstein system*

$$\begin{cases} \psi' = -\dfrac{\varepsilon \psi}{r^3}(w')^2 \\[2ex] \zeta' = \dfrac{(1-\zeta)\zeta}{r} + \dfrac{\varepsilon}{r^3}((1-w^2)\zeta^2 - (w')^2\zeta) \\[2ex] w'' = \left(\dfrac{3-\zeta}{r} + \dfrac{\varepsilon\zeta}{r^3}(1-w^2) \right) w' + \zeta w \end{cases} \tag{1.1.13}$$

of a static point charge admits a solution $(\psi_\varepsilon, \zeta_\varepsilon, w_\varepsilon)$ in $(0, \infty)$ satisfying the asymptotic properties described in (1.1.10) and (1.1.12), and such that, pointwise at any $r > 0$,

$$\lim_{\varepsilon\to 0} (\psi_\varepsilon(r), \zeta_\varepsilon(r), w_\varepsilon(r)) = (\psi_0(r), \zeta_0(r), w_0(r)) \; . \tag{1.1.14}$$

The argument is as follows:

- We show that, for any fixed $r_0 > 0$, a family of solutions exists on $[r_0, \infty)$ satisfying (1.1.10) and (1.1.11), as long as $\varepsilon > 0$ is small enough (the lower bound on ε gets worse the smaller we make r_0). This family is parametrized by two arbitrary real parameters μ and α, the first one having physical significance (it is related to the ADM mass). Our method consists of writing the solution as a power series in the small parameter ε, with the $\varepsilon = 0$ solution corresponding to the flat-space solution of the Maxwell-BLTP system, and then employing a novel technique for estimating the growth of the coefficients in order to get a lower bound for the radius of convergence.

- We find a suitable rewriting of the system that permits us to study it, for small r, as a first-order, 4D autonomous dynamical system around a hyperbolic equilibrium point. The new unknowns will be called (x, y, z, s). The 2-dimensional unstable manifold of this equilibrium point is analytic and consists of a 1-parameter family (we call σ the parameter) of solutions to the system satisfying (1.1.12), and we can use the same estimation techniques as above (this time for power series in two real variables) to find points on this manifold to arbitrarily small error.

- With the above work, we will have constructed (in 4-dimensional (x, y, z, s)-space):

  - a 3-dimensional hypersurface $\mathcal{Z}$ (comprising values of the coordinate s away from 0) which corresponds to solutions satisfying the good asymptotic conditions for large r; and
  - a 2-dimensional surface $\mathcal{W}$ (comprising only small values of the coordinate s) which corresponds to solutions satisfying the good asymptotic conditions for small r.

  To complete the proof, one needs to show that $\mathcal{W}$ and $\mathcal{Z}$ intersect. To this end we consider the 3D hypersurface of (x, y, z, s)-space that corresponds to $r = r_0$. Intersected with it, $\mathcal{W}$ becomes a curve $\mathcal{C}$ and $\mathcal{Z}$ becomes a surface $\mathcal{S}$. By looking at the x, y, z coordinates of points on $\mathcal{C}$ and $\mathcal{S}$ as continuous functions of numbers σ, ν, β that parametrize them, and by considering that an intersection exists when $\varepsilon = 0$, the *Poincaré-Miranda theorem* can be applied to ensure an intersection for small $\varepsilon > 0$, provided that suitable estimates are in place for how a change in ε perturbs the manifolds $\mathcal{Z}$ and $\mathcal{W}$.

The novel summation technique developed for the study of convergence of the ε- and σ-power series that appear as solutions to the Maxwell-BLTP-Einstein system is explained in remark 1.4.10. In the case of a power series in one variable, as in section 1.4, lemma 1.4.11 contains the main ingredient necessary for this technique, while theorem 1.4.13 is where it can be seen applied. In the case of power series in two variables, as in section 1.5, lemma 1.5.10 explains the generalization to multi-variable series and theorem 1.5.11 contains its application to our series.

1.2 Obtaining the differential system

In this section we show how to obtain the stress-energy tensor $T_{\mu\nu}$ and a tensorial form $\mathrm{d}M = 0$ for the vacuum law. Then we write out the system of Einstein equations

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \frac{8\pi G}{c^4}T_{\mu\nu} \tag{1.2.1}$$

and show that, under the assumption of staticity and spherical symmetry, it reduces to a second-order system of 3 ordinary differential equations. In (1.2.1), $(R_{\mu\nu})$ is the *Ricci curvature tensor* of g, containing first- and second-order derivatives of the metric components, and $(T_{\mu\nu})$ is the *stress-(energy density)-(momentum density) tensor*, or simply *stress tensor*, which is a symmetric 2-covariant tensor that models how the electromagnetic effects act as a source for gravity.

1.2.1 Set-up

We consider a Lorentzian manifold homeomorphic to $\mathbb{R}^4$ minus a line that is supposed to model the spacetime of a universe containing a single, static point charge. It is foliated by spacelike slices, each one homeomorphic to $\mathbb{R}^3$ minus a point, with this removed point (a spacetime singularity) representing the position of the particle. Therefore the spacetime itself is devoid of matter, like the Schwarzschild spacetime, but we assume that a smooth 2-form F, called the **Faraday tensor** of the electromagnetic field of the particle, is defined globally - hence this is an *electrovacuum spacetime.* The constants and parameters that we need, together with their physical dimension measured in Gaussian units of mass, length, time, are:

- c: the speed of light in vacuum ((length)(time)$^{-1}$),
- G: Newton's gravitational constant ((mass)$^{-1}$(length)^3(time)$^{-2}$),
- Q: the charge of the particle ((mass)$^{1/2}$(length)$^{3/2}$(time)$^{-1}$),
- $\varkappa$: the parameter postulated in the Maxwell-BLTP equations (1.1.3) of electromagnetism ((length)$^{-1}$).

A global coordinate system (ct, r, θ, ϕ), with $t \in \mathbb{R}$, $r > 0$, $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$, is assumed to exist, with (r, θ, ϕ) representing polar coordinates in any spacelike slice. The metric takes the general static and spherically symmetric form

$$g = -e^{2\lambda(r)}c^2\mathrm{d}t^2 + e^{2\nu(r)}\mathrm{d}r^2 + r^2\mathrm{d}\theta^2 + r^2\sin^2\theta\mathrm{d}\phi^2\ , \tag{1.2.2}$$

assumed to hold everywhere in spacetime. We also use g to denote the determinant

$$g(r,\theta) = -e^{2(\lambda(r)+\nu(r))}r^4\sin^2\theta\ . \tag{1.2.3}$$

A sign choice for the metric volume form must be made, since we will be working soon with the *Hodge star* $\star$ operation; we fix it as

$$\mathrm{vol}_g = e^{\lambda+\nu}r^2\sin\theta\ \mathrm{d}(ct)\wedge\mathrm{d}r\wedge\mathrm{d}\theta\wedge\mathrm{d}\phi\ . \tag{1.2.4}$$

By definition, $\star$ takes p-forms into $(4-p)$-forms according to

$$(\star\omega)_{\mu_{p+1}\cdots\mu_4} = \frac{1}{p!}\sqrt{-g}\omega^{\nu_1\cdots\nu_p}\varepsilon_{\nu_1\cdots\nu_p\mu_{p+1}\cdots\mu_4}\ , \tag{1.2.5}$$

where ε represents the Levi-Civita symbol

$$\varepsilon_I = \begin{cases} 1 \quad, \text{ if } I \text{ is an even permutation of } \{1,\ldots,p\}, \\ -1\ , \text{ if } I \text{ is an odd permutation of } \{1,\ldots,p\}, \\ 0 \text{ otherwise.}\end{cases} \ . \tag{1.2.6}$$

The main property of the $\star$ map is that, for any two p-forms α,β,

$$\alpha\wedge\star\beta = \beta\wedge\star\alpha = \frac{1}{p!}\alpha_{\mu_1\ldots\mu_p}\beta^{\mu_1\cdots\mu_p}\mathrm{vol}_g\ . \tag{1.2.7}$$

Also recall that, for each fixed index μ, the *interior product operation* i_μ, taking p-forms into $(p-1)$-forms, is defined by the following property (where α is a p form):

$$i_\mu(\alpha\wedge\beta) = i_\mu\alpha\wedge\beta + (-1)^p\alpha\wedge i_\mu\beta\ . \tag{1.2.8}$$

Since our spacetime is static, there are no magnetic effects. The only other unknown of the problem is the electric potential $\varphi(r)$, from which the Faraday tensor $F = \mathrm{d}A$ can be constructed, with the potential 1-form A being given in coordinates as

$$A_{ct} = \varphi(r) \quad , \quad A_r = A_\theta = A_\phi = 0\ . \tag{1.2.9}$$

We immediately get

$$F = \mathrm{d}A = \mathrm{d}(\varphi(r)\mathrm{d}(ct)) = \varphi'(r)\mathrm{d}r \wedge \mathrm{d}(ct) = -\varphi'(r)\mathrm{d}(ct) \wedge \mathrm{d}r \ . \tag{1.2.10}$$

We shall see in this section that the Maxwell (1.1.2) and BLTP (1.1.3) vacuum laws can be written in tensor form as

$$\mathrm{d}M = 0 \ , \tag{1.2.11}$$

where the 2-form M is defined, respectively in each case, by

$$M = \star F \quad \text{or} \quad M = \star F + \frac{1}{\varkappa^2} \star \mathrm{d} \star \mathrm{d} \star F \ . \tag{1.2.12}$$

The first choice yields the Maxwell-Maxwell-Einstein system, and the second choice, Maxwell-BLTP-Einstein system.

The Einstein tensor $G_{\mu\nu}$ for our metric is diagonal (adapted from [Str04], whose author utilizes the $(+---)$ signature convention):

$$\begin{aligned} G_{(ct)(ct)} &= \frac{e^{2\lambda}}{r^2} - e^{2(\lambda-\nu)}\left(\frac{1}{r^2} - \frac{2\nu'}{r}\right) \\ G_{rr} &= -\frac{e^{2\nu}}{r^2} + \frac{1}{r^2} + \frac{2\lambda'}{r} \\ G_{\theta\theta} &= r^2 e^{-2\nu}\left((\lambda')^2 + \lambda'' - \lambda'\nu' + \frac{\lambda' - \nu'}{r}\right) \\ G_{\phi\phi} &= r^2 \sin\theta e^{-2\nu}\left((\lambda')^2 + \lambda'' - \lambda'\nu' + \frac{\lambda' - \nu'}{r}\right) \end{aligned} \tag{1.2.13}$$

We shall also need to know the Christoffel symbols, which can be found in the same reference:

$$\begin{aligned} &\Gamma^{ct}_{(ct)r} = \lambda' \\ &\Gamma^{r}_{rr} = \nu' \quad , \quad \Gamma^{r}_{(ct)(ct)} = \lambda' e^{2(\lambda-\nu)} \quad , \quad \Gamma^{r}_{\theta\theta} = -re^{-2\nu} \quad , \quad \Gamma^{r}_{\phi\phi} = -re^{-2\nu}\sin^2\theta \\ &\Gamma^{\theta}_{\phi\phi} = -\sin\theta\cos\theta \quad , \quad \Gamma^{\theta}_{\theta r} = \frac{1}{r} \\ &\Gamma^{\phi}_{\phi\theta} = \cot\theta \quad , \quad \Gamma^{\phi}_{\phi r} = \frac{1}{r} \end{aligned} \tag{1.2.14}$$

All other $\Gamma^{\lambda}_{\mu\nu}$ (not obtained from these by swapping the two lower indices) are zero.

1.2.2 Stress-energy tensor and vacuum law

The computations here follow what is done in [GPT15] and [DGT07] and are included for completeness.

Using F, the **BLTP Lagrangian 4-form** can be defined on the manifold by

$$\Lambda = \Lambda(r) = \frac{1}{8\pi}\left(F \wedge \star F - \frac{1}{\varkappa^2} H \wedge \star H\right) \ , \tag{1.2.15}$$

where we abbreviated

$$H = H(r) = \mathrm{d} \star F \ . \tag{1.2.16}$$

We remark that this Lagrangian consists of a perturbation of the usual Schwarzschild Lagrangian for the Maxwell-Maxwell system (the first term), to which a term containing higher-order derivatives of φ was added, with the small $\varkappa^{-2}$ appearing as the coupling constant.

To compute $T_{\mu\nu}$ and the vacuum law from the Lagrangian Λ, we need to compute the variation of Λ with respect to compactly supported variations of the metric (which yields $T_{\mu\nu}$) and the 1-form A (which yields the vacuum law).

We start by considering the following orthonormal coframe (a basis for the cotangent space of the manifold):

$$e^{(0)} = e^{\lambda}\mathrm{d}t \quad , \quad e^{(1)} = e^{\nu}\mathrm{d}r \quad , \quad e^{(2)} = r\mathrm{d}\theta \quad , \quad e^{(3)} = r\sin\theta\mathrm{d}\phi \ . \tag{1.2.17}$$

Note that

$$g = \eta_{\mu\nu} e^{(\mu)} \otimes e^{(\nu)} \tag{1.2.18}$$

where

$$\eta = \mathrm{diag}(-1, 1, 1, 1) \tag{1.2.19}$$

is the Minkowski metric. When we write numerical indices on tensors, it will mean their coordinates with respect to this coframe and its dual frame. Note for example $G_{00} = e^{-2\lambda} G_{(ct)(ct)}$ etc. In this new coframe, we have

$$\begin{aligned} G_{00} &= \frac{1}{r^2} - e^{-2\nu}\left(\frac{1}{r^2} - \frac{2\nu'}{r}\right) \\ G_{11} &= -\frac{1}{r^2} + e^{-2\nu}\left(\frac{1}{r^2} + \frac{2\lambda'}{r}\right) \\ G_{22} = G_{33} &= e^{-2\nu}\left((\lambda')^2 + \lambda'' - \lambda'\nu' + \frac{\lambda' - \nu'}{r}\right) \end{aligned} \tag{1.2.20}$$

Let $\mathcal{U}$ be an arbitrary open set of spacetime. Suppose that a one-parameter family of coframes is given, $\{e_s^{(\mu)}\}_{\mu=0,1,2,3}$, $s \in (-a, a)$ for some small $a > 0$, with $e_0^{(\mu)} = e^{(\mu)}$, as in [DGT07] (formulas 56 and 57). This family defines a family of metrics by

$$g_s = \eta_{\mu\nu} e_s^{(\mu)} \otimes e_s^{(\nu)} \qquad \text{where } (\eta_{\mu\nu}) = \mathrm{diag}(-1, 1, 1, 1) \ . \tag{1.2.21}$$

We define the variation $\dot{e}^{(\mu)}$ as the derivative of $e_s^{(\mu)}$ with respect to s evaluate at $s = 0$:

$$e_s^{(\mu)} = e^{(\mu)} + s\dot{e}^{(\mu)} + O(s^2)\ . \tag{1.2.22}$$

Suppose also that each $\dot{e}^{(\mu)}$ is compactly supported on $\mathcal{U}$.

We also consider an independent variation of the potential 1-form A: suppose that a one-parameter family of 1-forms A_s is given, like above, and define the variation $\dot{A}$ (assumed compactly supported on $\mathcal{U}$) by

$$A_s = A + s\dot{A} + O(s^2)\ . \tag{1.2.23}$$

Tensors such as Λ that depend on the metric and on A also inherit their own one-parameter families, whose elements can be denoted by a subscript s, and variations, denoted with a dot on top, defined similarly:

$$\Lambda_s = \Lambda + s\dot{\Lambda} + O(s^2)\ . \tag{1.2.24}$$

The variation $\dot{\Lambda}$ is a tensor of the same rank as Λ (a 4-form). The Einstein Field Equations (1.2.1) are obtained by imposing zero variation of the *Einstein-Hilbert action* on $\mathcal{U}$ with respect to arbitrary $\dot{e}^{(\mu)}$ and $\dot{A}$. This action is defined by

$$S(g, A) = \int_{\mathcal{U}} \left(\frac{R}{2} + \frac{8\pi G}{c^4} \star \Lambda \right) \sqrt{-g}\ \mathrm{d}(ct)\mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi \tag{1.2.25}$$

where R is the Ricci scalar of g. The computation of $\dot{\Lambda}$ included here will reveal that its expression is formed by the sum of three parts:

- an exact differential, which has no effect in the action due to Stokes' theorem;
- a term of the form $\dot{A} \wedge \mathrm{d}X$, where X is a 2-form;
- a term of the form $\dot{e}^{(\mu)} \wedge \tau_{(\mu)}$, where $\tau_{(\mu)}$ are 3-forms.

The second term can only yield a zero contribution to the action, for a general $\dot{A}$, when $\mathrm{d}X = 0$ on $\mathcal{U}$, which we shall see that will produce the BLTP vacuum law as given by (1.2.11) and (1.2.12), upon defining $M = X$:

$$\mathrm{d}M = 0 \quad , \quad M = \star F + \frac{1}{\varkappa^2} \star \mathrm{d} \star \mathrm{d} \star F\ . \tag{1.2.26}$$

Finally, setting to zero the contribution of the third term to the action, for general $\dot{e}^{(\mu)}$, amounts to defining the stress-energy tensor (in the coframe (1.2.17)) by

$$T_{\mu\nu} = \eta_{\nu\lambda} \star (\tau_{(\mu)} \wedge e^{(\lambda)}) \tag{1.2.27}$$

(See [GPT15] formulas 106 and 107 for a derivation of this).

Lemma 1.2.1. *Given a p-form Ψ, the variation of its Hodge dual is computed as*

$$(\star\Psi)^{\cdot} = \dot{e}^{(\mu)} \wedge i_\mu(\star\Psi) \; - \; \star(\dot{e}^{(\mu)} \wedge i_\mu \Psi) \; + \; \star\dot{\Psi} \; . \tag{1.2.28}$$

Proof. This proof is adapted from the appendix of [DGT07]. It is for this to work that we need the chosen coframe $\{e^{(\mu)}\}$ to be orthonormal. Using this coframe we can construct a basis for the space of p-forms, containing elements of the form $e^{(\mu_1)} \wedge \cdots \wedge e^{(\mu_p)}$, $\mu_1 < \ldots, \mu_p$, which we can abbreviate as $e^{(I)}$, for I being the multiindex $(\mu_1, \ldots, \mu_p)$. Note that the Leibniz rule implies that

$$\dot{e}^{(I)} = \dot{e}^{(\mu)} \wedge i_\mu e^{(I)} \tag{1.2.29}$$

because, when computing the right side, the possible minus sign introduced by the wedge is canceled by the possible minus sign introduced by i_μ. By the same reasoning,

$$(\star e^{(I)})^{\cdot} = \dot{e}^{(\mu)} \wedge i_\mu(\star e^{(I)}) \tag{1.2.30}$$

this time also because the basis is orthonormal - that is, the computation of $\star e^{(I)}$ yields an element of the form $e^{(J)}$ without a scalar factor in front. Therefore, writing $\Psi = \Psi_I e^{(I)}$, we have

$$\begin{aligned} \dot{\Psi} &= \dot{\Psi}_I e^{(I)} + \Psi_I \dot{e}^{(I)} \\ &= \dot{\Psi}_I e^{(I)} + \Psi_I \dot{e}^{(\mu)} \wedge i_\mu e^{(I)} \\ &= \dot{\Psi}_I e^{(I)} + \dot{e}^{(\mu)} \wedge i_\mu \Psi \; , \end{aligned} \tag{1.2.31}$$

and thus

$$\star \dot{\Psi} = \dot{\Psi}_I \star e^{(I)} + \star(\dot{e}^{(\mu)} \wedge i_\mu \Psi) \; . \tag{1.2.32}$$

Now we can calculate

$$\begin{aligned} (\star\Psi)^{\cdot} &= (\Psi_I \star e^{(I)})^{\cdot} \\ &= \dot{\Psi}_I \star e^{(I)} + \Psi_I(\dot{e}^{(\mu)} \wedge i_\mu \star e^{(I)}) \\ &= \dot{\Psi}_I \star e^{(I)} + \dot{e}^{(\mu)} \wedge i_\mu \star \Psi \; . \end{aligned} \tag{1.2.33}$$

Using (1.2.32) yields (1.2.28). □

Now we explain how to use this lemma to find $\dot{\Lambda}$, following [GPT15] (equation 114). For this we will use the graded-commutativity property of the wedge product $\wedge$, the graded derivative property of the exterior derivative d, the property (1.2.7) of the Hodge dual map, and commutativity of d with variations (they are derivations with respect to distinct variables). First we have:

$$\begin{aligned}(F \wedge \star F)^{\cdot} &= \dot{F} \wedge \star F + F \wedge (\star F)^{\cdot} \\ &= \dot{F} \wedge \star F + F \wedge (\dot{e}^{(\mu)} \wedge i_\mu \star F - \star(\dot{e}^{(\mu)} \wedge i_\mu F) + \star\dot{F}) \\ &= \dot{F} \wedge \star F + \dot{e}^{(\mu)} \wedge F \wedge i_\mu \star F - \dot{e}^{(\mu)} \wedge i_\mu F \wedge \star F + \dot{F} \wedge \star F \\ &= 2\dot{F} \wedge \star F + \dot{e}^{(\mu)} \wedge (F \wedge i_\mu \star F - i_\mu F \wedge \star F) \\ &= 2\mathrm{d}\dot{A} \wedge \star F + \dot{e}^{(\mu)} \wedge (F \wedge i_\mu \star F - i_\mu F \wedge \star F) \\ &= 2\mathrm{d}(\dot{A} \wedge \star F) + 2\dot{A} \wedge \mathrm{d} \star F + \dot{e}^{(\mu)} \wedge (F \wedge i_\mu \star F - i_\mu F \wedge \star F)\ .\end{aligned} \tag{1.2.34}$$

and

$$\begin{aligned}(H \wedge \star H)^{\cdot} &= \dot{H} \wedge \star H + H \wedge (\star H)^{\cdot} \\ &= \dot{H} \wedge \star H + H \wedge (\dot{e}^{(\mu)} \wedge i_\mu \star H - \star(\dot{e}^{(\mu)} \wedge i_\mu H) + \star\dot{H}) \\ &= \dot{H} \wedge \star H - \dot{e}^{(\mu)} \wedge H \wedge i_\mu \star H - \dot{e}^{(\mu)} \wedge i_\mu H \wedge \star H + \dot{H} \wedge \star H \\ &= 2\dot{H} \wedge \star H - \dot{e}^{(\mu)} \wedge (H \wedge i_\mu \star H + i_\mu H \wedge \star H)\ .\end{aligned} \tag{1.2.35}$$

Expanding the first summand in (1.2.35) above (without its factor 2) according to the definition (1.2.16) of H:

$$\begin{aligned}\dot{H} \wedge \star H &= \mathrm{d}(\star F)^{\cdot} \wedge \star H \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H) - (\star F)^{\cdot} \wedge \mathrm{d} \star H \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H) - (\dot{e}^{(\mu)} \wedge i_\mu \star F - \star(\dot{e}^{(\mu)} \wedge i_\mu F) + \star\dot{F}) \wedge \mathrm{d} \star H \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H) - \dot{e}^{(\mu)} \wedge i_\mu \star F \wedge \mathrm{d} \star H + \mathrm{d} \star H \wedge \star(\dot{e}^{(\mu)} \wedge i_\mu F) - \mathrm{d} \star H \wedge \star\dot{F} \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H) - \dot{e}^{(\mu)} \wedge i_\mu \star F \wedge \mathrm{d} \star H + \dot{e}^{(\mu)} \wedge i_\mu F \wedge \star\mathrm{d} \star H - \dot{F} \wedge \star\mathrm{d} \star H \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H) + \dot{e}^{(\mu)} \wedge (-i_\mu \star F \wedge \mathrm{d} \star H + i_\mu F \wedge \star\mathrm{d} \star H) - \mathrm{d}\dot{A} \wedge \star\mathrm{d} \star H \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H) + \dot{e}^{(\mu)} \wedge (-i_\mu \star F \wedge \mathrm{d} \star H + i_\mu F \wedge \star\mathrm{d} \star H) - \mathrm{d}(\dot{A} \wedge \star\mathrm{d} \star H) - \dot{A} \wedge \mathrm{d} \star \mathrm{d} \star H \\ &= \mathrm{d}((\star F)^{\cdot} \wedge \star H - \dot{A} \wedge \star\mathrm{d} \star H) - \dot{A} \wedge \mathrm{d} \star \mathrm{d} \star H + \dot{e}^{(\mu)} \wedge (-i_\mu \star F \wedge \mathrm{d} \star H + i_\mu F \wedge \star\mathrm{d} \star H)\ .\end{aligned} \tag{1.2.36}$$

Plug this back into (1.2.35):

$$\begin{aligned}(H \wedge \star H)^{\cdot} = {} & 2\mathrm{d}((\star F)^{\cdot} \wedge \star H - \dot{A} \wedge \star\mathrm{d} \star H) - 2\dot{A} \wedge \mathrm{d} \star \mathrm{d} \star H \\ & - \dot{e}^{(\mu)} \wedge (H \wedge i_\mu \star H + i_\mu H \wedge \star H + 2 i_\mu \star F \wedge \mathrm{d} \star H - 2 i_\mu F \wedge \star\mathrm{d} \star H)\ .\end{aligned} \tag{1.2.37}$$

This together with (1.2.34) gives the final expression for $\dot{\Lambda}$:

$$\begin{aligned} 8\pi\dot{\Lambda} = 2\mathrm{d}\Big[\ \dot{A}\wedge\star F\ -\ \frac{1}{\varkappa^2}\Big((\star F)^{\cdot}\wedge\star H\ -\ \dot{A}\wedge\star\mathrm{d}\star H\Big)\ \Big]\ + \\ +\ 2\dot{A}\wedge\Big[\ \mathrm{d}\star F\ +\ \frac{1}{\varkappa^2}\mathrm{d}\star\mathrm{d}\star H\ \Big]\ + \\ +\ \dot{e}^{(\mu)}\wedge\Big[\ F\wedge i_\mu\star F\ -\ i_\mu F\wedge\star F\ + \\ +\ \frac{1}{\varkappa^2}\Big(H\wedge i_\mu\star H\ +\ i_\mu H\wedge\star H\ +\ 2i_\mu\star F\wedge\mathrm{d}\star H\ -\ 2i_\mu F\wedge\star\mathrm{d}\star H\Big)\Big]\ . \end{aligned} \tag{1.2.38}$$

Write this compactly in the form

$$\dot{\Lambda} = 2\mathrm{d}\Big[\ \dot{A}\wedge\star F\ -\ \frac{1}{\varkappa^2}\Big((\star F)^{\cdot}\wedge\star H\ -\ \dot{A}\wedge\star\mathrm{d}\star H\Big)\ \Big]\ +\ 2\dot{A}\wedge\mathrm{d}M\ +\ \dot{e}^{(\mu)}\wedge\tau_{(\mu)} \tag{1.2.39}$$

where M and $\tau_{(\mu)}$ are defined as

$$M = \star F\ +\ \frac{1}{\varkappa^2}\star\mathrm{d}\star H \tag{1.2.40}$$

and

$$\begin{aligned} \tau_{(\mu)} = F\wedge i_\mu\star F\ -\ i_\mu F\wedge\star F \\ +\ \frac{1}{\varkappa^2}\Big(H\wedge i_\mu\star H\ +\ i_\mu H\wedge\star H - 2i_\mu F\wedge\star\mathrm{d}\star H\ +\ 2i_\mu\star F\wedge\mathrm{d}\star H\Big) \end{aligned} \tag{1.2.41}$$

These formulas and the definition (1.2.27) of $T_{\mu\nu}$ from $\tau_{(\mu)}$ conclude the computation of the Maxwell and stress-energy tensors.

1.2.3 In coordinates

To expand out the coordinates of T and the equation $\mathrm{d}M = 0$, we will need to compute all expressions involving d and $\star$ of F and H in them. As we compute each one, we keep track of their coordinates in both the original coordinate coframe $(\mathrm{d}(ct), \mathrm{d}r, \mathrm{d}\theta, \mathrm{d}\phi)$ (in order to compute exterior derivatives) as well as in the orthonormal coframe $(e^{(0)}, e^{(1)}, e^{(2)}, e^{(3)})$ (in which the Hodge dual is most easily computed).

$$F = -\varphi'\mathrm{d}(ct)\wedge\mathrm{d}r = -e^{-\lambda-\nu}\varphi' e^{(0)}\wedge e^{(1)} \tag{1.2.42}$$

$$\begin{aligned} (\star F)_{23} = \frac{1}{2}(F^{01}\varepsilon_{0123} + F^{10}\varepsilon_{1023}) = F^{01} = -F_{01} \\ \implies\quad \star F = e^{-\lambda-\nu}\varphi' e^{(2)}\wedge e^{(3)} = r^2\sin\theta e^{-\lambda-\nu}\varphi'\mathrm{d}\theta\wedge\mathrm{d}\phi \end{aligned} \tag{1.2.43}$$

$$H = \mathrm{d}\star F = \sin\theta \frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\mathrm{d}r\wedge\mathrm{d}\theta\wedge\mathrm{d}\phi = \frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')e^{(1)}\wedge e^{(2)}\wedge e^{(3)} \tag{1.2.44}$$

$$\begin{aligned} (\star H)_0 &= H^{123}\varepsilon_{1230} = -H^{123} = -H_{123} \\ \Longrightarrow \quad \star H &= -\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')e^{(0)} = -\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\mathrm{d}(ct) \end{aligned} \tag{1.2.45}$$

$$\mathrm{d}\star H = \frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)\mathrm{d}(ct)\wedge\mathrm{d}r = e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)e^{(0)}\wedge e^{(1)} \tag{1.2.46}$$

$$\begin{aligned} (\star\mathrm{d}\star H)_{23} &= \frac{1}{2}((\mathrm{d}\star H)^{01}\varepsilon_{0123} + (\mathrm{d}\star H)^{10}\varepsilon_{1023}) = (\mathrm{d}\star H)^{01} = -(\mathrm{d}\star H)_{01} \\ \Longrightarrow \quad \star\mathrm{d}\star H &= -e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)e^{(2)}\wedge e^{(3)} \\ &= -r^2\sin\theta e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)\mathrm{d}\theta\wedge\mathrm{d}\phi \end{aligned} \tag{1.2.47}$$

$$\begin{aligned} \mathrm{d}\star\mathrm{d}\star H &= -\sin\theta\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)\right)\mathrm{d}r\wedge\mathrm{d}\theta\wedge\mathrm{d}\phi \\ &= -\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)\right)e^{(1)}\wedge e^{(2)}\wedge e^{(3)} \end{aligned} \tag{1.2.48}$$

Having all these at hand, we expand the vacuum law $\mathrm{d}M = 0$:

$$\begin{aligned} 0 = \mathrm{d}M &= H + \frac{1}{\varkappa^2}\mathrm{d}\star\mathrm{d}\star H \\ &= \left[\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi') - \frac{1}{\varkappa^2}\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)\right)\right]e^{(1)}\wedge e^{(2)}\wedge e^{(3)}\ , \end{aligned} \tag{1.2.49}$$

implying that, for some constant q,

$$-q = r^2 e^{-\lambda-\nu}\varphi' - \frac{1}{\varkappa^2}r^2 e^{-\lambda-\nu}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2 e^{-\lambda-\nu}\varphi')\right)\ . \tag{1.2.50}$$

By defining the following function:

$$w(r) = r^2 e^{-(\lambda(r)+\nu(r))}\varphi'(r) + q\ , \tag{1.2.51}$$

this becomes a homogeneous equation:

$$0 = w - \frac{1}{\varkappa^2} r^2 e^{-(\lambda+\nu)} \frac{\mathrm{d}}{\mathrm{d}r} \left(\frac{e^{\lambda-\nu}}{r^2} w' \right) , \tag{1.2.52}$$

which we rewrite as

$$\frac{w e^{\lambda+\nu}}{r^2} = \frac{1}{\varkappa^2} \frac{\mathrm{d}}{\mathrm{d}r} \left(\frac{e^{\lambda-\nu}}{r^2} w' \right) . \tag{1.2.53}$$

We shall see in subsection 1.3.3 that q can be identified with the charge content Q in the spacetime (but we keep writing q until we've proven this).

Next we find $T_{\mu\nu}$ using (1.2.27) and the $\tau_{(\mu)}$ just defined. This requires expanding each of the 6 summands in the formula for $\tau_{(\mu)}$:

$$F \wedge i_\mu \star F = \begin{cases} -(e^{-\lambda-\nu}\varphi')^2 e^{(0)} \wedge e^{(1)} \wedge e^{(3)} & \text{if } \mu = 2 \\ (e^{\lambda-\nu}\varphi')^2 e^{(0)} \wedge e^{(1)} \wedge e^{(2)} & \text{if } \mu = 3 \end{cases} \tag{1.2.54}$$

$$-i_\mu F \wedge \star F = \begin{cases} (e^{-\lambda-\nu}\varphi')^2 e^{(1)} \wedge e^{(2)} \wedge e^{(3)} & \text{if } \mu = 0 \\ -(e^{-\lambda-\nu}\varphi')^2 e^{(0)} \wedge e^{(2)} \wedge e^{(3)} & \text{if } \mu = 1 \end{cases} \tag{1.2.55}$$

$$H \wedge i_\mu \star H = \begin{cases} -\left(\frac{e^{-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right)^2 e^{(1)} \wedge e^{(2)} \wedge e^{(3)} & \text{if } \mu = 0 \end{cases} \tag{1.2.56}$$

$$i_\mu H \wedge \star H = \begin{cases} -\left(\frac{e^{-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right)^2 e^{(0)} \wedge e^{(2)} \wedge e^{(3)} & \text{if } \mu = 1 \\ \left(\frac{e^{-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right)^2 & \text{if } \mu = 2 \\ -\left(\frac{e^{-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right)^2 & \text{if } \mu = 3 \end{cases} \tag{1.2.57}$$

$$-2 i_\mu F \wedge \star \mathrm{d} \star H = \begin{cases} -2\varphi'(e^{-\lambda-\nu})^2 \frac{\mathrm{d}}{\mathrm{d}r} \left(\frac{e^{\lambda-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right) e^{(1)} \wedge e^{(2)} \wedge e^{(3)} & \text{if } \mu = 0 \\ 2\varphi'(e^{-\lambda-\nu})^2 \frac{\mathrm{d}}{\mathrm{d}r} \left(\frac{e^{\lambda-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right) e^{(0)} \wedge e^{(2)} \wedge e^{(3)} & \text{if } \mu = 1 \end{cases} \tag{1.2.58}$$

$$2 i_\mu \star F \wedge \mathrm{d} \star H = \begin{cases} 2\varphi'(e^{-\lambda-\nu})^2 \frac{\mathrm{d}}{\mathrm{d}r} \left(\frac{e^{\lambda-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right) e^{(0)} \wedge e^{(1)} \wedge e^{(3)} & \text{if } \mu = 2 \\ -2\varphi'(e^{-\lambda-\nu})^2 \frac{\mathrm{d}}{\mathrm{d}r} \left(\frac{e^{\lambda-\nu}}{r^2} \frac{\mathrm{d}}{\mathrm{d}r} (r^2 e^{-\lambda-\nu}\varphi') \right) e^{(0)} \wedge e^{(1)} \wedge e^{(2)} & \text{if } \mu = 3 \end{cases} \tag{1.2.59}$$

Then we conclude:

$$8\pi\tau_{(0)} = \bigg\{(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 - 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\bigg\}e^{(1)}\wedge e^{(2)}\wedge e^{(3)} \quad (1.2.60)$$

$$8\pi\tau_{(1)} = \bigg\{-(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 + 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\bigg\}e^{(1)}\wedge e^{(2)}\wedge e^{(3)} \quad (1.2.61)$$

$$8\pi\tau_{(2)} = \bigg\{-(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 + 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\bigg\}e^{(1)}\wedge e^{(2)}\wedge e^{(3)} \quad (1.2.62)$$

$$8\pi\tau_{(3)} = \bigg\{(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 - 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\bigg\}e^{(1)}\wedge e^{(2)}\wedge e^{(3)} \quad (1.2.63)$$

Now we see from (1.2.27) that $(T_{\mu\nu})$ is diagonal with

$$\begin{aligned}
8\pi T_{00} &= +(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 - 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\\
8\pi T_{11} &= -(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 + 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\\
8\pi T_{22} &= +(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 - 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]\\
8\pi T_{33} &= +(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\bigg[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 - 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\bigg]
\end{aligned} \quad (1.2.64)$$

We can simplify these four equations considerably using w instead of φ' and using the vacuum law

(1.2.53). For example, let us work with the first one:

$$\begin{aligned}
8\pi T_{00} &= +(e^{-\lambda-\nu}\varphi')^2 + \frac{1}{\varkappa^2}\left[-\left(\frac{e^{-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)^2 - 2\varphi'(e^{-\lambda-\nu})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2e^{-\lambda-\nu}\varphi')\right)\right] \\
&= \left(\frac{w-q}{r^2}\right)^2 + \frac{1}{\varkappa^2}\left[-\left(\frac{e^{-\nu}}{r^2}w'\right)^2 - 2\varphi'(e^{-(\lambda+\nu)})^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{e^{\lambda-\nu}}{r^2}w'\right)\right] \\
&= \frac{1}{r^4}(w-q)^2 + -\frac{1}{\varkappa^2}\frac{e^{-2\nu}}{r^4}(w')^2 - \frac{2}{\varkappa^2}\varphi'(e^{-(\lambda+\nu)})^2\frac{\varkappa^2we^{\lambda+\nu}}{r^2} \\
&= \frac{1}{r^4}(w-q)^2 + -\frac{1}{\varkappa^2}\frac{e^{-2\nu}}{r^4}(w')^2 - 2\varphi'e^{-(\lambda+\nu)}\frac{w}{r^2} \\
&= \frac{1}{r^4}(w-q)^2 + -\frac{1}{\varkappa^2}\frac{e^{-2\nu}}{r^4}(w')^2 - \frac{2}{r^4}w(w-q) \\
&= \frac{1}{r^4}\left(-w^2+q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \, .
\end{aligned} \tag{1.2.65}$$

Note that, in all equations in (1.2.64), the signs of the first and third terms are flipped (so that the same simplification that happened between them in the above calculation will take place), while the sign of the second term remains the same (so that all will yield the same multiple of $\varkappa^{-2}$ as in the above calculation). Hence we have:

$$\begin{aligned}
8\pi T_{00} &= \frac{1}{r^4}\left(-w^2+q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \\
8\pi T_{11} &= \frac{1}{r^4}\left(+w^2-q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \\
8\pi T_{22} &= \frac{1}{r^4}\left(-w^2+q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \\
8\pi T_{33} &= \frac{1}{r^4}\left(-w^2+q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right)
\end{aligned} \tag{1.2.66}$$

1.2.4 Einstein Field Equations

We have concluded that both sides of the Einstein system (1.2.1) are diagonal. Also comparing the equations for G_{22} and G_{33} reveals that their left sides are one and the same, and the same is true for their right sides. Hence the system reduces to 3 independent equations:

$$\begin{aligned}
\frac{1}{r^2} - e^{-2\nu}\left(\frac{1}{r^2}-\frac{2\nu'}{r}\right) &= \frac{G}{c^4r^4}\left(-w^2+q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \, , \\
-\frac{1}{r^2} + e^{-2\nu}\left(\frac{1}{r^2}+\frac{2\lambda'}{r}\right) &= \frac{G}{c^4r^4}\left(w^2-q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \, , \\
e^{-2\nu}\left((\lambda')^2-\lambda'\nu'+\lambda''+\frac{\lambda'-\nu'}{r}\right) &= \frac{G}{c^4r^4}\left(-w^2+q^2-\frac{1}{\varkappa^2}e^{-2\nu}(w')^2\right) \, .
\end{aligned} \tag{1.2.67}$$

Proposition 1.2.2. *The third equation above is a consequence of the first two and the vacuum law (1.2.53).*

Proof. Consider the *Bianchi identity*:

$$G^{\mu\nu}_{;\mu} = 0 \quad , \quad \nu = 0, 1, 2, 3 \ , \tag{1.2.68}$$

where semicolon denotes covariant derivative in the Levi-Civita connection of g. Using the expression

$$G^{\alpha\beta}_{;\gamma} = G^{\alpha\beta}_{,\gamma} + \Gamma^{\alpha}_{\mu\gamma}G^{\mu\beta} + \Gamma^{\beta}_{\mu\gamma}G^{\alpha\mu} \tag{1.2.69}$$

and the Christoffel symbols as given in (1.2.14), we can work out that the $\nu = 1$ equation in (1.2.68) is the only nontrivial one, equivalent to

$$\frac{2}{r}G_{22} = \frac{2}{r}G_{33} = G'_{11} + G_{11}\left(\lambda' + \frac{2}{r}\right) + \lambda' G_{00} \ . \tag{1.2.70}$$

Use the first two equations from (1.2.67) to rewrite the left-hand side in terms of $(T_{\mu\nu})$:

$$\frac{2}{r}G_{22} = \frac{2}{r}G_{33} = 8\pi G\left(T'_{11} + T_{11}\left(\lambda' + \frac{2}{r}\right) + \lambda' T_{00}\right) \ . \tag{1.2.71}$$

Therefore, we will be able to deduce the equations $G_{22} = 8\pi G T_{22}$ and $G_{33} = 8\pi G T_{33}$ if we can check that $(T_{\mu\nu})$ satisfies

$$T'_{11} + T_{11}\left(\lambda' + \frac{2}{r}\right) + \lambda' T_{00} = \frac{2}{r}T_{22} = \frac{2}{r}T_{33} \ . \tag{1.2.72}$$

Adding and subtracting the first two equations in (1.2.67) yields

$$\begin{aligned} (\lambda + \nu)' &= -\frac{G}{c^4 \varkappa^2}\frac{(w')^2}{r^3} \\ (\lambda - \nu)' &= \frac{e^{2\nu} - 1}{r} + \frac{G}{c^4}\frac{e^{2\nu}}{r^3}(w^2 - q^2) \end{aligned} \tag{1.2.73}$$

which are equivalent to

$$\begin{aligned} \lambda' &= +\frac{e^{2\nu} - 1}{2r} + \frac{G}{2c^4 r^3}\left(+e^{2\nu}(w^2 - q^2) - \frac{1}{\varkappa^2}(w')^2\right) \\ \nu' &= -\frac{e^{2\nu} - 1}{2r} + \frac{G}{2c^4 r^3}\left(-e^{2\nu}(w^2 - q^2) - \frac{1}{\varkappa^2}(w')^2\right) \end{aligned} \tag{1.2.74}$$

In particular note that λ' does not depend on λ. This means that, when expanding out the second-order w equation (1.2.53) (which contains e^{λ} on the left and its derivative on the right) by using (1.2.74), there will also be no λ terms present. One can check that it becomes

$$w'' = \left(\frac{3 - e^{2\nu}}{r} + \frac{Ge^{2\nu}}{c^4 r^3}(q^2 - w^2)\right) w' + \varkappa^2 e^{2\nu} w \ . \tag{1.2.75}$$

Upon expanding both sides of (1.2.72) by using the definition of $T_{\mu\nu}$ and the equations (1.2.74) and (1.2.75), one can verify that (1.2.72) is indeed an identity, as needed.

$\square$

Hence we can continue working only with the first two equations in (1.2.67) (or their equivalent (1.2.73)) as well as the w equation (1.2.53) (or its equivalent (1.2.75)). The most convenient form for the first two equations can be obtained by introducing new functions ψ, ζ:

$$\psi(r) = e^{\lambda(r)+\nu(r)} \quad , \quad \zeta(r) = e^{2\nu(r)} \ . \tag{1.2.76}$$

Given this definition, it will also be necessary to verify that the solutions we obtain for them satisfy

$$\psi(r) > 0 \quad , \quad \zeta(r) > 0 \tag{1.2.77}$$

for all $r > 0$.

Then we see from (1.2.73) that they satisfy a system of decoupled equations. With this we have found the Maxwell-BLTP-Einstein system for the functions ψ, ζ, w defined by (1.2.51) and (1.2.76):

$$\begin{cases} \psi' = -\dfrac{G}{c^4\varkappa^2}\dfrac{\psi}{r^3}(w')^2 \\[2ex] \zeta' = \dfrac{\zeta(1-\zeta)}{r} + \dfrac{G}{c^4 r^3}\left(q^2\zeta^2 - \zeta^2 w^2 - \dfrac{1}{\varkappa^2}(w')^2\zeta\right) \\[2ex] w'' = \left(\dfrac{3-\zeta}{r} + \dfrac{G\zeta}{c^4 r^3}(q^2 - w^2)\right) w' + \varkappa^2 \zeta w \end{cases} . \tag{1.2.78}$$

Note that ψ does not show up in the ζ and w equations. Therefore we can study those two equations separately, and only then draw conclusions about ψ using the first equation.

Remark 1.2.3. We will see in subsection 1.3.4 that the ψ and ζ corresponding to the RWN spacetime together with the w corresponding to the Coulomb potential $\varphi(r) = q/r$ are a solution to this system satisfying these asymptotic conditions, but we will quickly rule it out as a desirable solution due to the fact that its EM field energy density is not integrable in 3D space around the singularity.

1.3 *A priori* study of the differential system

1.3.1 Perturbation of the flat-space solution

We single out a special solution of the system (1.2.78) above in the case $G = 0$, called the **flat-space solution**, as defined in (1.1.4):

$$\varphi_0(r) = \frac{q - qe^{-\varkappa r}}{r} \quad , \quad \lambda_0(r) \equiv \nu_0(r) \equiv 0 \ . \tag{1.3.1}$$

The corresponding w as defined in (1.2.51) and ψ, ζ as defined in (1.2.76) are

$$w_0(r) = q(1 + \varkappa r)e^{-\varkappa r} \quad , \quad \psi_0(r) \equiv \zeta_0(r) \equiv 1 \ . \tag{1.3.2}$$

Considering that, in most physically interesting contexts, gravitational effects are several orders of magnitude less significant than electric ones, we would like to impose that the solution we seek for $G \neq 0$ be a perturbation of this flat-space solution. More precisely, if we indicate the dependence of the solution on the value of G with a subscript, then we seek solutions satisfying

$$\lim_{G \to 0} (\psi_G(r), \zeta_G(r), w_G(r)) = (\psi_0(r), \zeta_0(r), w_0(r)) \quad \text{for all } r > 0 \ . \tag{1.3.3}$$

(For the derivation of the flat-space solution, see subsection 1.3.4 ahead).

We can use the parameters $q, \varkappa, c$ to re-scale the potential φ and the coordinates r, t into dimensionless quantities:

$$\tilde{\lambda}(\tilde{r}) = \lambda(\tilde{r}/\varkappa) \quad , \quad \tilde{\nu}(\tilde{r}) = \nu(\tilde{r}/\varkappa) \quad , \quad \tilde{r} = \varkappa r \quad , \quad \tilde{t} = c\varkappa t \quad , \quad \tilde{\varphi}(\tilde{r}) = \frac{\varphi(\tilde{r}/\varkappa)}{q} \ . \tag{1.3.4}$$

The effect produced by this change is to replace $q, \varkappa, c$ by 1 in all formulas, while G gets replaced by the dimensionless constant

$$\varepsilon = \frac{Gq^2\varkappa^2}{c^4} \ . \tag{1.3.5}$$

We will implement this change in most formulas going forward, except when we want to carefully keep track of where each constant ends up. But we continue to use the notation without tildes even when the change has been implemented, to unburden the notation.

Remark 1.3.1. The flat-space potential (1.3.1) should be viewed as a small perturbation of the Coulomb potential q/r given by a *Yukawa potential* $-e^{-\varkappa r}/r$. The magnitude of $\varkappa$ controls the range of this deviation, which quickly becomes negligible after $r = 1/\varkappa$ due to its exponential decay. If our spacetime is supposed to model a charged particle, it is to be expected that $1/\varkappa$ should be a sub-atomic length.

Using the *cgs* values of the constants G, q, c (take q to be the elementary charge):

$$G = 6.67 \times 10^{-8}\text{cm}^3\text{g}^{-1}\text{s}^{-2} \quad , \quad q = 1.60 \times 10^{-10}\text{cm}^{3/2}\text{g}^{1/2}\text{s}^{-1} \quad , \quad c = 3.00 \times 10^{10}\text{cm s}^{-1} \ ,$$

we obtain

$$\frac{Gq^2}{c^4} = 1.90 \times 10^{-86}\text{cm}^2$$

This means that, even if $1/\varkappa$ is exceptionally small (say, the Planck length 1.62×10^{-33}cm), the resulting dimensionless constant ε still comes out small (7.24×10^{-21}).

1.3.2 Asymptotic conditions for large r

We do not wish to look for just any solution of (1.2.78), but rather only those that behave like what we observe in the physical world in the appropriate scales. Namely, we impose conditions of an **asymptotically Minkowski metric**

$$\lim_{r\to\infty} \lambda(r) = \lim_{r\to\infty} \nu(r) = 0 \ , \tag{1.3.6}$$

which ensure that the spacetime gets closer and closer to being flat away from the singularity, as well as conditions of an **asymptotically Coulomb potential**:

$$\lim_{r\to\infty} \varphi(r) = 0 \quad , \quad \lim_{r\to\infty} r^2\varphi'(r) = -Q \ . \tag{1.3.7}$$

The first of these limits simply fixes a value at ∞ for the potential, as is usually done. The second one says that the radial derivative φ' looks more and more like the one obtained from the Coulomb potential in flat-space, equal to Q/r. The significance of this will be clear in subsection 1.3.3, where we calculate that the electric field is a multiple of φ', just like in the case of Maxwell-Maxwell electromagnetism, and hence, under (1.3.7), the expression for the Coulomb field from a distance in the Maxwell-BLTP case will look like that of Maxwell-Maxwell.

Note that, in terms of the functions ψ, ζ defined in (1.2.76) and w defined in (1.2.51), the asymptotic conditions (1.3.6) and (1.3.7) at $r = \infty$ are written as

$$\lim_{r\to\infty} \psi(r) = \lim_{r\to\infty} \zeta(r) = 1 \quad , \quad \lim_{r\to\infty} w(r) = -Q + q \ . \tag{1.3.8}$$

Remark 1.3.2. For a metric like ours and under the conditions (1.3.6), the notion of the **ADM mass** M of the spacetime can be defined by

$$e^{-2\nu(r)} = 1 + \frac{2GM}{c^2 r} + O\left(\frac{1}{r^2}\right) \quad \text{as } r \to \infty \ . \tag{1.3.9}$$

It has the physical interpretation of the total mass content of the spacetime. For example, it is the M appearing in the RWN solution (1.1.7). When working with dimensionless units as explained in subsection 1.3.1, the **dimensionless ADM mass** can be defined as

$$\mu = \frac{c^2 M}{q^2 \varkappa} \ , \tag{1.3.10}$$

and (1.3.9) now looks like

$$e^{-2\nu(r)} = 1 + \frac{2\varepsilon\mu}{r} + O\left(\frac{1}{r^2}\right) \quad \text{as } r \to \infty \ . \tag{1.3.11}$$

The first two coefficients in the RWN metric (1.1.7) corresponding to charge q and ADM mass M are written in dimensionless variables as

$$e^{2\lambda(r)} = 1 - \frac{2\mu\varepsilon}{r} + \frac{\varepsilon}{r^2} \quad , \quad e^{2\nu(r)} = \left(1 - \frac{2\mu\varepsilon}{r} + \frac{\varepsilon}{r^2}\right)^{-1} \ . \tag{1.3.12}$$

When $\varepsilon\mu^2 < 1$, these expressions are positive for all $r > 0$, that is, the spacetime is free of horizons and the coordinate system is global. Using the electron mass $M = 9.11 \times 10^{-28}$ g and charge as above, we can calculate that this is the case, and by several orders of magnitude:

$$\varepsilon\mu^2 = \left(\frac{Gq^2\varkappa^2}{c^4}\right)\left(\frac{c^4 M^2}{q^4 \varkappa^2}\right) = \frac{GM^2}{q^2} = 2.40 \times 10^{-43} \ . \tag{1.3.13}$$

1.3.3 Charge and electric fields

Next we show that the integration constant q can be identified with the charge Q. This will have the consequence that the asymptotic condition for w as $r \to \infty$ becomes simpler:

$$\lim_{r\to\infty} w(r) = 0 \ . \tag{1.3.14}$$

In the tensorial formulation of electromagnetism, the electric fields E, D are 4-vectors obtained by raising indices from 1-forms $E^\flat, D^\flat$, which in turn are obtained from the tensors F and M by taking an interior product with the Killing vector field corresponding to time (see [Tah11]):

$$E^\flat = i_{\partial_{ct}} F \quad , \quad D^\flat = -i_{\partial_{ct}}(\star M) \ . \tag{1.3.15}$$

We can find $F, \star F, M, \star M$ written in coordinates, as well as the H tensor that appears in the definition of M, in equations (1.2.42), (1.2.43), (1.2.40), (1.2.16) and (1.2.47). The φ equation (1.2.50) simplifies M and $\star M$ considerably and brings in the constant q into them:

$$F = -\varphi' \,\mathrm{d}(ct) \wedge \mathrm{d}r \quad , \quad \star F = r^2 e^{-(\lambda+\nu)} \sin\theta \varphi' \,\mathrm{d}\theta \wedge \mathrm{d}\phi \ , \tag{1.3.16}$$

$$M = -q \sin\theta \,\mathrm{d}\theta \wedge \mathrm{d}\phi \quad , \quad \star M = -\frac{q e^{\lambda+\nu}}{r^2} \,\mathrm{d}(ct) \wedge \mathrm{d}r \ . \tag{1.3.17}$$

In particular

$$E^\flat = -\varphi' \,\mathrm{d}r \quad , \quad D^\flat = \frac{q e^{\lambda+\nu}}{r^2} \,\mathrm{d}r \ , \tag{1.3.18}$$

and raising indices:

$$E = -\varphi' e^{-2\nu} \frac{\partial}{\partial r} \quad , \quad D = \frac{q e^{\lambda-\nu}}{r^2} \frac{\partial}{\partial r} \ . \tag{1.3.19}$$

Rewriting these using the unit vector $\hat{e_r} = e^{-\nu}\partial_r$, we have

$$E = -\varphi' e^{-\nu} \hat{e_r} \quad , \quad D = \frac{q e^{\lambda}}{r^2} \hat{e_r} \ . \tag{1.3.20}$$

We see that, as we claimed in subsection 1.3.2, φ' enters in the calculation of the electric field E, while the electric displacement field D looks similar to its $\varkappa = \infty$ counterpart, with the difference being the presence of e^λ.

To understand the role of the constant q, assume that our spacetime can be extended to include the worldline $r = 0$ of the point charge. The equation $\mathrm{d}M = 0$ is true only on open sets away from this line; but, in general, the covariant formulation of electromagnetism imposes the following equation:

$$\mathrm{d}M = \frac{4\pi}{c} \star J^\flat \ , \tag{1.3.21}$$

where $J^\flat$ is the 1-form obtained by lowering indices of the **four-current vector**

$$J = c\rho \frac{\partial}{\partial(ct)} + \boldsymbol{j} \ . \tag{1.3.22}$$

In the above, ρ is a scalar field representing charge density, while the spatial part $\boldsymbol{j}$ represents current density. In a static spacetime like ours, ρ is a function of only r, and $\boldsymbol{j} = 0$. Furthermore, our spacetime consists only of a point-like charge at $r = 0$, which is modeled by a delta measure: $\rho(r) = Q\delta_0$. To avoid working with distributional fields like this, we will make use of an integral of ρ performed on a sphere centered at $r = 0$ to represent the charge Q, and then the expression for

M above will relate it to q. Namely, for any fixed time instant t_0 and radius $R > 0$, the charge Q should be the total amount of charge inside the sphere

$$B_r = \{(t_0, r, \theta, \phi) \mid r \leq R, \theta \in [0, \pi], \phi \in [0, 2\pi]\} \ , \tag{1.3.23}$$

which is written as

$$Q = \iiint_{B_R} \rho \, \mathrm{d}V \ . \tag{1.3.24}$$

In the above,

$$\mathrm{d}V = e^{\lambda+\nu} r^2 \sin\theta \, \mathrm{d}r \wedge \mathrm{d}\theta \wedge \mathrm{d}\phi \tag{1.3.25}$$

is the volume element induced by the metric on the slice of constant $t = t_0$. Now compute $J^\flat$ from the definition (1.3.22) of J, and then

$$\star \, J^\flat = -c\rho e^{\lambda+\nu} r^2 \sin\theta \, \mathrm{d}r \wedge \mathrm{d}\theta \wedge \mathrm{d}\phi \ . \tag{1.3.26}$$

In particular

$$\mathrm{d}M = -4\pi\rho e^{\lambda+\nu} r^2 \sin\theta \, \mathrm{d}r \wedge \mathrm{d}\theta \wedge \mathrm{d}\phi = -4\pi\rho \, \mathrm{d}V \ , \tag{1.3.27}$$

and the integral (1.3.24) for Q becomes

$$Q = -\frac{1}{4\pi} \iiint_{B_R} \mathrm{d}M = -\frac{1}{4\pi} \iint_{\partial B_R} M = -\frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} (-q \sin\theta) \mathrm{d}\theta \mathrm{d}\phi = q \ , \tag{1.3.28}$$

in which the Stokes theorem and the expression (1.3.17) for M were used. Henceforth, we will write Q in place of q.

1.3.4 Particular solutions

When $G = 0$, we can check that the flat-space solution of the Maxwell-BLTP equations is a solution to our system, as expected. Indeed, in that case the system becomes

$$\begin{cases} \psi' = 0 \\[2ex] \zeta' = \dfrac{\zeta(1-\zeta)}{r} \\[2ex] w'' - \dfrac{3-\zeta}{r} w' - \varkappa^2 \zeta w = 0 \end{cases} \tag{1.3.29}$$

The general solution for the metric variables $e^{2\lambda} = \psi^2/\zeta$, $e^{2\nu} = \zeta$ is the *Schwarzschild spacetime*

$$e^{2\lambda(r)} = 1 - \frac{M}{c^2 r} \quad , \quad e^{2\nu(r)} = \left(1 - \frac{M}{c^2 r}\right)^{-1} \tag{1.3.30}$$

where $M \in \mathbb{R}$ is a parameter. If we set $M = 0$ to force the manifold to be flat-space, we obtain the following general solution for w:

$$w(r) = C_1(1 + \varkappa r)e^{-\varkappa r} + C_2(1 - \varkappa r)e^{\varkappa r} \tag{1.3.31}$$

Imposing $w \to 0$ as $r \to \infty$ reduces it to just

$$w(r) = C_1(1 + \varkappa r)e^{-\varkappa r} , \tag{1.3.32}$$

which implies, for the electric potential $\varphi(r)$,

$$\varphi'(r) = \frac{w(r) - Q}{r^2} = -\frac{Q}{r^2} + C_1\left(\frac{\varkappa}{r} + \frac{1}{r^2}\right)e^{-\varkappa r} . \tag{1.3.33}$$

By also imposing $\varphi \to 0$ as $r \to \infty$, we can unambiguously integrate:

$$\varphi(r) = \frac{Q}{r} - C_1\frac{e^{-\varkappa r}}{r} . \tag{1.3.34}$$

Now the choice $C_1 = Q$ is the only one that makes $\varphi(0)$ finite. Thus φ is as stated in (1.1.4). In dimensionless units, this case corresponds to $\varepsilon = 0$, with the solution taking the form

$$\psi \equiv \zeta \equiv 1 \quad , \quad w(r) = (1 + r)e^{-r} . \tag{1.3.35}$$

If instead $G \neq 0$, we should be able to check that RWN is the solution of our equations in the Maxwell-Maxwell case, that is, when $\varkappa = \infty$. We cannot use the form of the w equation given in the main system (1.2.78), since there is a $\varkappa^2 = \infty$ present in there. Instead we use the equivalent equation (1.2.53) which uses $1/\varkappa^2 = 0$; it reads

$$\frac{\psi w}{r^2} = \frac{1}{\varkappa^2}\left(\frac{\psi w'}{\zeta r^2}\right)' . \tag{1.3.36}$$

The system is then

$$\begin{cases} \psi' = 0 \\ \\ \zeta' = \dfrac{\zeta(1-\zeta)}{r} + \dfrac{GQ^2\zeta^2}{c^4 r^3}(1 - w^2) \\ \\ \dfrac{\psi w}{r^2} = 0 \end{cases} \tag{1.3.37}$$

Immediately we get $\psi \equiv 1$ (if we impose that $\psi \to 1$ as $r \to \infty$) and $w \equiv 0$ (which then gives φ the expression of the Coulomb potential). The general solution for ζ can be written

$$e^{-2\nu(r)} = \frac{1}{\zeta(r)} = 1 - \frac{2GM}{c^2 r} + \frac{GQ^2}{c^4 r^2} \ , \tag{1.3.38}$$

where M is an integration constant. Together with the fact that $e^{\lambda+\nu} = \psi \equiv 1$, this gives the RWN metric, as claimed.

Remark 1.3.3. The RWN metric with the Coulomb potential above (that is, $w \equiv 0$) also solves our main system (1.2.78) in the case $0 < \varkappa < \infty$. Indeed, in that system, all terms involving $\varkappa^2$ or $1/\varkappa^2$ are accompanied by w or w' and will still vanish if we plug in $w = 0$. What is more, RWN is the only solution of (1.2.78) satisfying $\psi \equiv 1$ (that is, $g_{tt}g_{rr} = -1$), because in this case the ψ equation in (1.2.78) implies that w is constant, hence zero under the assumption $w \to 0$ as $r \to \infty$. But this solution is not acceptable as a candidate for the solution we seek for the Maxwell-BLTP-Einstein system, since, as we shall see now, its corresponding total EM field energy is infinite.

1.3.5 Energy and asymptotic conditions at $r = 0$

We will now find the expression that defines the electromagnetic energy contained in a constant time slice of the spacetime. As in [Tah11], we can find it as the conserved quantity associated with the Killing field ∂_t (it is true that any quantity defined on a spacelike slice is conserved in time in our case, since we have a static spacetime, but the procedure outlined here is valid in more general settings to identify the specific quantity that should be called *energy*).

We work under the simplification $Q = \varkappa = c = 1$, $G = \varepsilon$ as explained in subsection 1.3.1. Consider the 1-form

$$P(Y) = T(\partial_t, Y) \ , \tag{1.3.39}$$

defined on vector fields Y, where T is the stress-energy tensor that appears as right-hand side of the Einstein equations (1.2.1) (which is necessarily divergence-free). Calculate the divergence of P:

$$\star \, \mathrm{d} \star P = \mathrm{div} P = \nabla_\mu P^\mu = T^{\mu\nu} \nabla_\mu (\partial_t)_\nu = \frac{1}{2}(\nabla_\mu (\partial_t)_\nu + \nabla_\nu (\partial_t)_\mu) = 0 \ . \tag{1.3.40}$$

In this we used $\nabla_\mu T^{\mu\nu} = 0$ and, in the last step, the fact that ∂_t is Killing. This implies $\mathrm{d} \star P = 0$, and then Stokes' Theorem implies that the quantity

$$\mathcal{E}(t_0) = \int_{\{t=t_0\}} \star P \tag{1.3.41}$$

is constant as t_0 varies:

$$\mathcal{E}(t_1) - \mathcal{E}(t_0) = \int_{\{t_0 \leq t \leq t_1\}} \mathrm{d} \star P = 0 \ . \tag{1.3.42}$$

It is this constant that is called the *energy* contained in any hypersurface of constant time in our spacetime. We shall omit the (t) dependence from it. (Note that we could have defined it also with a minus sign in front; we will soon see that the definition we chose leads to a positive value for the energy).

We can explicitly compute the 3-form $\star P$: by the definition of P and the fact that T is diagonal,

$$P = T_{tt} \mathrm{d}t \ , \tag{1.3.43}$$

and the Hodge dual works out to be

$$\star P = -e^{\lambda+\nu} r^2 \sin\theta e^{-2\lambda} T_{tt} \ \mathrm{d}r \mathrm{d}\theta \mathrm{d}\phi \ . \tag{1.3.44}$$

Therefore, after performing the θ, ϕ integrals, we find

$$\begin{aligned} \mathcal{E} &= \frac{1}{2} \int_0^\infty \frac{e^{\lambda(r)+\nu(r)}}{r^2} \left(1 - w(r)^2 - e^{-2\nu(r)} (w'(r))^2\right) \mathrm{d}r \\ &= \frac{1}{2} \int_0^\infty \frac{\psi}{r^2} \left(1 - w^2 - \frac{1}{\zeta} (w')^2\right) \mathrm{d}r \ . \end{aligned} \tag{1.3.45}$$

Remark 1.3.4. Plugging in (ψ, ζ, w) as in the RWN solution (in particular $\psi \equiv 1$ and $w \equiv 0$), this expression becomes

$$\mathcal{E} = \frac{1}{2} \int_0^\infty \frac{\mathrm{d}r}{r^2} = \infty \tag{1.3.46}$$

(it is not integrable around the singularity). This is what deems the RWN solution inadequate for our purposes.

Now let us rewrite the energy integral by using

$$1 - w^2 = -(w-1)^2 - 2(w-1) \ . \tag{1.3.47}$$

We see that we can split it into a negative integral plus another one that we are able to simplify, given the definition (1.2.51) of w in terms of φ':

$$\begin{aligned} \mathcal{E} &= \frac{1}{2} \int_0^\infty \frac{\psi}{r^2} (-(w-1)^2 - \zeta^{-1} (w')^2) \mathrm{d}r - \frac{1}{2} \int_0^\infty \frac{\psi}{r^2} 2(w-1) \mathrm{d}r \\ &= -\frac{1}{2} \int_0^\infty \frac{\psi}{r^2} ((w-1)^2 + \zeta^{-1} (w')^2) \mathrm{d}r - \int_0^\infty \varphi' \mathrm{d}r \ . \end{aligned} \tag{1.3.48}$$

Using the boundary conditions that we will prove are true for φ when we solve the system, that is, $\varphi(\infty) = 0$ and $\lim_{r\to 0} \varphi(r) \in \mathbb{R}$, we have

$$\mathcal{E} = -\frac{1}{2}\int_0^\infty \frac{\psi}{r^2}((w-1)^2 + \zeta^{-1}(w')^2)\mathrm{d}r + \varphi(0) \ . \tag{1.3.49}$$

Then the energy will be finite if and only if each of the two negative integrals in this expression is finite:

$$\left|\int_0^\infty \frac{\psi(w-1)^2}{r^2}\mathrm{d}r\right| < \infty \quad , \quad \left|\int_0^\infty \frac{\psi\zeta^{-1}(w')^2}{r^2}\mathrm{d}r\right| < \infty \ . \tag{1.3.50}$$

Note that we can also write the condition $|\varphi(0)| < \infty$ in terms of finiteness of an integral, again by rewriting φ' in terms of w:

$$\left|\int_0^\infty \frac{\psi(w-1)}{r^2}\mathrm{d}r\right| < \infty \ . \tag{1.3.51}$$

Given the asymptotic conditions at $r = \infty$ for ψ, ζ, w, w', there are no divergence problems in these integrals for large r. It is at the point $r = 0$ where there is a possibility of divergence, as in the case of the RWN solution.

Now go back to the equation satisfied by ψ in the main system (1.2.78). We see that it is a decreasing function:

$$\psi' = -\frac{\varepsilon\psi}{r^3}(w')^2 < 0 \ .$$

Since we also require $\lim_{r\to\infty} \psi(r) = 1$, we must have

$$\psi(r) \geq 1 \quad \text{for all } r \geq 0 \ .$$

Therefore the presence of ψ in (1.3.50) and (1.3.51) is not helping with finiteness of the integrals. To obtain finite integrals, it will be necessary (but possibly not sufficient, depending on whether ψ diverges and how fast) to have the following conditions:

$$\left|\int_0^\infty \frac{w-1}{r^2}\mathrm{d}r\right| < \infty \quad , \quad \left|\int_0^\infty \frac{(w-1)^2}{r^2}\mathrm{d}r\right| < \infty \quad , \quad \left|\int_0^\infty \frac{\zeta^{-1}(w')^2}{r^2}\mathrm{d}r\right| < \infty \ . \tag{1.3.52}$$

Remark 1.3.5. The first of the 3 inequalities above tells us that $w(0)$ must be defined and equal to 1; in fact, since $1/r$ is not integrable near 0, it must be true that $(w-1)/r \to 0$ as $r \to 0$, that is, $w'(0) = 0$. Also note that the second one follows from the first. In section 1.5, we will let these necessary values of $w(0), w'(0)$ guide our choice of new variables to study the system for small r. We will be able to prove that, for any small ε, there is a 1-parameter family of solutions which satisfy

$$0 < |X| < \infty \quad , \quad 0 < |Y| < \infty \quad , \quad 0 < |Z| < \infty \ , \tag{1.3.53}$$

where

$$X = \lim_{r\to 0} \zeta(r) \quad , \quad Y = \lim_{r\to 0} \frac{w'(r)}{r} \quad , \quad Z = \lim_{r\to 0} \frac{w(r)-1}{r^2} \ . \tag{1.3.54}$$

These imply that the integrals (1.3.52) (performed only on a neighborhood of 0) are indeed finite. Then we will be able to study the behavior of ψ along these solutions and conclude that also (1.3.50) and (1.3.51) are finite (around 0). Once we manage to connect the solutions coming from $r = 0$ to those coming from $r = \infty$ to obtain a solution on $(0, \infty)$, these statements prove that $|\mathcal{E}| < \infty$ and $|\varphi(0)| < \infty$.

Remark 1.3.6. Once the statements made in the above remark are proved, there's a further simplification to be made in the energy integral. First note that

$$\lim_{r\to 0} \frac{\psi(w-1)w'}{\zeta r^2} = \lim_{r\to 0} \frac{w-1}{r^2} \cdot \frac{1}{\zeta} \cdot \frac{r}{w'} \cdot \frac{(w')^2\psi}{r} = \frac{Z}{XY} \lim_{r\to 0} \frac{(w')^2\psi}{r} = 0 \tag{1.3.55}$$

(the last limit is zero since the second integral in (1.3.50) converges). Now consider again the w equation (1.2.53)

$$\frac{\psi w}{r^2} - \left(\frac{\psi w'}{\zeta r^2}\right)' = 0 \ . \tag{1.3.56}$$

Add ψ/r^2 on both sides and multiply by $w-1$:

$$\frac{\psi(w^2-1)}{r^2} - (w-1)\left(\frac{\psi w'}{\zeta r^2}\right)' = \frac{(w-1)\psi}{r^2} = \varphi' \ . \tag{1.3.57}$$

Integrating (by parts in the second term):

$$\int_0^\infty \frac{\psi(w^2-1)}{r^2}\mathrm{d}r - \left.\frac{\psi(w-1)w'}{\zeta r^2}\right|_0^\infty + \int_0^\infty \frac{\psi(w')^2}{\zeta r^2}\mathrm{d}r = \int_0^\infty \varphi'\mathrm{d}r = -\varphi(0) \ . \tag{1.3.58}$$

The two integrals on the left-hand side combine to make a multiple of the energy, as per formula (1.3.45):

$$-2\mathcal{E} - \left.\frac{\psi(w-1)w'}{\zeta r^2}\right|_0^\infty = -\varphi(0) \ , \tag{1.3.59}$$

while the boundary term vanishes at both ends (at $r = 0$ this is due to (1.3.55), while at $r = \infty$ it is due to the fact that $\lim_{r\to\infty} w'(r) = 0$, to be proven in section 1.4). Therefore we obtain

$$\mathcal{E} = \frac{\varphi(0)}{2} \ . \tag{1.3.60}$$

This proves that the flat-space formula (1.1.5) still holds true. We can also plug this back into (1.3.49) and solve for $\varphi(0)$:

$$\varphi(0) = \int_0^\infty \frac{e^{\lambda+\nu}}{r^2}((w-1)^2 + e^{-2\nu}(w')^2)\mathrm{d}r \geq 0 \ , \tag{1.3.61}$$

showing that the sign we chose for the energy in (1.3.41) was correct (yielded a positive energy).

1.4 Radial variable away from 0

In this section we focus on solving the Maxwell-BLTP-Einstein system (1.1.13) for values of r satisfying $r \geq r_0 > 0$, where r_0 is fixed (later we will impose also $r_0 < 1$ for convenience). The system is recalled here:

$$\begin{cases} \psi' = -\dfrac{\varepsilon\psi}{r^3}(w')^2 \\ \\ \zeta' = \dfrac{(1-\zeta)\zeta}{r} + \dfrac{\varepsilon}{r^3}((1-w^2)\zeta^2 - (w')^2\zeta) \\ \\ w'' = \left(\dfrac{3-\zeta}{r} + \dfrac{\varepsilon\zeta}{r^3}(1-w^2)\right) w' + \zeta w \end{cases} \tag{1.4.1}$$

We focus almost all of the attention on the ζ and w equations, which are independent of ψ, and only study the solution for ψ in the very end of this section.

The number $\varepsilon \geq 0$ is considered a parameter. We will find solutions that are power series in ε, convergent at any large enough r with a uniform lower bound on the radius of convergence. The solutions will be written as $\psi_\varepsilon(r), \zeta_\varepsilon(r), w_\varepsilon(r)$ when we need to consider what happens to them as ε changes, but we will mostly write just $\psi(r), \zeta(r), w(r)$ when that is not needed. The main result to be proven in this section is:

Theorem 1.4.1. *Let $\mu_*, \alpha_* > 0$. For every $0 < r_0 < 1$, there exists*

$$\varepsilon_* = \frac{r_0^7}{240(15 + 4r_0\mu_* + r_0^4\alpha_*)} \tag{1.4.2}$$

such that, for any choice of the parameter $\varepsilon \in [0, \varepsilon_*)$ satisfying

$$\varepsilon\mu_*^2 < 1 \ , \tag{1.4.3}$$

the Maxwell-BLTP-Einstein system (1.1.13) admits a 2-parameter family of solutions $\psi_\varepsilon, \zeta_\varepsilon, w_\varepsilon$ in $[r_0, \infty)$, parametrized by $\mu, \alpha \in \mathbb{R}$, with $|\mu| \leq \mu_*$ and $|\alpha| \leq \alpha_*$, which are continuous on (μ, α) at any $r \in [r_0, \infty)$ and satisfy the following asymptotic conditions *at $r = \infty$:*

$$\lim_{r\to\infty} \zeta_\varepsilon(r) = \lim_{r\to\infty} \psi_\varepsilon(r) = 1 \ , \tag{1.4.4}$$

$$\lim_{r\to\infty} w_\varepsilon(r) = \lim_{r\to\infty} w'_\varepsilon(r) = 0 \ , \tag{1.4.5}$$

and the following perturbation conditions *at any fixed* $r \in (r_0, \infty)$*:*

$$\lim_{\varepsilon\to 0^+} \zeta_\varepsilon(r) = \lim_{\varepsilon\to 0^+} \psi_\varepsilon(r) = 1 \ , \tag{1.4.6}$$

$$\lim_{\varepsilon\to 0^+} w_\varepsilon(r) = (1+r)e^{-r} \ . \tag{1.4.7}$$

Furthermore, we have, for all $r \geq r_0$*,*

$$\psi_\varepsilon(r) > 0 \quad , \quad \zeta_\varepsilon(r) > 0 \ , \tag{1.4.8}$$

and, for a given choice of the parameter μ *(and an arbitrary one for* α*),*

$$\zeta_\varepsilon(r) = 1 + \frac{2\mu\varepsilon}{r} + O\left(\frac{1}{r^2}\right) \quad as \quad r \to \infty \ , \tag{1.4.9}$$

so that μ *can be identified with the* dimensionless ADM mass *of the spacetime represented by the system.*

The big O notation above is, as usual, employed to indicate that a function asymptotically dominates another as r increases; that is, a statement of the form $x(r) = y(r) + O(z(r))$ means that there exists C such that $|x(r) - y(r)| \leq C|z(r)|$ for $r \geq r_0$.

The steps in the proof, each one contained in one subsection, can be described as follows:

- (Subsection 1.4.1) We fix $r_0 > 0$ and **assume** that, at each $r > r_0$, we can write ζ, w as convergent power series $\zeta(r,\varepsilon) = \sum_j \zeta_j(r)\varepsilon^j$ and $w(r,\varepsilon) = \sum_j w_j(r)\varepsilon^j$. We find recursion formulas for the coefficients. They will involve two free parameters $\mu, \alpha \in \mathbb{R}$ whose values will be considered fixed for the rest of the argument. The main task that is left is proving the convergence of the series.

- (Subsection 1.4.2) We introduce new functions η, u, v of (r, ε), which are also given as ε-power series with coefficients denoted by η_j, u_j, v_j, and read off the recursion formulas for them using the ones found for ζ_j, w_j. Proving the convergence of these new series is readily seen to be equivalent to proving that of the original ones. The reason for considering the η variable in place of ζ will only become apparent in subsection 1.4.4 (it is better suited for our technique because it decays exponentially with r, while ζ doesn't), while the reason for considering the u, v variables in place of w, w' is for convenience only (the formulas become shorter).

- (Subsection 1.4.3) We put absolute values on those recursion formulas and find good ways to estimate away the r dependence. It is proven that there exist numerical sequences $(A_j), (B_j)$, defined via a polynomial recursion, such that

$$|\eta_j(r)| \leq A_j e^{-r/2} \quad , \quad |u_j(r)|, |v_j(r)| \leq B_j e^{-r/2} \ . \tag{1.4.10}$$

  Another numerical sequence (C_j) is used in order to define A_j, B_j and will also figure in the sequel.

- (Subsection 1.4.4) A summation technique is developed in order to prove by induction that

$$A_j, B_j, C_j \leq \frac{SR^j}{(j+\delta)^2} \tag{1.4.11}$$

  for some $R, S, \delta > 0$, establishing the convergence of the power series for any $\varepsilon < 1/R$.

- (Subsection 1.4.5) The estimates (1.4.10) can be used to obtain bounds which are uniform in $r \geq r_0$. This is used to finish proving some of the leftover details, such as the desired asymptotics of the series as $r \to \infty$ and the fact that r-derivatives can be taken term by term. We also quickly check the desired behavior of the ψ function from the original system (positivity, asymptotic behavior) and continuity of the solutions with respect to the parameters μ and α.

1.4.1 ε power series

In this subsection, we *assume* that

$$\zeta_\varepsilon(r) = \sum_{j=0}^{\infty} \zeta_j(r)\varepsilon^j \quad , \quad w_\varepsilon(r) = \sum_{j=0}^{\infty} w_j(r)\varepsilon^j \tag{1.4.12}$$

with convergence for any large enough r and small enough ε, and with the possibility to take r-derivatives term by term. Our goal is to find recursive formulas for the series coefficients.

The desired perturbation conditions (1.4.6) and (1.4.7) immediately imply that the zeroth terms are determined:

$$\zeta_0 \equiv 1 \quad , \quad w_0(r) = (1+r)e^{-r} \quad , \quad w_0'(r) = -re^{-r} \ . \tag{1.4.13}$$

Furthermore, the desired asymptotic conditions (1.4.4) and (1.4.5) suggest (although they don't necessarily imply) that it should be true that

$$\begin{aligned} \lim_{r\to\infty} \zeta_j(r) = 0 \quad \text{for all } j \geq 1 \ , \\ \lim_{r\to\infty} w_j(r) = \lim_{r\to\infty} w_j'(r) = 0 \quad \text{for all } j \geq 0 \ . \end{aligned} \tag{1.4.14}$$

We will look for solutions satisfying these limits, and later prove (subsection 1.4.5) that they imply (1.4.4) and (1.4.5).

Every polynomial expression $P(\zeta, w, w')$ involving ζ, w, w' is also given as a power series in ε, converging wherever ζ, w, w' converge. We will use the notation $[P(\zeta, w, w')]_j$ to denote the j-th coefficient in the series for any such polynomial expression ($j \geq 0$), which depends on the coefficients ζ_k, w_k, w_k' for all $k = 0, \ldots, j$ and is given as a sum over indices adding up to j. So for example

$$[\zeta^2]_j = \sum_{k=0}^{j} \zeta_k \zeta_{j-k} \quad , \quad [\zeta^2 w^2]_j = \sum_{k=0}^{j} [\zeta^2]_k [w^2]_{j-k} = \sum_{k=0}^{j} \left(\sum_{l=0}^{k} \zeta_l \zeta_{k-l} \right) \left(\sum_{m=0}^{j-k} w_m w_{j-k-m} \right) \ . \tag{1.4.15}$$

Proposition 1.4.2. *Let $\varepsilon \geq 0$. Fix $r_0 > 0$ and two parameters $\mu, \alpha \in \mathbb{R}$. Define sequences of functions ζ_j, f_j, w_j of $r \in [r_0, \infty)$ by:*

$$\zeta_0(r) = 1 \quad , \quad f_0(r) = 0 \quad , \quad w_0(r) = (1+r)e^{-r} \ ; \tag{1.4.16}$$

$$\begin{aligned} \zeta_1(r) &= \left(\frac{2\mu}{r} - \frac{1}{r^2} \right) + \left(\frac{1}{r} + \frac{1}{r^2} \right) e^{-2r} \\ f_1(r) &= \left(2\mu + \frac{4\mu - 1}{r} - \frac{2}{r^2} \right) e^{-r} + \left(2 + \frac{5}{r} + \frac{3}{r^2} \right) e^{-3r} \ , \\ w_1(r) &= \frac{1}{2} \left(\alpha(1+r)e^{-r} + (1+r)e^{-r} \int_{r_0}^{r} \frac{(1-s)e^s}{s^2} f_1(s) \, \mathrm{d}s + (1-r)e^r \int_r^\infty \frac{(1+s)e^{-s}}{s^2} f_1(s) \, \mathrm{d}s \right) \ ; \end{aligned} \tag{1.4.17}$$

and, for all $j > 0$,

$$\zeta_{j+1}(r) = \frac{1}{r} \int_r^\infty \left(\sum_{k=1}^{j} \zeta_k(s) \zeta_{j+1-k}(s) + \frac{[-\zeta(s)^2 + \zeta(s)^2 w(s)^2 + \zeta(s)(w'(s))^2]_j}{s^2} \right) \mathrm{d}s \ , \tag{1.4.18}$$

$$f_{j+1}(r) = \sum_{k=0}^{j} \zeta_{j+1-k} \left[w - \frac{w'}{r} \right]_k + \frac{[\zeta w' - \zeta w^2 w']_j}{r^3} \ , \tag{1.4.19}$$

$$w_{j+1}(r) = \frac{1}{2} \left((1+r)e^{-r} \int_{r_0}^{r} \frac{(1-s)e^s}{s^2} f_{j+1}(s) \, \mathrm{d}s + (1-r)e^r \int_r^\infty \frac{(1+s)e^{-s}}{s^2} f_{j+1}(s) \, \mathrm{d}s \right) \ . \tag{1.4.20}$$

Then these sequences are well-defined, in the sense that the recursive definition is non-circular and the improper integrals converge, and they satisfy

$$\zeta_j(r) = O\left(\frac{1}{r^j}\right) \quad , \quad w_j(r) = O(e^{-r/2}) \quad , \quad w_j'(r) = O(e^{-r/2}) \quad \text{as } r \to \infty \ . \tag{1.4.21}$$

Furthermore, the analytic functions of ε defined by

$$\zeta(r,\varepsilon) = \sum_{j=0}^{\infty} \zeta_j(r)\varepsilon^j \quad , \quad w(r,\varepsilon) = \sum_{j=0}^{\infty} w_j(r)\varepsilon^j \tag{1.4.22}$$

are solutions of (1.1.13) for $r \geq r_0$ (provided that they converge and can be differentiated in the r variable term-by-term).

Proof. System (1.1.13) determines differential equations satisfied by each ζ_{j+1} and w_{j+1} which we can solve in order to recursively define them in terms of all previous coefficients ζ_k, w_k, w_k', $k = 0, \ldots, j$. First look at the $(j+1)^{\text{st}}$ coefficient of the ζ equation:

$$\zeta_{j+1}' = \frac{\zeta_{j+1} - [\zeta^2]_{j+1}}{r} + \frac{[\zeta^2 - \zeta^2 w^2 - \zeta(w')^2]_j}{r^3} \ . \tag{1.4.23}$$

In the expansion for $[\zeta^2]_{j+1}$, there are two terms equal to $\zeta_0\zeta_{j+1} = \zeta_{j+1}$. Other than these and the very first ζ_{j+1} above, nothing else involves any coefficient of degree $j+1$. So we collect these ζ_{j+1} terms on the left side and obtain:

$$\zeta_{j+1}' + \frac{\zeta_{j+1}}{r} = -\frac{1}{r}\sum_{k=1}^{j} \zeta_k\zeta_{j+1-k} + \frac{[\zeta^2 - \zeta^2 w^2 - \zeta(w')^2]_j}{r^3} \ . \tag{1.4.24}$$

One possible way to write the general solution to this equation is by fixing a number $a \geq r_0$ as an integration starting point (to be used for all j) and including an integration constant C_j:

$$\zeta_{j+1}(r) = \frac{C_j}{r} + \frac{1}{r}\int_a^r \left(-\sum_{k=1}^{j} \zeta_k(s)\zeta_{j+1-k}(s) + \frac{[\zeta(s)^2 - \zeta(s)^2 w(s)^2 - \zeta(s)(w'(s))^2]_j}{s^2} \right) \mathrm{d}s \ . \tag{1.4.25}$$

But it turns out that choosing $a = \infty$, $C_1 \in \mathbb{R}$ and $C_{j+1} = 0$ for all $j > 0$ will yield the asymptotic condition (1.4.21) (this will be proven soon). In fact, choosing $C_1 = 2\mu$ gives the stronger form (1.4.9) of the asymptotic condition for ζ. This gives the recursion for the ζ coefficients as stated in this proposition:

$$\begin{aligned} \zeta_{j+1}(r) &= \frac{1}{r}\int_r^{\infty} \left(\sum_{k=1}^{j} \zeta_k\zeta_{j+1-k} + \frac{[-\zeta^2 + \zeta^2 w^2 + \zeta(w')^2]_j}{s^2} \right) \mathrm{d}s \quad \text{for all } j > 0 \ , \\ \zeta_1(r) &= \frac{2\mu}{r} + \frac{1}{r}\int_r^{\infty} \frac{[-\zeta^2 + \zeta^2 w^2 + \zeta(w')^2]_0}{s^2} \mathrm{d}s \ . \end{aligned} \tag{1.4.26}$$

Using the zeroth coefficients we can calculate

$$\zeta_1(r) = \left(\frac{2\mu}{r} - \frac{1}{r^2}\right) + \left(\frac{1}{r} + \frac{1}{r^2}\right) e^{-2r} \ . \tag{1.4.27}$$

Next we analyze the w equation. First rewrite it as

$$w'' - \frac{2}{r}w' - w = (\zeta - 1)\left(w - \frac{w'}{r}\right) + \frac{\varepsilon}{r^3}\zeta(1 - w^2)w' \ , \tag{1.4.28}$$

so that, when computing the $(j+1)^{\text{st}}$ coefficient on both sides, the right side will not involve any w_{j+1} or w'_{j+1}. Indeed, these terms can only possibly show up in the term not including ε, and only in the first term of the expansion

$$\left[(\zeta - 1)\left(w - \frac{w'}{r}\right)\right]_{j+1} = [\zeta - 1]_0 \left[w - \frac{w'}{r}\right]_{j+1} + \cdots \ , \tag{1.4.29}$$

but this first term is zero, since $[\zeta - 1]_0 = 1 - 1 = 0$. This means that, after having computed ζ_{j+1}, we can proceed with computing w_{j+1} by

$$\begin{aligned} w''_{j+1} - \frac{2}{r}w'_{j+1} - w_{j+1} &= \sum_{k=0}^{j} [\zeta - 1]_{j+1-k} \left[w - \frac{w'}{r}\right]_k + \frac{[\zeta w' - \zeta w^2 w']_j}{r^3} \\ &= \sum_{k=0}^{j} \zeta_{j+1-k} \left[w - \frac{w'}{r}\right]_k + \frac{[\zeta w' - \zeta w^2 w']_j}{r^3} \\ &= f_{j+1} \ . \end{aligned} \tag{1.4.30}$$

We can calculate f_1 defined by this formula and it will be precisely as stated in the proposition:

$$f_1(r) = \left(2\mu + \frac{4\mu - 1}{r} - \frac{2}{r^2}\right) e^{-r} + \left(2 + \frac{5}{r} + \frac{3}{r^2}\right) e^{-3r} \ . \tag{1.4.31}$$

The general solution of (1.4.30) can be found by the method of variation of parameters. It involves a linear combination of the two solutions $(1 + r)e^{-r}$ and $(1 - r)e^{r}$ of the homogeneous equation, each multiplied by a particular integral involving the non-homogeneity f_{j+1} as part of the integrand. In writing the most general solution, we can let the lower integration endpoint be a free parameter b_{j+1} in the second of these integrals, and leave it fixed as r_0 in the first, as long as we also include a general multiple $\alpha_{j+1}(1 + r)e^{-r}$ of the corresponding homogeneous solution together with this integral. This form will prove the most convenient later. The result of this procedure can be calculated to be:

$$\begin{aligned} w_{j+1}(r) = \frac{1}{2}\Bigg(&\alpha_{j+1}(1 + r)e^{-r} + (1 + r)e^{-r} \int_{r_0}^{r} \frac{(1 - s)e^{s}}{s^2} f_{j+1}(s)\, \mathrm{d}s \\ &- (1 - r)e^{r} \int_{b_{j+1}}^{r} \frac{(1 + s)e^{-s}}{s^2} f_{j+1}(s)\, \mathrm{d}s\Bigg) \ . \end{aligned} \tag{1.4.32}$$

Note that the $1/s^2$ terms in the integrals come from the Wronskian determinant of the two fundamental solution.

The asymptotic condition of w_j and w'_j (1.4.21) can only be satisfied by choosing $b_{j+1} = \infty$ for all $j \geq 0$. It will also be enough for our purposes to let only α_1 be nonzero among all of the α_{j+1} (we call α_1 just α). Hence, we have the recursion as given in the proposition statement:

$$w_{j+1}(r) = \frac{1}{2}\left((1+r)e^{-r}\int_{r_0}^{r}\frac{(1-s)e^{s}}{s^2}f_{j+1}(s)\,\mathrm{d}s + (1-r)e^{r}\int_{r}^{\infty}\frac{(1+s)e^{-s}}{s^2}f_{j+1}(s)\,\mathrm{d}s\right) \quad , \quad j > 0 \tag{1.4.33}$$

and

$$w_1(r) = \frac{1}{2}\left(\alpha(1+r)e^{-r} + (1+r)e^{-r}\int_{r_0}^{r}\frac{(1-s)e^{s}}{s^2}f_1(s)\,\mathrm{d}s \right.$$
$$\left. + (1-r)e^{r}\int_{r}^{\infty}\frac{(1+s)e^{-s}}{s^2}f_1(s)\,\mathrm{d}s\right) . \tag{1.4.34}$$

Next let us compute w'_{j+1} by differentiating the expressions above. Nothing comes from when the derivative hits the integrals (a cancellation between the two terms takes place); the only surviving expression is obtained from when the derivative hits the functions $(1\pm r)e^{\mp r}$ outside of the integrals:

$$w'_{j+1}(r) = -\frac{r}{2}\left(e^{-r}\int_{r_0}^{r}\frac{(1-s)e^{s}}{s^2}f_{j+1}(s)\,\mathrm{d}s + e^{r}\int_{r}^{\infty}\frac{(1+s)e^{-s}}{s^2}f_{j+1}(s)\,\mathrm{d}s\right) \quad , \quad j > 0 \tag{1.4.35}$$

and

$$w'_1(r) = -\frac{r}{2}\left(\alpha e^{-r} + e^{-r}\int_{r_0}^{r}\frac{(1-s)e^{s}}{s^2}f_1(s)\,\mathrm{d}s + e^{r}\int_{r}^{\infty}\frac{(1+s)e^{-s}}{s^2}f_1(s)\,\mathrm{d}s\right) . \tag{1.4.36}$$

We now have a non-circular recursion for all ζ_j, f_j, w_j, w'_j. What is left is the proof that the improper integrals in the formulas converge and that the asymptotics (1.4.21) hold; we will prove both at the same time by induction. To start, note that (1.4.21) is immediately true for $j = 0$.

(1.4.21) is also true for ζ_1 (the dominant term in ζ_1 is $2\mu/r$ when r is made large). For w_1, we will use its defining formula (1.4.34) to prove that $|w_1(r)e^{r/2}|$ is bounded. First estimate the f_1 term inside the integrals in the w_1 formula by some multiple C of $e^{-r/2}$ (which can be done considering the expression for f_1), so that we can write:

$$2|w_1(r)|e^{r/2} \leq |\alpha|(1+r)e^{-r/2} + C(1+r)e^{-r/2}\int_{r_0}^{r}\frac{(1+s)e^{s/2}}{s^2}\mathrm{d}s + C(1+r)e^{3r/2}\int_{r}^{\infty}\frac{(1+s)e^{-3s/2}}{s^2}\mathrm{d}s . \tag{1.4.37}$$

The first of these three terms is clearly bounded. To see that the second one is also bounded, since we are only concerned with the region $[r_0, \infty)$, away from 0, all we have to do is prove that it has a finite limit as $r \to \infty$, which can be done by the L'Hôpital Rule (observe that the integral itself diverges, so L'Hôpital is justified):

$$\lim_{r\to\infty}(1+r)e^{-r/2}\int_{r_0}^{r}\frac{(1+s)e^{s/2}}{s^2}\mathrm{d}s = \lim_{r\to\infty}\frac{\int_{r_0}^{r}\frac{(1+s)e^{s/2}}{s^2}\mathrm{d}s}{\frac{e^{r/2}}{1+r}} = \lim_{r\to\infty}\frac{\frac{(1+r)e^{r/2}}{r^2}}{\left(\frac{1}{2(1+r)}-\frac{1}{(1+r)^2}\right)e^{r/2}} = 2\ . \tag{1.4.38}$$

As for the third term, we estimate the decreasing function $(1+s)/s$ by $(1+r)/r^2$ and integrate:

$$(1+r)e^{3r/2}\int_{r}^{\infty}\frac{(1+s)e^{-3s/2}}{s^2} \le \frac{2}{3}\frac{(1+r)^2}{r^2}e^{3r/2}e^{-3r/2} \le \frac{2}{3}\left(1+\frac{2}{r_0}+\frac{1}{r_0^2}\right)\ . \tag{1.4.39}$$

An entirely analogous argument proves (1.4.21) for w_1'.

So we have (1.4.21) for $j = 0, 1$. Now fix $j > 0$ and assume by induction that, for all $k = 0, \dots, j$, the coefficients ζ_k, w_k are well-defined and there exist constants $D_k > 0$ such that

$$|\zeta_k(r)| \le \frac{D_k}{r^k} \quad , \quad |w_k(r)|, |w_k'(r)| \le D_k e^{-r/2} \quad , \quad r \ge r_0\ . \tag{1.4.40}$$

Then we have:

$$\begin{aligned}
|\zeta_{j+1}(r)| \le \frac{1}{r}\int_r^\infty \Bigg(&\sum_{k=1}^{j}\frac{D_kD_{j+1-k}}{s^{j+1}} + \sum_{k=0}^{j}\frac{D_kD_{j-k}}{s^{j+2}} + \sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k}\frac{D_lD_{k-l}D_mD_{j-k-m}}{s^{k+2}}e^{-s} \\
&+ \sum_{k=0}^{j}\sum_{m=0}^{j-k}\frac{D_kD_mD_{j-k-m}}{s^{k+2}}e^{-s}\Bigg)\mathrm{d}s \\
\le \frac{1}{r}\Bigg(&\frac{1}{jr^j}\sum_{k=1}^{j}D_kD_{j+1-k} + \frac{1}{(j+1)r^{j+1}}\sum_{k=0}^{j}D_kD_{j-k} + e^{-r}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k}\frac{D_lD_{k-l}D_mD_{j-k-m}}{(k+1)r^{k+1}} \\
&+ e^{-r}\sum_{k=0}^{j}\sum_{m=0}^{j-k}\frac{D_kD_mD_{j-k-m}}{(k+1)r^{k+1}}\Bigg)\ ,
\end{aligned} \tag{1.4.41}$$

where we have estimated the decreasing factor of e^{-s} by its maximum e^{-r} in the integration domain. It is clear that the end result is dominated, for $r \ge r_0$, by a multiple of $1/r^{j+1}$, since the exponential

e^{-r} is dominated by a multiple of any function of the form $1/r^{j-k}$. Similarly, we have

$$\begin{aligned}|f_{j+1}(r)| &\leq \sum_{k=0}^{j} |\zeta_{j+1-k}||w_k| + \frac{1}{r}\sum_{k=0}^{j} |\zeta_{j+1-k}||w_k'| + \frac{1}{r^3}\sum_{k=0}^{j} |\zeta_{j-k}||w_k'| \\ &\qquad + \frac{1}{r^3}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{l} |\zeta_{j-k}||w_m||w_{l-m}||w_{k-l}'| \\ &\leq \sum_{k=0}^{j} \frac{D_{j+1-k}D_k}{r^{j+1-k}}e^{-r/2} + \frac{D_{j+1-k}D_k}{r^{j+2-k}}e^{-r/2} + \sum_{k=0}^{j} \frac{D_{j-k}D_k}{r^{j+3-k}}e^{-r/2} \\ &\qquad + \sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{l} \frac{D_{j-k}D_m D_{l-m} D_{k-l}}{r^{j+3-k}}e^{-3r/2} \ ,\end{aligned} \tag{1.4.42}$$

which we can write as

$$|f_{j+1}(r)| \leq E_{j+1}e^{-r/2} \tag{1.4.43}$$

for some constant E_{j+1}. Now the exact same argument that led to the bound on $|w_1 e^{r/2}|$ will work also for w_{j+1}, w_{j+1}'. Then the induction hypothesis (1.4.40) is proven for $k = j+1$. □

Remark 1.4.3. The proof above does not attempt to keep track of the growth in j of the constants C_j, D_j, E_j, which is necessary before we can prove convergence. The rest of this section will deal with this.

Remark 1.4.4. In section 1.6, we will actually need to know the exact expressions for w_1, w_1', and not just estimates for their absolute values. So we provide them here. They are written in terms of the following non-elementary function, called the *exponential integral*:

$$\mathrm{Ei}(-r) := \int_r^\infty \frac{e^{-s}}{s}\mathrm{d}s \quad , \quad r > 0 \tag{1.4.44}$$

(the minus sign in the argument is the most common convention for this function). Note its exponential decay as $r \to \infty$:

$$\mathrm{Ei}(-r) < \frac{1}{r}\int_r^\infty e^{-s}\mathrm{d}s = \frac{e^{-r}}{r} \ . \tag{1.4.45}$$

Computing w_1, w_1' using the f_1 formula gives:

$$\begin{aligned} w_1(r) = &-\frac{5}{6}e^{-r} + 2e^{-3r} + \frac{1}{3}\Big(2\mathrm{Ei}(-2r) - 9\mathrm{Ei}(-4r)\Big)(r-1)e^r - 2\mathrm{Ei}(-2r)(r+1)e^{-r} \\ &+ \left[\frac{1}{12}\left(\frac{1}{r_0} + \frac{3}{r_0^2} - \frac{4}{r_0^3}\right) + \frac{1}{2}\left(-\frac{3}{r_0} + \frac{1}{r_0^3}\right)e^{-2r_0} + 2\mathrm{Ei}(-2r_0)\right](r-1)e^{-r} \\ &+ \mu\left[\mathrm{Ei}(-2r)(r-1)e^r + \left(-\frac{1}{r_0} + \frac{1}{r_0^2} - \log\left(\frac{r}{r_0}\right)\right)(r+1)e^{-r}\right] + \frac{\alpha}{2}(r+1)e^{-r} \end{aligned} \tag{1.4.46}$$

$$w_1'(r) = \frac{1}{6}\left(1+\frac{4}{r}\right)e^{-r} - \left(1+\frac{1}{r}\right)e^{-3r} + 2\mathrm{Ei}(-2r)re^{-r} + \frac{1}{3}\Big(2\mathrm{Ei}(-2r) - 9\mathrm{Ei}(-4r)\Big)re^{r}$$
$$+\left[\frac{1}{12}\left(-\frac{1}{r_0} - \frac{3}{r_0^2} + \frac{4}{r_0^3}\right) - 2\mathrm{Ei}(-2r_0) + \frac{1}{2}\left(\frac{3}{r_0} - \frac{1}{r_0^2}\right)e^{-2r_0}\right]re^{-r}$$
$$+\mu\left[-2e^{-r} + \left(\frac{1}{r_0} - \frac{1}{r_0^2}\right)re^{-r} + \mathrm{Ei}(-2r)re^{r} + re^{-r}\log\left(\frac{r}{r_0}\right)\right] - \frac{\alpha}{2}re^{-r} \quad (1.4.47)$$

In particular, when evaluated at $r = r_0$, we have:

$$w_1(r_0) = \frac{1}{12}\left(-9 + \frac{4}{r_0} - \frac{1}{r_0^2} - \frac{4}{r_0^3}\right)e^{-r_0} + \frac{1}{2}\left(1 - \frac{3}{r_0} + \frac{1}{r_0^2} + \frac{1}{r_0^3}\right)e^{-3r_0}$$
$$+\frac{1}{3}\Big(2\mathrm{Ei}(-2r_0) - 9\mathrm{Ei}(-4r_0)\Big)(r_0-1)e^{r_0} + \mu\left[\left(-1+\frac{1}{r_0^2}\right)e^{-r_0} + \mathrm{Ei}(-2r_0)(r_0-1)e^{r_0}\right] + \frac{\alpha}{2}(1+r_0)e^{-r_0}$$
$$(1.4.48)$$

$$w_1'(r_0) = \frac{1}{12}\left(1 + \frac{5}{r_0} + \frac{4}{r_0^2}\right)e^{-r_0} + \frac{1}{2}\left(1 - \frac{2}{r_0} - \frac{1}{r_0^2}\right)e^{-3r_0}$$
$$+\frac{1}{3}\Big(2\mathrm{Ei}(-2r_0) - 9\mathrm{Ei}(-4r_0)\Big)r_0e^{r_0} + \mu\left[-\left(1+\frac{1}{r_0}\right)e^{-r_0} + \mathrm{Ei}(-2r_0)r_0e^{r_0}\right] - \frac{\alpha}{2}r_0e^{-r_0} \quad (1.4.49)$$

1.4.2 New variables

It will turn out to be the case that, for large r, the metric can be realized as an exponentially small correction to the RWN metric. More precisely:

$$\zeta_\varepsilon(r) = \zeta_{\mathrm{RWN}}(\varepsilon, r) + O(e^{-r/2}) \quad \text{as } r \to \infty \quad (1.4.50)$$

where ζ_{RWN} is the second metric coefficient in the RWN metric (using the same parameter μ), which in our dimensionless variables reads

$$\zeta_{\mathrm{RWN}}(\varepsilon, r) = \left(1 - \frac{2\mu\varepsilon}{r} + \frac{\varepsilon}{r^2}\right)^{-1} . \quad (1.4.51)$$

We remark that, at any fixed $r > 0$, the latter can be written as a power series in ε:

$$\zeta_{\mathrm{RWN}}(\varepsilon, r) = \sum_{j=0}^{\infty} \rho(r)^j \varepsilon^j \quad , \quad \rho(r) := \frac{2\mu}{r} - \frac{1}{r^2} . \quad (1.4.52)$$

with radius of convergence at a fixed r equal to $1/|\rho(r)|$ (which decreases to 0 as $r \to 0^+$, and grows unboundedly with r when $r \geq 1/\mu$, in case $\mu > 0$, or for all $r > 0$, when $\mu \leq 0$). Also note that ζ_{RWN} is well-defined for any $r > 0$ because we are under the assumption that $\varepsilon\mu^2 \leq \varepsilon\mu_*^2 < 1$, which is the necessary and sufficient condition for $1/\zeta_{\mathrm{RWN}}(r) > 0$ for all $r > 0$.

So we consider a new function that measures the deviation from the RWN metric:

$$\eta(r) = \zeta(r) - \zeta_{\mathrm{RWN}}(r) \ . \tag{1.4.53}$$

Define also

$$\eta_j(r) = \zeta_j(r) - [\zeta_{\mathrm{RWN}}(r)]_j = \zeta_j(r) - \rho(r)^j \ . \tag{1.4.54}$$

Remark 1.4.5. Our technique for proving convergence of the power series would not have worked if we attempted to apply it for ζ, and the reason is that $|\zeta(r)|$ becomes much larger than $|w(r)|$ as r increases (the first approaches 1, the second decays exponentially), whereas the technique requires working with functions comparable in size as r increases. The first two coefficients in the η series are found from ζ_0 and ζ_1 given in (1.4.16), (1.4.17):

$$\eta_0(r) \equiv 0 \quad , \quad \eta_1(r) = \left(\frac{1}{r} + \frac{1}{r^2}\right) e^{-2r} \ . \tag{1.4.55}$$

Note their exponential decay as $r \to \infty$. When we compute the recursion satisfied by η_{j+1} for $j \geq 1$, we will see that all terms in it involve the coefficients w_k and/or w_k', as well as η_k, hence all η_j coefficients will decay exponentially with r, just like those of w and w'.

On the other hand, because we explicitly separate out the RWN term from the metric (which does not have a uniform radius of convergence on $(0, \infty)$), our work in this section cannot be extended all the way to $r = 0$. This is why we can only apply it to an interval of the form $[r_0, \infty)$, and later we have to study the system at small r and ensure that the two regimes connect.

We also introduce new functions $u(r), v(r)$ to consider in place of $w(r)$ and $w'(r)$. They are of comparable magnitude to them. The reason for introducing them is simply to make the formulas more compact; there will only be one integral instead of two in their recursion. Define:

$$\begin{aligned} u(r) &= \frac{w(r)}{r} + \left(\frac{1}{r} + \frac{1}{r^2}\right) w'(r) \ , \\ v(r) &= -\frac{w(r)}{r} + \left(\frac{1}{r} - \frac{1}{r^2}\right) w'(r) \ , \end{aligned} \tag{1.4.56}$$

with inverse transformation $(u, v) \mapsto (w, w')$ given by

$$\begin{aligned} w(r) &= \frac{1}{2}\Big((r-1)u(r) - (r+1)v(r)\Big) \ , \\ w'(r) &= \frac{r}{2}(u(r) + v(r)) \ . \end{aligned} \tag{1.4.57}$$

Define also the coefficients $u_j(r)$ and $v_j(r)$ by taking the j-th coefficients of $w(r)$ and $w'(r)$ in (1.4.56) just above.

Remark 1.4.6. We now have 3 power series to consider in place of the original ones:

$$\eta(\varepsilon, r) = \sum_{j=0}^{\infty} \eta_j(r)\varepsilon^j \quad , \quad u(\varepsilon, r) = \sum_{j=0}^{\infty} u_j(r)\varepsilon^j \quad , \quad v(\varepsilon, r) = \sum_{j=0}^{\infty} v_j(r)\varepsilon^j \ . \tag{1.4.58}$$

Proving the convergence of u, v also proves that of w, w' for the same radius at each r, due to (1.4.57). Proving the convergence of η also proves that of ζ, albeit possibly for a smaller radius, since $\zeta - \eta = \zeta_{\mathrm{RWN}}$ has a radius given by $1/|\rho(r)|$ at each $r > 0$. It will turn out that the radius that we will end up obtaining for η, u, v will be much smaller than $1/|\rho(r)|$ when r_0 is small, hence it will also be the one that works for ζ, w.

Before writing the recursion for η_j, u_j, v_j, we state:

Lemma 1.4.7. *Let $\rho(r)$ be defined as in (1.4.52). Then, for all $r > 0$ and $j \geq 0$,*

$$\frac{1}{r}\int_r^{\infty} \left(j\rho(s)^{j+1} - \frac{(j+1)\rho(s)^j}{s^2} \right) \mathrm{d}s = \rho(r)^{j+1} \ . \tag{1.4.59}$$

Proof. Consider the expressions

$$G_1(r) = \int_r^{\infty} \left(j\rho(s)^{j+1} - \frac{(j+1)\rho(s)^j}{s^2} \right) \mathrm{d}s \quad , \quad G_2(r) = r\rho(r)^{j+1} \ . \tag{1.4.60}$$

Both have a limit of 0 as $r \to \infty$; hence, if we show that $G_1' \equiv G_2'$, we will have proven that $G_1 \equiv G_2$, as the lemma states. Simply compute:

$$G_1'(r) = -j\rho(r)^{j+1} + \frac{(j+1)\rho(r)^j}{r^2} = \rho(r)^j \left(-j\left(\frac{2\mu}{r} - \frac{1}{r^2} \right) + \frac{j+1}{r^2} \right) = \rho(r)^j \left(-\frac{2j\mu}{r} + \frac{2j+1}{r^2} \right) \tag{1.4.61}$$

and

$$\begin{aligned} G_2'(r) &= \rho(r)^{j+1} + (j+1)r\rho(r)^j \left(-\frac{2\mu}{r^2} + \frac{2}{r^3} \right) \\ &= \rho(r)^j \left(\frac{2\mu}{r} - \frac{1}{r^2} - \frac{2(j+1)\mu}{r} + \frac{2(j+1)}{r^2} \right) = \rho(r)^j \left(-\frac{2j\mu}{r} + \frac{2j+1}{r^2} \right) \ . \end{aligned} \tag{1.4.62}$$

$\square$

Now we're ready to find the formula for η_{j+1}, $j \geq 1$, using the one for ζ_{j+1} (1.4.18), which reads:

$$\begin{aligned}\rho(r)^{j+1} + \eta_{j+1} &= \frac{1}{r}\int_r^\infty \left(\sum_{k=1}^{j} \zeta_k \zeta_{j+1-k} + \frac{[-\zeta^2 + \zeta^2 w^2 + \zeta (w')^2]_j}{s^2}\right) \mathrm{d}s \\ &= \frac{1}{r}\int_r^\infty \Bigg(\sum_{k=1}^{j} \zeta_k \zeta_{j+1-k} - \frac{1}{s^2}\sum_{k=0}^{j} \zeta_k \zeta_{j-k} + \frac{1}{s^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} \zeta_l \zeta_{k-l} w_m w_{j-k-m} \\ &\qquad + \frac{1}{s^2}\sum_{k=0}^{j}\sum_{m=0}^{j-k} \zeta_k w'_m w'_{j-k-m}\Bigg) \mathrm{d}s \ . \end{aligned} \tag{1.4.63}$$

Look at the ζ_* factors appearing in each of the 4 sums in this integral: the first 3 involve two of them, the 4$^{\text{th}}$ only one of them. Replace each ζ_* with $\rho^* + \eta_*$ and multiply out: each of the first 3 sums will become a sum of 3 terms (the first containing $\rho^*\rho^*$, the second $2\rho^*\eta_*$, and the third $\eta_*\eta_*$), while the last sum will become a sum of 2 terms (one containing ρ^k, the other η_k), for a total of 11 terms. Now look specifically at the 2 that contain only powers of ρ, and no η_*, w_*, w'_* terms:

$$\frac{1}{r}\int_r^\infty \left(\sum_{k=1}^{j} \rho^k \rho^{j+1-k} - \frac{1}{s^2}\sum_{k=0}^{j} \rho^k \rho^{j-k} + \cdots\right) \mathrm{d}s = \frac{1}{r}\int_r^\infty \left(j\rho^{j+1} - \frac{(j+1)\rho^j}{s^2} + \cdots\right) \mathrm{d}s \ . \tag{1.4.64}$$

Due to lemma 1.4.7, this produces precisely $\rho(r)^{j+1}$, a term already present on the left side of (1.4.63). We subtract this term from both sides to get the recursion for η_{j+1}. It contains a total of 9 sums inside the integral on the right side. Finally, rewrite all w_*, w'_* in these sums in terms of u_*, v_* by using (1.4.57). We obtain:

$$\eta_{j+1}(r) = \frac{1}{r}\int_r^\infty \sum_{i=1}^{9} H_i(s)\mathrm{d}s \quad , \quad j \geq 0 \ , \tag{1.4.65}$$

where

$$H_1 = 2\sum_{k=1}^{j} \rho^{j+1-k}\eta_k \ , \ H_2 = \sum_{k=1}^{j} \eta_k \eta_{j+1-k} \ , \ H_3 = -\frac{2}{r^2}\sum_{k=0}^{j} \rho^{j-k}\eta_k \ , \ H_4 = -\frac{1}{r^2}\sum_{k=0}^{j} \eta_k \eta_{j-k} \ , \tag{1.4.66}$$

$$H_5 = \frac{1}{r^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} \rho^{k-l}\rho^l \frac{(r-1)u_m - (r+1)v_m}{2} \frac{(r-1)u_{j-k-m} - (r+1)v_{j-k-m}}{2} \ , \tag{1.4.67}$$

$$H_6 = \frac{2}{r^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} \rho^{k-l}\eta_l \frac{(r-1)u_m - (r+1)v_m}{2} \frac{(r-1)u_{j-k-m} - (r+1)v_{j-k-m}}{2} \ , \tag{1.4.68}$$

$$H_7 = \frac{1}{r^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} \eta_l \eta_{k-l} \frac{(r-1)u_m - (r+1)v_m}{2} \frac{(r-1)u_{j-k-m} - (r+1)v_{j-k-m}}{2} \ , \tag{1.4.69}$$

$$H_8 = \frac{1}{r^2}\sum_{k=0}^{j}\sum_{m=0}^{j-k}\rho^k \frac{ru_m + rv_m}{2}\frac{ru_{j-k-m}+rv_{j-k-m}}{2} = \sum_{k=0}^{j}\sum_{m=0}^{j-k}\rho^k \frac{u_m + v_m}{2}\frac{u_{j-k-m}+v_{j-k-m}}{2} \ , \tag{1.4.70}$$

$$H_9 = \frac{1}{r^2}\sum_{k=0}^{j}\sum_{m=0}^{j-k}\eta_k \frac{ru_m + rv_m}{2}\frac{ru_{j-k-m}+rv_{j-k-m}}{2} = \sum_{k=0}^{j}\sum_{m=0}^{j-k}\eta_k \frac{u_m + v_m}{2}\frac{u_{j-k-m}+v_{j-k-m}}{2} \ . \tag{1.4.71}$$

(all $H_i, \rho^k, \eta_k, u_k, v_k$ applied to r).

Next we turn to the recursion for u and v. Simply apply the map (1.4.57) to the formulas for all terms w_j, w_j':

$$u_0(r) \equiv 0 \quad , \quad v_0(r) = -2e^{-r} \ ; \tag{1.4.72}$$

$$\begin{aligned} u_1(r) &= -e^r \int_r^\infty \left(\frac{1}{s} + \frac{1}{s^2}\right) e^{-s} f_1(s)\mathrm{d}s \ , \\ v_1(r) &= -\alpha e^{-r} + e^{-r}\int_{r_0}^{r}\left(\frac{1}{s} - \frac{1}{s^2}\right) e^{s} f_1(s)\mathrm{d}s \ ; \end{aligned} \tag{1.4.73}$$

and, for $j > 0$,

$$\begin{aligned} u_{j+1}(r) &= -e^r \int_r^\infty \left(\frac{1}{s} + \frac{1}{s^2}\right) e^{-s} f_{j+1}(s)\mathrm{d}s \ , \\ v_{j+1}(r) &= e^{-r}\int_{r_0}^{r}\left(\frac{1}{s} - \frac{1}{s^2}\right) e^{s} f_{j+1}(s)\mathrm{d}s \ . \end{aligned} \tag{1.4.74}$$

But here the recursion for the f_j terms should be rewritten using the η_k, u_k, v_k variables. We expand the f_{j+1} formula (1.4.19) by writing all ζ_* as $\rho^* + \eta_*$ and all w_*, w_*' in terms of u_*, v_*. There are no simplifications like the one above which used lemma 1.4.7. The result is

$$f_{j+1}(r) = \sum_{i=1}^{6} F_i(r) \quad , \quad j \geq 0 \ , \tag{1.4.75}$$

with

$$F_1 = \sum_{k=1}^{j+1}\rho^k \frac{(r-2)u_{j+1-k} - (r+2)v_{j+1-k}}{2} \quad , \quad F_2 = \sum_{k=1}^{j+1}\eta_k \frac{(r-2)u_{j+1-k} - (r+2)v_{j+1-k}}{2} \ , \tag{1.4.76}$$

$$F_3 = \frac{1}{r^2}\sum_{k=0}^{j}\rho^{j-k}\frac{u_k + v_k}{2} \quad , \quad F_4 = \frac{1}{r^2}\sum_{k=0}^{j}\eta_{j-k}\frac{u_k + v_k}{2} \ , \tag{1.4.77}$$

$$F_5 = -\frac{1}{r^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l}\rho^{j-k}\frac{u_l + v_l}{2}\frac{(r-1)u_m - (r+1)v_m}{2}\frac{(r-1)u_{k-l-m} - (r+1)v_{k-l-m}}{2} \ , \tag{1.4.78}$$

$$F_6 = -\frac{1}{r^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l}\eta_{j-k}\frac{u_l + v_l}{2}\frac{(r-1)u_m - (r+1)v_m}{2}\frac{(r-1)u_{k-l-m} - (r+1)v_{k-l-m}}{2} \ . \tag{1.4.79}$$

This concludes the definition of the new power series to be considered in what follows in this section.

1.4.3 Estimates and separation of r and j

Here we will find useful estimates for $|\eta_j|, |u_j|, |v_j|$, working the cases $j = 0, 1$ separately and the rest by induction. We assume that $r_0 > 0$, $\mu, \alpha \in \mathbb{R}$ have been fixed, as in proposition 1.4.2, and that we are restricted to $r \geq r_0$.

For our purposes in this subsection, it will be necessary to bound the 1^{st}-degree coefficients $|\eta_1(r)|$, $|u_1(r)|$, $|v_1(r)|$ by multiples of $e^{-r/2}$. Let's compute these multiples now. First,

$$|\eta_1(r)| = \left(\frac{1}{r} + \frac{1}{r^2}\right) e^{-2r} < \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) e^{-r/2} = \frac{1 + r_0}{r_0^2} e^{-r/2} \ , \tag{1.4.80}$$

Next, from the expression (1.4.17) for f_1, we have:

$$\begin{aligned} |f_1(r)| &\leq \left|2\mu + \frac{4\mu - 1}{r} - \frac{2}{r^2}\right| e^{-r} + \left(2 + \frac{5}{r} + \frac{3}{r^2}\right) e^{-3r} \\ &\leq \left(\left(2 + \frac{4}{r_0}\right)|\mu| + \frac{1}{r_0} + \frac{2}{r_0^2} + \left(2 + \frac{5}{r_0} + \frac{3}{r_0^2}\right) e^{-2r_0}\right) e^{-r} \\ &< \left(\left(2 + \frac{4}{r_0}\right)|\mu| + 2 + \frac{6}{r_0} + \frac{5}{r_0^2}\right) e^{-r} \\ &= \frac{5 + 6r_0 + 2r_0^2 + (4r_0 + 2r_0^2)|\mu|}{r_0^2} e^{-r} \ , \end{aligned} \tag{1.4.81}$$

and therefore

$$\begin{aligned} |u_1(r)| &\leq e^r \int_r^\infty e^{-s}\left(\frac{1}{s} + \frac{1}{s^2}\right)|f_1(s)|\mathrm{d}s \\ &< \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right)\frac{5 + 6r_0 + 2r_0^2 + (4r_0 + 2r_0^2)|\mu|}{r_0^2} e^r \int_r^\infty e^{-2s}\mathrm{d}s \\ &= \frac{1}{2}\left(\frac{1}{r_0} + \frac{1}{r_0^2}\right)\frac{5 + 6r_0 + 2r_0^2 + (4r_0 + 2r_0^2)|\mu|}{r_0^2} e^{-r} \\ &< \left(\frac{2 + 3r_0 + r_0^2}{r_0^3}|\mu| + \frac{\frac{5}{2} + \frac{11}{2}r_0 + 4r_0^2 + r_0^3}{r_0^4}\right) e^{-r/2} \ , \end{aligned} \tag{1.4.82}$$

and

$$\begin{aligned}
|v_1(r)| &\le e^{-r}\left(|\alpha| + \int_{r_0}^{r} e^s \left|\frac{1}{s} - \frac{1}{s^2}\right| |f_1(s)| \mathrm{d}s\right) \\
&< e^{-r}\left(|\alpha| + \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) \frac{5 + 6r_0 + 2r_0^2 + (4r_0 + 2r_0^2)|\mu|}{r_0^2}(r - r_0)\right) \\
&< |\alpha| e^{-r/2} + \frac{5 + 11r_0 + 8r_0^2 + 2r_0^3 + (4r_0 + 6r_0^2 + 2r_0^3)|\mu|}{r_0^4} r e^{-r} \\
&< \left(|\alpha| + \frac{4 + 6r_0 + 2r_0^2}{r_0^3}|\mu| + \frac{5 + 11r_0 + 8r_0^2 + 2r_0^3}{r_0^4}\right) e^{-r/2} \ ,
\end{aligned} \tag{1.4.83}$$

where we bounded $r - r_0$ by just r and then used the fact that the maximum of the expression $re^{-r/2}$ over the domain $r > 0$ is $2e^{-1} < 1$.

Having found estimates for the 1^{st}-degree coefficients, we turn to estimating the recursive formulas for the coefficients $j+1$, $j \ge 1$.

Estimate each sum H_i in formula (1.4.65) for η_{j+1} by taking absolute values everywhere. We bound the factors $1/r^2$ in front of H_3, H_4 by $1/r_0^2$, the ensuing expression $(r+1)^2/r^2$ in front of H_5, H_6, H_7 by $(r_0+1)^2/r_0^2$, and the overall factor of $1/r$ outside the integral by $1/r_0$. Hence:

$$|\eta_{j+1}(r)| \le \frac{1}{r_0} \int_r^\infty \sum_{i=1}^{9} \tilde{H}_i(s) \mathrm{d}s \quad , \quad j \ge 1 \ , \tag{1.4.84}$$

where

$$|H_1(r)| \le 2\sum_{k=1}^{j} |\rho(r)|^{j+1-k} |\eta_k(r)| =: \tilde{H}_1(r) \quad , \quad |H_2(r)| \le \sum_{k=1}^{j} |\eta_k(r)||\eta_{j+1-k}(r)| =: \tilde{H}_2(r) \ , \tag{1.4.85}$$

$$|H_3(r)| \le \frac{2}{r_0^2} \sum_{k=0}^{j} |\rho(r)|^{j-k} |\eta_k(r)| =: \tilde{H}_3(r) \quad , \quad |H_4(r)| \le \frac{1}{r_0^2} \sum_{k=0}^{j} |\eta_k(r)||\eta_{j-k}(r)| =: \tilde{H}_4(r) \ , \tag{1.4.86}$$

$$|H_5(r)| \le \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{j-k} |\rho(r)|^{k-m} |\rho(r)|^m \frac{|u_l(r)| + |v_l(r)|}{2} \frac{|u_{j-k-l}(r)| + |v_{j-k-l}(r)|}{2} =: \tilde{H}_5(r) \ , \tag{1.4.87}$$

$$|H_6(r)| \le \frac{2(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{j-k} |\rho(r)|^{k-m} |\eta_m(r)| \frac{|u_l(r)| + |v_l(r)|}{2} \frac{|u_{j-k-l}(r)| + |v_{j-k-l}(r)|}{2} =: \tilde{H}_6(r) \ , \tag{1.4.88}$$

$$|H_7(r)| \le \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{j-k} |\eta_m(r)||\eta_{k-m}(r)| \frac{|u_l(r)| + |v_l(r)|}{2} \frac{|u_{j-k-l}(r)| + |v_{j-k-l}(r)|}{2} =: \tilde{H}_7(r) \ , \tag{1.4.89}$$

$$|H_8(r)| \leq \sum_{k=0}^{j}\sum_{m=0}^{j-k} |\rho(r)|^k \frac{|u_m(r)|+|v_m(r)|}{2}\frac{|u_{j-k-m}(r)|+|v_{j-k-m}(r)|}{2} =: \tilde{H}_8(r) \ , \tag{1.4.90}$$

$$|H_9(r)| \leq \sum_{k=0}^{j}\sum_{m=0}^{j-k} |\eta_k(r)| \frac{|u_m(r)|+|v_m(r)|}{2}\frac{|u_{j-k-m}(r)|+|v_{j-k-m}(r)|}{2} =: \tilde{H}_9(r) \ . \tag{1.4.91}$$

Do the same for the F_i's in formula (1.4.75):

$$|f_{j+1}(r)| \leq \sum_{i=1}^{6} \tilde{F}_i(r) \ , \tag{1.4.92}$$

where

$$|F_1(r)| \leq (r_0+2)\sum_{k=1}^{j+1} |\rho(r)|^k \frac{|u_{j+1-k}(r)|+|v_{j+1-k}(r)|}{2} =: \tilde{F}_1(r) \ , \tag{1.4.93}$$

$$|F_2(r)| \leq (r_0+2)\sum_{k=1}^{j+1} |\eta_k(r)| \frac{|u_{j+1-k}(r)|+|v_{j+1-k}(r)|}{2} =: \tilde{F}_2(r) \ , \tag{1.4.94}$$

$$|F_3(r)| \leq \frac{1}{r_0^2}\sum_{k=0}^{j} |\rho(r)|^{j-k} \frac{|u_k(r)|+|v_k(r)|}{2} =: \tilde{F}_3(r) \ , \tag{1.4.95}$$

$$|F_4(r)| \leq \frac{1}{r_0^2}\sum_{k=0}^{j} |\eta_{j-k}(r)| \frac{|u_k(r)|+|v_k(r)|}{2} =: \tilde{F}_4(r) \ , \tag{1.4.96}$$

$$|F_5(r)| \leq \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l} |\rho(r)|^{j-k} \frac{|u_l(r)|+|v_l(r)|}{2}\frac{|u_m(r)|+|v_m(r)|}{2}\frac{|u_{k-l-m}(r)|+|v_{k-l-m}(r)|}{2}$$
$$=: \tilde{F}_5(r) \ , \tag{1.4.97}$$

$$|F_6(r)| \leq \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l} |\eta_{j-k}(r)| \frac{|u_l(r)|+|v_l(r)|}{2}\frac{|u_m(r)|+|v_m(r)|}{2}\frac{|u_{k-l-m}(r)|+|v_{k-l-m}(r)|}{2}$$
$$=: \tilde{F}_6(r) \ . \tag{1.4.98}$$

Plug this inside the integrals for u_{j+1}, v_{j+1}, $j \geq 1$:

$$|u_{j+1}(r)| \leq e^r \int_r^\infty \left(\frac{1}{s}+\frac{1}{s^2}\right) e^{-s}|f_{j+1}(s)|\mathrm{d}s \leq \left(\frac{1}{r_0}+\frac{1}{r_0^2}\right) e^r \int_r^\infty e^{-s}\sum_{i=1}^{6}\tilde{F}_i(s)\mathrm{d}s \ , \tag{1.4.99}$$

and similarly

$$|v_{j+1}(r)| \leq \left(\frac{1}{r_0}+\frac{1}{r_0^2}\right) e^{-r}\int_{r_0}^{r} e^s \sum_{i=1}^{6}\tilde{F}_i(s)\mathrm{d}s \ . \tag{1.4.100}$$

Our next step is to define scalar sequences $(A_j), (B_j)$ quantifying how $|\eta_j(r)|, |u_j(r)|, |v_j(r)|$ compare to $e^{-r/2}$ (see inequalities (1.4.101) below, which we like to think of as a form of *separation* *of variables* r and j). Then it will be the rate of growth of these coefficients that will determine the radius of convergence for the series for η, u, v, while the fact that $e^{-r/2}$ is uniformly bounded over $[r_0, \infty)$ will permit us to estimate the radius uniformly over this interval.

Proposition 1.4.8. *There exist sequences* $(A_j), (B_j)$ *of nonnegative numbers such that, for all* $j \geq 0$ *and* $r \geq r_0$,

$$|\eta_j(r)| \leq A_j e^{-r/2} \quad , \quad |u_j(r)|, |v_j(r)| \leq B_j e^{-r/2} \ , \tag{1.4.101}$$

and they can be defined recursively, together with an auxiliary sequence (C_j), *as follows:*

$$\begin{cases} A_0 = 0 \\ B_0 = 2 \\ C_0 = 1 \end{cases} , \quad \begin{cases} A_1 = \dfrac{1+r_0}{r_0^2} \\ B_1 = |\alpha| + \dfrac{4+6r_0+2r_0^2}{r_0^3}|\mu| + \dfrac{5+11r_0+8r_0^2+2r_0^3}{r_0^4} \\ C_1 = \dfrac{2|\mu|}{r_0} + \dfrac{1}{r_0^2} \end{cases} \tag{1.4.102}$$

and, for $j \geq 1$,

$$\begin{aligned} A_{j+1} = \frac{1}{r_0}\Bigg(4\sum_{k=1}^{j} A_k C_{j+1-k} + \sum_{k=1}^{j} A_k A_{j+1-k} \\ + \frac{4}{r_0^2}\sum_{k=0}^{j} A_k C_{j-k} + \frac{1}{r_0^2}\sum_{k=0}^{j} A_k A_{j-k} \\ + \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} C_m C_{k-m} B_l B_{j-k-l} + \frac{4(r_0+1)^2}{3r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} A_m C_{k-m} B_l B_{j-k-l} \\ + \frac{(r_0+1)^2}{2r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} A_m A_{k-m} B_l B_{j-k-l} \\ + \sum_{k=0}^{j}\sum_{m=0}^{j-k} C_k B_m B_{j-k-m} + \frac{2}{3}\sum_{k=0}^{j}\sum_{m=0}^{j-k} A_k B_m B_{j-k-m} \Bigg) \ , \end{aligned} \tag{1.4.103}$$

$$B_{j+1} = \frac{1+r_0}{r_0^2}\Bigg(2(r_0+2)\sum_{k=1}^{j+1} C_k B_{j+1-k} + (r_0+2)\sum_{k=1}^{j+1} A_k B_{j+1-k}$$
$$+ \frac{2}{r_0^2}\sum_{k=0}^{j} C_{j-k}B_k + \frac{1}{r_0^2}\sum_{k=0}^{j} A_{j-k}B_k$$
$$+ \frac{2(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l} C_{j-k}B_l B_m B_{k-l-m} + \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l} A_{j-k}B_l B_m B_{k-l-m}\Bigg) , \tag{1.4.104}$$

$$C_{j+1} = \left(\frac{2|\mu|}{r_0} + \frac{1}{r_0^2}\right) C_j \ . \tag{1.4.105}$$

Proof. The recursion is well-posed since, by inspection, A_{j+1} and C_{j+1} only depend on terms of index at most j, while B_{j+1} depends only on A_{j+1} and C_{j+1} in addition to those. Also note that the recursion for (C_j) is easily solved:

$$C_j = \left(\frac{2|\mu|}{r_0} + \frac{1}{r_0^2}\right)^j \ , \tag{1.4.106}$$

and in particular, for any $k \geq 0$ and $r \geq r_0$,

$$|\rho(r)|^k = \left|\frac{2\mu}{r} - \frac{1}{r^2}\right|^k \leq \left(\frac{2|\mu|}{r_0} + \frac{1}{r_0^2}\right)^k = C_k \ . \tag{1.4.107}$$

But we choose to keep writing C_k in all formulas, instead of its known value (1.4.106), so that later we can apply the same technique to all sums appearing in the recursive formulas for $(A_j), (B_j)$.

The claim (1.4.101) is true for $j = 0$, given that

$$\eta_0 \equiv u_0 \equiv 0 \quad , \quad |v_0(r)| = 2e^{-r} < 2e^{-r/2} \ . \tag{1.4.108}$$

It is also true for $j = 1$, due to the 1^{st}-degree coefficients estimates (1.4.80), (1.4.82), (1.4.83).

Now assume for induction that (1.4.101) are valid for all indices up to some $j \geq 1$. We will estimate the sums $\tilde{H}_i, \tilde{F}_i$ appearing in the formulas (1.4.84), (1.4.99) and (1.4.100) for $\eta_{j+1}, u_{j+1}, v_{j+1}$ by using the induction hypothesis on all factors $|\eta_k|, |u_k|, |v_k|$ in them, and bounding all $|\rho(r)|^k$ by C_k. Note that $|u_k|$ and $|v_k|$ always appear in the form $(|u_k| + |v_k|)/2$, which can be bounded by $B_k e^{-r/2}$. Since each sum involves at least one factor η_k or $(|u_k| + |v_k|)/2$, they will all yield some power of $e^{-s/2}$, to be integrated in s.

For η_{j+1}, we get

$$|\eta_{j+1}(r)| \le \frac{1}{r_0}\int_r^\infty \Bigg(2\sum_{k=1}^{j} A_k C_{j+1-k} e^{-s/2} + \sum_{k=1}^{j} A_k A_{j+1-k} e^{-s}$$
$$+ \frac{2}{r_0^2}\sum_{k=0}^{j} A_k C_{j-k} e^{-s/2} + \frac{1}{r_0^2}\sum_{k=0}^{j} A_k A_{j-k} e^{-s}$$
$$+ \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} C_m C_{k-m} B_l B_{j-k-l} e^{-s} + \frac{2(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} A_m C_{k-m} B_l B_{j-k-l} e^{-3s/2}$$
$$+ \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} A_m A_{k-m} B_l B_{j-k-l} e^{-2s}$$
$$+ \sum_{k=0}^{j}\sum_{m=0}^{j-k} C_k B_m B_{j-k-m} e^{-s} + \sum_{k=0}^{j}\sum_{m=0}^{j-k} A_k B_m B_{j-k-m} e^{-3s/2}\Bigg) \mathrm{d}s\ . \quad (1.4.109)$$

Integrating the exponentials e^{-as} (where $a = 1/2, 1, 3/2$ or 2) yields e^{-ar}/a, which does not exceed $e^{-r/2}/a$. Therefore,

$$|\eta_{j+1}(r)| \le \frac{e^{-r/2}}{r_0}\Bigg(4\sum_{k=1}^{j} A_k C_{j+1-k} + \sum_{k=1}^{j} A_k A_{j+1-k}$$
$$+ \frac{4}{r_0^2}\sum_{k=0}^{j} A_k C_{j-k} + \frac{1}{r_0^2}\sum_{k=0}^{j} A_k A_{j-k}$$
$$+ \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} C_m C_{k-m} B_l B_{j-k-l} + \frac{4(r_0+1)^2}{3r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} A_m C_{k-m} B_l B_{j-k-l}$$
$$+ \frac{(r_0+1)^2}{2r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} A_m A_{k-m} B_l B_{j-k-l}$$
$$+ \sum_{k=0}^{j}\sum_{m=0}^{j-k} C_k B_m B_{j-k-m} + \frac{2}{3}\sum_{k=0}^{j}\sum_{m=0}^{j-k} A_k B_m B_{j-k-m}\Bigg)\ . \quad (1.4.110)$$

The η_{j+1} bound in (1.4.101) is verified. Proceed similarly with the u_{j+1} formula (1.4.99):

$$|u_{j+1}(r)| \le \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) e^r \int_r^\infty e^{-s}\Bigg((r_0+2)\sum_{k=1}^{j+1} C_k B_{j+1-k} e^{-s/2} + (r_0+2)\sum_{k=1}^{j+1} A_k B_{j+1-k} e^{-s}$$
$$+ \frac{1}{r_0^2}\sum_{k=0}^{j} C_{j-k} B_k e^{-s/2} + \frac{1}{r_0^2}\sum_{k=0}^{j} A_{j-k} B_k e^{-s}$$
$$+\frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l} C_{j-k} B_l B_m B_{k-l-m} e^{-3s/2} + \frac{(r_0+1)^2}{r_0^2}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{k-l} A_{j-k} B_l B_m B_{k-l-m} e^{-2s}\Bigg) \mathrm{d}s\ .$$
$$(1.4.111)$$

Each factor contains an exponential e^{-as} where $a = 3/2, 2, 5/2$ or 3 (observe that there is an overall e^{-s} factor inside the integral). Integrate and then bound the resulting e^{-ar} by $e^{-3r/2}$ in each term, which together with the e^{r} outside makes $e^{-r/2}$. We have then

$$
\begin{aligned}
|u_{j+1}(r)| \leq \frac{1+r_0}{r_0^2} e^{-r/2} \Bigg(& \frac{2(r_0+2)}{3} \sum_{k=1}^{j+1} C_k B_{j+1-k} + \frac{r_0+2}{2} \sum_{k=1}^{j+1} A_k B_{j+1-k} \\
& + \frac{2}{3r_0^2} \sum_{k=0}^{j} C_{j-k} B_k + \frac{1}{2r_0^2} \sum_{k=0}^{j} A_{j-k} B_k \\
& + \frac{2(r_0+1)^2}{5r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} C_{j-k} B_l B_m B_{k-l-m} + \frac{(r_0+1)^2}{3r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} A_{j-k} B_l B_m B_{k-l-m} \Bigg) .
\end{aligned}
\tag{1.4.112}
$$

Each r_0-dependent coefficient in front of the sums in this formula is smaller or equal to the corresponding one in the definition of B_{j+1} given in the proposition statement, so the u_{j+1} bound is proven. Do the same for v_{j+1} from (1.4.100):

$$
\begin{aligned}
|v_{j+1}(r)| \leq \left(\frac{1}{r_0} + \frac{1}{r_0^2} \right) e^{-r} \int_{r_0}^{r} e^{s} \Bigg(& (r_0+2) \sum_{k=1}^{j+1} C_k B_{j+1-k} e^{-s/2} + (r_0+2) \sum_{k=1}^{j+1} A_k B_{j+1-k} e^{-s} \\
& + \frac{1}{r_0^2} \sum_{k=0}^{j} C_{j-k} B_k e^{-s/2} + \frac{1}{r_0^2} \sum_{k=0}^{j} A_{j-k} B_k e^{-s} \\
+ \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} C_{j-k} B_l B_m B_{k-l-m} e^{-3s/2} & + \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} A_{j-k} B_l B_m B_{k-l-m} e^{-2s} \Bigg) \mathrm{d}s .
\end{aligned}
\tag{1.4.113}
$$

Upon integrating:

$$
\begin{aligned}
|v_{j+1}(r)| \leq \left(\frac{1}{r_0} + \frac{1}{r_0^2} \right) e^{-r} \Bigg(& 2(r_0+2) \sum_{k=1}^{j+1} C_k B_{j+1-k} (e^{r/2} - e^{r_0/2}) + (r_0+2) \sum_{k=1}^{j+1} A_k B_{j+1-k} (r - r_0) \\
& + \frac{2}{r_0^2} \sum_{k=0}^{j} C_{j-k} B_k (e^{r/2} - e^{r_0/2}) + \frac{1}{r_0^2} \sum_{k=0}^{j} A_{j-k} B_k (r - r_0) \\
& + \frac{2(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} C_{j-k} B_l B_m B_{k-l-m} (e^{-r_0/2} - e^{-r/2}) \\
& + \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} A_{j-k} B_l B_m B_{k-l-m} (e^{-r_0} - e^{-r}) \Bigg) .
\end{aligned}
\tag{1.4.114}
$$

Keep only the positive term from each of the expressions $(e^{r/2} - e^{r_0/2})$, $(r - r_0)$, $(e^{-r_0/2} - e^{-r/2})$

and $(e^{-r_0} - e^{-r})$, then bound the last two by 1 and distribute the overall factor e^{-r}:

$$\begin{aligned}|v_{j+1}(r)| \leq \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) \Bigg(& 2(r_0+2) \sum_{k=1}^{j+1} C_k B_{j+1-k} e^{-r/2} + (r_0+2) \sum_{k=1}^{j+1} A_k B_{j+1-k} r e^{-r} \\ & + \frac{2}{r_0^2} \sum_{k=0}^{j} C_{j-k} B_k e^{-r/2} + \frac{1}{r_0^2} \sum_{k=0}^{j} A_{j-k} B_k r e^{-r} \\ & + \frac{2(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} C_{j-k} B_l B_m B_{k-l-m} e^{-r} \\ & + \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} A_{j-k} B_l B_m B_{k-l-m} e^{-r} \Bigg) . \qquad (1.4.115)\end{aligned}$$

Now keep only a factor of $e^{-r/2}$ from the last two terms, and (just like when we estimated $|v_1|$) use $re^{-r} \leq e^{-r/2}$ where re^{-r} appears:

$$\begin{aligned}|v_{j+1}(r)| \leq \frac{1+r_0}{r_0^2} e^{-r/2} \Bigg(& 2(r_0+2) \sum_{k=1}^{j+1} C_k B_{j+1-k} + (r_0+2) \sum_{k=1}^{j+1} A_k B_{j+1-k} \\ & + \frac{2}{r_0^2} \sum_{k=0}^{j} C_{j-k} B_k + \frac{1}{r_0^2} \sum_{k=0}^{j} A_{j-k} B_k \\ & + \frac{2(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} C_{j-k} B_l B_m B_{k-l-m} + \frac{(r_0+1)^2}{r_0^2} \sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{k-l} A_{j-k} B_l B_m B_{k-l-m} \Bigg) .\end{aligned}$$

$$(1.4.116)$$

This proves the v_{j+1} bound. □

Remark 1.4.9. As we noted, the formula for B_{j+1} includes the terms A_{j+1} and C_{j+1}. If we plug the recursive formulas for these two terms into the places where they appear in the B_{j+1} formula (the first two sums), we obtain an expression for B_{j+1} involving only indices at most equal to j:

$$\begin{aligned}B_{j+1} = \frac{1+r_0}{r_0^2} \Bigg[& 2(r_0+2) B_0 C_{j+1} + (r_0+2) B_0 A_{j+1} \\ & + 2(r_0+2) \sum_{k=1}^{j} C_k B_{j+1-k} + (r_0+2) \sum_{k=1}^{j} A_k B_{j+1-k} + \cdots \Bigg] \qquad (1.4.117)\end{aligned}$$

We don't attempt to fully write it down. It is just a polynomial recursion involving A, B, C coefficients, but soon we will bound all A, C coefficients using B coefficients and the formula will get shortened.

1.4.4 Sub-exponential growth of the coefficients

Having separated r and j in our estimates for the series coefficients, our next step (the most technical, and the one where a novel technique appears) will be to prove that

$$\limsup_{j\to\infty} A_j^{1/j} < \infty \quad , \quad \limsup_{j\to\infty} B_j^{1/j} < \infty \ , \tag{1.4.118}$$

which we refer to as $(A_j), (B_j)$ having **sub-exponential growth**. Once this is established, the bounds (1.4.101) proven in proposition 1.4.8 yield a positive lower bound for the radius of convergence of the η, u, v series. For example, for any given $r \geq r_0$, the radius of convergence of $\sum_{j=0}^{\infty} \eta_j(r)\varepsilon^j$ will be the inverse of

$$\limsup_{j\to\infty} |\eta_j(r)|^{1/j} \leq \lim_{j\to\infty} (A_j e^{-r/2})^{1/j} = \lim_{j\to\infty} A_j^{1/j} < \infty \ , \tag{1.4.119}$$

that is, it will be at least some positive number, independent of $r \in [r_0, \infty)$.

Remark 1.4.10. Some words about our technique are in order now. The recursion formulas (1.4.103) and (1.4.104) make it clear that A_j, B_j are polynomial expressions, with coefficients depending on r_0, of the initial terms A_0, A_1, B_0, B_1, and it is not difficult to prove that the degree of these polynomials is at most $4j$. But knowing this is still far from being able to establish something like (1.4.118), which would require us to also control the growth of the coefficients of the polynomials. Our technique will pursue a different path, which we now briefly explain.

If (1.4.118) is to be true, there must exist positive numbers R, S such that, for all $j \geq 0$,

$$A_j, B_j \leq SR^j. \tag{1.4.120}$$

But trying to establish an inequality like this by induction proves to be a problem: when using the induction hypothesis on each term in the sums appearing in the recursive definition of A_{j+1} and B_{j+1}, the several resulting powers of R^k combine to produce R^j or R^{j+1}, as needed, but they leave behind sums that make quadratic, cubic or quartic expressions of j. For example:

$$\sum_{k=0}^{j}\sum_{m=0}^{j-k} A_k B_m B_{j-k-m} \leq \sum_{k=0}^{j}\sum_{m=0}^{j-k} SR^k SR^m SR^{j-k-m} = S^3 R^j \sum_{k=0}^{j}\sum_{m=0}^{j-k} 1 \approx SR^{j+1}\frac{S^2}{R} j^3 \ . \tag{1.4.121}$$

It becomes impossible to bound this by a uniform constant times SR^{j+1} as j increases.

Our technique deals with this issue by instead trying to establish an inequality of the form

$$A_j, B_j \leq \frac{SR^j}{(j+\delta)^2} \tag{1.4.122}$$

for some $R, S, \delta > 0$. Such an inequality is also equivalent to (1.4.118), since the quadratic expression in j in the denominator can always be absorbed into the exponential R^j when j grows. However, this form is better suited for an induction proof because, as it turns out, the convolutional sums analogous to (1.4.121) that are produced by the induction hypothesis can be bounded by something which also includes a similar quadratic term in j in the denominator, as is needed to complete the induction. This is due to the next lemma.

Lemma 1.4.11. *For all $\delta_1, \delta_2 > 0$, we have*

$$\sum_{k=0}^{j} \frac{1}{(k+\delta_1)^2(j-k+\delta_2)^2} \le \frac{8+2\left(\dfrac{1}{\delta_1}+\dfrac{1}{\delta_2}\right)^2}{(j+\delta_1+\delta_2)^2} \quad , \quad j \ge 0 \tag{1.4.123}$$

and

$$\sum_{k=1}^{j-1} \frac{1}{(k+\delta_1)^2(j-k+\delta_2)^2} \le \frac{8}{(j+\delta_1+\delta_2)^2} \quad , \quad j \ge 2\ . \tag{1.4.124}$$

Proof. By partial fractions in the variable k:

$$\frac{1}{(k+\delta_1)^2(j-k+\delta_2)^2} = \frac{1}{(j+\delta_1+\delta_2)^2}\left(\frac{2/(j+\delta_1+\delta_2)}{k+\delta_1} + \frac{1}{(k+\delta_1)^2} + \frac{2/(j+\delta_1+\delta_2)}{j-k+\delta_2} + \frac{1}{(j-k+\delta_2)^2}\right)\ . \tag{1.4.125}$$

First we will establish (1.4.124). When summing (1.4.125) over $k = 1, \ldots, j-1$, the terms including $j-k$ in the denominator can be rewritten with k, since $j-k$ and k both sweep the same range in the sum:

$$\sum_{k=1}^{j-1} \frac{1}{(k+\delta_1)^2(j-k+\delta_2)^2} = \frac{1}{(j+\delta_1+\delta_2)^2}\sum_{k=1}^{j-1}\left(\frac{2/(j+\delta_1+\delta_2)}{k+\delta_1} + \frac{1}{(k+\delta_1)^2} + \frac{2/(j+\delta_1+\delta_2)}{k+\delta_2} + \frac{1}{(k+\delta_2)^2}\right)\ . \tag{1.4.126}$$

Now distribute the sum and get rid of any δ's in the denominators inside parenthesis:

$$\sum_{k=1}^{j-1} \frac{1}{(k+\delta_1)^2(j-k+\delta_2)^2} < \frac{1}{(j+\delta_1+\delta_2)^2}\left(\frac{4}{j}\sum_{k=1}^{j-1}\frac{1}{k} + 2\sum_{k=1}^{j-1}\frac{1}{k^2}\right)\ . \tag{1.4.127}$$

The second sum is bounded above by the value $\pi^2/6$ of the infinite p-series ($p = 2$). The first sum can be estimated using an integral:

$$\frac{1}{j}\sum_{k=1}^{j-1}\frac{1}{k} = \frac{1}{j}\left(1+\sum_{k=2}^{j-1}\right) < \frac{1}{j}\left(1+\int_1^{j-1}\frac{\mathrm{d}x}{x}\right) = \frac{1}{j}\left(1+\log(j-1)\right) < \frac{1}{j}(1+j-1) = 1\ , \tag{1.4.128}$$

where we used the fact that $\log(x) < x$ for all $x > 0$. Hence

$$\sum_{k=1}^{j-1} \frac{1}{(k+\delta_1)^2(j-k+\delta_2)^2} < \frac{1}{(j+\delta_1+\delta_2)^2}\left(4+\frac{\pi^2}{3}\right) < \frac{8}{(j+\delta_1+\delta_2)^2} \ . \tag{1.4.129}$$

To prove (1.4.123), we use the bound just proved for $\sum_{k=1}^{j-1}$, and add to it the terms given by (1.4.125) with $k=0$ and $k=j$, which are:

$$\frac{1}{(j+\delta_1+\delta_2)^2}\left(\frac{2}{j+\delta_1+\delta_2}\left(\frac{1}{\delta_1}+\frac{1}{\delta_2}+\frac{1}{j+\delta_1}+\frac{1}{j+\delta_2}\right)+\frac{1}{\delta_1^2}+\frac{1}{\delta_2^2}+\frac{1}{(j+\delta_1)^2}+\frac{1}{(j+\delta_2)^2}\right) \ .$$

Bound the expression in parenthesis above by replacing j with 0 to obtain

$$\frac{4}{\delta_1+\delta_2}\left(\frac{1}{\delta_1}+\frac{1}{\delta_2}\right)+\frac{2}{\delta_1^2}+\frac{2}{\delta_2^2} = \frac{4\delta_1\delta_2+2\delta_2^2+2\delta_1^2}{\delta_1^2\delta_2^2} = 2\left(\frac{\delta_1+\delta_2}{\delta_1\delta_2}\right)^2 = 2\left(\frac{1}{\delta_1}+\frac{1}{\delta_2}\right)^2 \ .$$

This proves the claim. □

Remark 1.4.12. There is nothing special about the power 2 in the denominator in this lemma; a similar result would hold with any power greater than 1, but we chose to work with 2 because the simple proof by partial fractions is available for it.

Now, a tricky aspect of our technique is the fact that the bounds (1.4.122) need to be satisfied for all j, not just j large enough. For proving the sub-exponential growth property (1.4.118), it would of course be enough to have them be satisfied only for large enough j, but the point is that, in order to prove the bounds for some j, we will need to use the bounds themselves inductively — and since the recursion for the $(j+1)^{\text{st}}$ coefficients includes all coefficients A_k, B_k, C_k with $k = 0, \dots, j$, the inequality is needed for all these indices. One could also decide to treat the first few indices in the formulas by a different means, but that would require opening up the sums to separate them out and would be impractical.

This need for the inequality to be satisfied for all indices suggests how to obtain the constants R, S, δ: the value of the zeroth coefficients will dictate the relationship between S and δ, then the value of the first coefficients will impose a δ-dependent lower bound for R, and finally the recursion for $j+1 \geq 2$ will impose a small value for δ to close the induction and in turn determine R.

Theorem 1.4.13. *There exist numbers $R, S, \delta > 0$ such that the sequences $(A_j), (B_j), (C_j)$ of proposition 1.4.2 satisfy*

$$A_j, B_j, C_j \leq \frac{SR^j}{(j+\delta)^2} \quad , \quad j \geq 0 \ . \tag{1.4.130}$$

Furthermore, R, δ, S can be selected as such:

$$R = \frac{240(15 + 4r_0|\mu| + r_0^4|\alpha|)}{r_0^7} \quad , \quad \delta < \frac{1}{\sqrt{48}} \quad , \quad S = 2\delta^2 \ . \tag{1.4.131}$$

Proof. Let $\delta > 0$ (we will specify a value later, in order to also demonstrate how a suitable δ can be found). Define

$$S = B_0\delta^2 = 2\delta^2 \quad , \quad R = \frac{B_1}{B_0}\left(1 + \frac{1}{\delta}\right)^2 = (1+\delta)^2 \frac{|\alpha| + \frac{4+6r_0+2r_0^2}{r_0^3}|\mu| + \frac{5+11r_0+8r_0^2+2r_0^3}{r_0^4}}{2\delta^3} \ . \tag{1.4.132}$$

Observe, for later use, that

$$\frac{1}{R} = \frac{B_0}{B_1}\frac{\delta^2}{(1+\delta)^2} < \frac{B_0}{B_1}\delta^2 \ . \tag{1.4.133}$$

Then (1.4.130) are true for $j = 0, 1$. Indeed, it is enough to verify these only for the (B_j) sequence, since one can see that $\max\{A_j, B_j, C_j\} = B_j$ for $j = 0, 1$; and in this case we actually have equality:

$$\frac{SR^0}{(0+\delta)^2} = \frac{B_0\delta^2}{\delta^2} = B_0 \quad , \quad \frac{SR^1}{(1+\delta)^2} = \frac{B_0\delta^2}{(1+\delta)^2}\frac{B_1}{B_0}\left(1 + \frac{1}{\delta}\right)^2 = B_1 \ . \tag{1.4.134}$$

Now fix $j \geq 1$ and assume for induction that (1.4.130) is true for all indices up to j. We will use the recursive definition of $A_{j+1}, B_{j+1}, C_{j+1}$ to prove it for $j+1$ as well. The giant formula (1.4.117) for B_{j+1} makes it clear that $B_{j+1} \geq A_{j+1}, C_{j+1}$ for all $j \geq 1$, hence we only need to prove the induction hypothesis for B_{j+1}. Since also $B_j \geq A_j, C_j$ for $j = 0, 1$, we can bound every A_* and C_* term in this formula by the corresponding B_* term and group together similar sums:

$$\begin{aligned} B_{j+1} \leq{}& \frac{20 + 36r_0 + 19r_0^2 + 3r_0^3}{r_0^3}\sum_{k=1}^{j} B_k B_{j+1-k} + \left(\frac{16 + 24r_0 + 8r_0^2}{r_0^3}|\mu| \frac{8 + 12r_0 + 4r_0^2}{r_0^4}\right) B_j \\ &+ \frac{20 + 33r_0 + 13r_0^2}{r_0^5}\sum_{k=0}^{j} B_k B_{j-k} + \frac{20 + 30r_0 + 10r_0^2}{3r_0^3}\sum_{k=0}^{j}\sum_{m=0}^{j-k} B_k B_m B_{j-k-m} \\ &+ \frac{34 + 128r_0 + 180r_0^2 + 112r_0^3 + 26r_0^4}{3r_0^5}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} B_m B_{k-m} B_l B_{j-k-l} \ . \end{aligned} \tag{1.4.135}$$

We will now estimate each sum in this expression by first using the induction hypothesis in each B_* and then lemma 1.4.11 in the ensuing sums. Each time we will look for the particular expression $SR^{j+1}/(j+1+\delta)^2$ that is needed to complete the induction.

- In the first sum ($\sum_{k=1}^{j}$), since the index k is never 0 or $j+1$, we can use (1.4.123) with $j+1$ in place of j:

$$\sum_{k=1}^{j} B_k B_{j+1-k} \leq \sum_{k=1}^{j} \frac{SR^k SR^{j+1-k}}{(k+\delta)^2(j+1-k+\delta)^2} \leq \frac{8S^2R^{j+1}}{(j+1+2\delta)^2} < \frac{SR^{j+1}}{(j+1+\delta)^2}16\delta^2 \ , \tag{1.4.136}$$

where we used $S = 2\delta^2$ and bounded 2δ in the denominator by just δ. It was important here to be able to use the part of lemma 1.4.11 that guarantees a δ-uniform constant, 8, instead of one that diverges when δ is small, $8 + 2(2/\delta)^2$. Because of this, we were able to get a bound proportional to δ^2, which, we shall see, will be important.

- In the second term (the one without a summation sign), simply do

$$B_j \leq \frac{SR^j}{(j+\delta)^2} = \frac{SR^{j+1}}{(j+1+\delta)^2}\frac{1}{R}\left(\frac{j+1+\delta}{j+\delta}\right)^2 < \frac{SR^{j+1}}{(j+1+\delta)^2}\frac{4}{R} \ , \tag{1.4.137}$$

where we used the fact that

$$\frac{j+1+\delta}{j+\delta} = 1 + \frac{1}{j+\delta} < 1 + \frac{1}{1+0} = 2 \ . \tag{1.4.138}$$

Note how it is important that $j \geq 1$ for this calculation; if we were to attempt it for $j = 0$ too, there would not be a δ-independent bound when δ is made small. This is part of the reason why we have to consider the $j = 0, 1$ terms separately in this proof and only let the recursion kick off at $j + 1 \geq 2$.

- In the third sum ($\sum_{k=0}^{j}$), proceed similarly to the first, but applying (1.4.124) this time since the summation index k spans the whole $\{0, \ldots, j\}$. Note that the indices of the B terms in this sum add up to only j, meaning they will produce an R^j after the induction hypothesis is applied; so we include an extra $1/R$ and substitute R^j with R^{j+1}:

$$\begin{aligned}\sum_{k=0}^{j} B_k B_{j-k} &\leq \sum_{k=0}^{j} \frac{SR^k SR^{j-k}}{(k+\delta)^2(j-k+\delta)^2} \leq \frac{S^2R^j}{(j+2\delta)^2}\left(8 + 2\left(\frac{1}{\delta}+\frac{1}{\delta}\right)^2\right) \\ &= \frac{S^2R^j}{(j+2\delta)^2}\left(8 + \frac{8}{\delta^2}\right) = \frac{SR^{j+1}}{(j+1+\delta)^2}\frac{2}{R}\left(8\delta^2+8\right)\left(\frac{j+1+\delta}{j+2\delta}\right)^2 < \frac{SR^{j+1}}{(j+1+\delta)^2}\frac{8}{R}\left(8\delta^2+8\right) \ ,\end{aligned} \tag{1.4.139}$$

where we used $S = 2\delta^2$ and also bounded $(j+1+\delta)/(j+2\delta)$ by 2, similarly to what we did for $(j+1+\delta)/(j+\delta)$ above.

- In the double sum term ($\sum_{k=0}^{j} \sum_{m=0}^{j-k}$), after applying the induction hypothesis, we can use the lemma once just in the part whose indices add to $j-k$, then once more together with the other k index:

$$\begin{aligned}\sum_{k=0}^{j}\sum_{m=0}^{j-k} B_k B_m B_{j-k-m} &\leq \sum_{k=0}^{j} \frac{SR^k}{(k+\delta)^2} \sum_{m=0}^{j-k} \frac{SR^m SR^{j-k-m}}{(m+\delta)^2 (j-k-m+\delta)^2} \\ &\leq S^3 R^j \sum_{k=0}^{j} \frac{1}{(k+\delta)^2} \frac{1}{(j-k+2\delta)^2} \left(8+\frac{8}{\delta^2}\right) \leq S^3 R^j \left(8+\frac{8}{\delta^2}\right) \frac{8+2\left(\frac{1}{\delta}+\frac{1}{2\delta}\right)^2}{(j+3\delta)^2} \\ = \frac{S^3 R^{j+1}}{(j+3\delta)^2} \frac{1}{R} \left(8+\frac{8}{\delta^2}\right)\left(8+\frac{9}{2\delta^2}\right) &= \frac{SR^{j+1}}{(j+1+\delta)^2} \frac{4}{R} (8\delta^2+1) \left(8\delta^2+\frac{9}{2}\right) \left(\frac{j+1+\delta}{j+3\delta}\right)^2 \\ &< \frac{SR^{j+1}}{(j+1+\delta)^2} \frac{16}{R} (8\delta^2+1) \left(8\delta^2+\frac{9}{2}\right) . \end{aligned} \tag{1.4.140}$$

- In the triple sum term ($\sum_{k=0}^{j} \sum_{l=0}^{k} \sum_{m=0}^{j-k}$), we need three applications of the lemma:

$$\begin{aligned}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{m=0}^{j-k} B_m B_{k-m} B_l B_{j-k-l} &< S^4 R^j \sum_{k=0}^{j} \frac{8+8/\delta^2}{(k+2\delta)^2} \frac{8+8/\delta^2}{(j-k+2\delta)^2} \\ &\leq \frac{S^4 R^j}{(j+4\delta)^2} \left(8+\frac{8}{\delta^2}\right)^2 \left(8+2\left(\frac{1}{2\delta}+\frac{1}{2\delta}\right)^2\right) \\ = \frac{SR^{j+1}}{(j+1+\delta^2)^2} \frac{8}{R} (8\delta^2+8)^2 (8\delta^2+2) \left(\frac{j+1+\delta}{j+4\delta}\right)^2 &< \frac{SR^{j+1}}{(j+1+\delta^2)^2} \frac{32}{R} (8\delta^2+8)^2 (8\delta^2+2) . \end{aligned} \tag{1.4.141}$$

Putting all of this together, we conclude

$$B_{j+1} \leq \frac{SR^{j+1}}{(j+1+\delta)^2} b_{R,\delta} , \tag{1.4.142}$$

where $b_{R,\delta}$ is given by

$$\begin{aligned} b_{R,\delta} = \frac{20+36r_0+19r_0^2+3r_0^3}{r_0^3} 16\delta^2 + \frac{1}{R}\Bigg[\left(\frac{16+24r_0+8r_0^2}{r_0^3}|\mu| + \frac{8+12r_0+4r_0^2}{r_0^4}\right) 4 \\ + \frac{20+33r_0+13r_0^2}{r_0^5} 8(8\delta^2+8) + \frac{20+30r_0+10r_0^2}{3r_0^3} 16(8\delta^2+1)\left(8\delta^2+\frac{9}{2}\right) \\ + \frac{34+128r_0+180r_0^2+112r_0^3+26r_0^4}{3r_0^5} 32(8\delta^2+8)^2(8\delta^2+2)\Bigg] . \end{aligned} \tag{1.4.143}$$

To complete the induction, we must be able to select $\delta > 0$ making $b_{R,\delta} < 1$. First note that, for any δ, we can use (1.4.133) to bound $1/R$ in terms of δ^2. Then all terms in the above definition of $b_{R,\delta}$ will include a δ^2, which is what we will take advantage of to make it less than 1. Also bringing out a factor B_0/B_1, present in all but the first term, we have:

$$\begin{aligned} b_{R,\delta} < \frac{B_0}{B_1}\delta^2 \Bigg[& \frac{20+36r_0+19r_0^2+3r_0^3}{r_0^3}\frac{16B_1}{B_0} + \left(\frac{16+24r_0+8r_0^2}{r_0^3}|\mu| + \frac{8+12r_0+4r_0^2}{r_0^4}\right)4 \\ & + \frac{20+33r_0+13r_0^2}{r_0^5}8(8\delta^2+8) + \frac{20+30r_0+10r_0^2}{3r_0^3}16(8\delta^2+1)\left(8\delta^2+\frac{9}{2}\right) \\ & + \frac{34+128r_0+180r_0^2+112r_0^3+26r_0^4}{3r_0^5}32(8\delta^2+8)^2(8\delta^2+2)\Bigg] . \end{aligned} \tag{1.4.144}$$

In particular, looking only at the first term, if we want to make $b_{R,\delta} < 1$, then it will be necessary that

$$\frac{B_0}{B_1}\delta^2 < \frac{r_0^3}{20+36r_0+19r_0^2+3r_0^3}\frac{B_0}{16B_1} < \frac{r_0^3}{320}\frac{B_0}{B_1} \quad \Longrightarrow \quad \delta^2 < \frac{r_0^3}{320} . \tag{1.4.145}$$

So assume this a priori and plug it into all instances of δ^2 inside parenthesis in (1.4.144) to obtain an upper bound for $b_{R,\delta}$. It becomes $b_{R,\delta} < (B_0/B_1)\delta^2 b$, where

$$\begin{aligned} b := & \frac{\begin{array}{l} 2400000 + 9600000r_0 + 158728000r_0^2 + 543968000r_0^3 + 747528000r_0^4 + 465071200r_0^5 \\ +117210200r_0^6 + 13875800r_0^7 + 8679840r_0^8 + 2064880r_0^9 + 65000r_0^{10} \\ +40637r_0^{11} + 9524r_0^{12} + 90r_0^{13} + 56r_0^{14} + 13r_0^{15} \end{array}}{3000r_0^7} \\ & + \frac{640+2112r_0+2656r_0^2+1648r_0^3+544r_0^4+80r_0^5}{r_0^6}|\mu| + \frac{160+288r_0+152r_0^2+24r_0^3}{r_0^3}|\alpha| \\ & > \frac{160}{r_0^7}\left(15+4r_0|\mu|+r_0^4|\alpha|\right) \end{aligned} \tag{1.4.146}$$

(the occurrence of $|\mu|$ and $|\alpha|$ here comes from the fraction B_1/B_0 in the first term of (1.4.144), as well as the presence of $|\mu|$ in the second term). Hence, by imposing

$$\delta^2 := \frac{B_1}{B_0}\frac{r_0^7}{160(15+4r_0|\mu|+r_0^4|\alpha|)} , \tag{1.4.147}$$

the a priori bound (1.4.145) holds and $b_{R,\delta} < 1$, closing the induction.

Now plug this into the definition of R:

$$R = \frac{B_1}{B_0}\left(\frac{1+\delta}{\delta}\right)^2 = \frac{160(15+4r_0|\mu|+r_0^4|\alpha|)(1+\delta)^2}{r_0^7} . \tag{1.4.148}$$

Finally, to get rid of δ in the above, note that the first inequality in (1.4.145) implies

$$\delta^2 < \frac{r_0^3}{(20+36r_0+19r_0^2+3r_0^3)16} < \frac{1}{48} . \tag{1.4.149}$$

Then the chosen R satisfies

$$R < \frac{160(15 + 4r_0|\mu| + r_0^4|\alpha|)}{r_0^7}\left(1 + \frac{1}{\sqrt{48}}\right)^2 < \frac{240(15 + 4r_0|\mu| + r_0^4|\alpha|)}{r_0^7} \ . \tag{1.4.150}$$

It is clear that increasing the value of R does not invalidate the theorem, so we might as well replace the chosen R with this exact upper bound, just as the theorem states.

□

Corollary 1.4.14. *The radius of convergence of the η, u and v power series, at any $r \in [r_0, \infty)$, is at least*

$$\frac{1}{R} = \frac{r_0^7}{240(15 + 4r_0|\mu| + r_0^4|\alpha|)} \ . \tag{1.4.151}$$

Proof. This was explained in equation (1.4.119). But now, with the inequalities (1.4.130) proven in the above theorem, we can find an upper bound for the inverse of the radius of convergence at any point, as in (1.4.119), given by

$$\limsup_{j\to\infty} A_j^{1/j} \le \lim_{j\to\infty} \frac{S^{1/j}R}{(j+\delta)^{2/j}} = R \ . \tag{1.4.152}$$

□

Corollary 1.4.15. *For $r_0 < 1$, the radius of convergence of the ζ and w power series, at any $r \in [r_0, \infty)$, is at least*

$$\frac{1}{R} = \frac{r_0^7}{240(15 + 4r_0|\mu| + r_0^4|\alpha|)} \ . \tag{1.4.153}$$

Proof. As noted in remark 1.4.6, the radii for w and w' at any $r \ge r_0$ are the same as for u and v, while the one for $\zeta(r)$ will be $\min\{1/R, 1/|\rho(r)|\}$, where

$$\frac{1}{|\rho(r)|} = \frac{r^2}{|1 - 2\mu r|} \ge \frac{r^2}{1 + 2r|\mu|} \ge \frac{r_0^2}{1 + 2r_0|\mu|} \ . \tag{1.4.154}$$

We see that, when $r_0 < 1$, this minimum also yields $1/R$. □

1.4.5 Remaining details

Assume $0 < r_0 < 1$ and $\mu_*, \alpha_* \in \mathbb{R}$ are fixed. We'll also need to assume that $\varepsilon > 0$ has been chosen such that

$$\varepsilon < \frac{1}{4R} = \frac{r_0^7}{960(15 + 4r_0\mu_* + r_0^4\alpha_*)} \ . \tag{1.4.155}$$

With this ε (actually also with $\varepsilon < 1/R$, however the reason for the $1/4$ factor will become clear soon), the power series for η, u, v, ζ, w are well-defined on $[r_0, \infty)$ for any choice of the parameters $\mu \in [-\mu_*, \mu_*]$ and $\alpha \in [-\alpha_*, \alpha_*]$. In this subsection, when we write η, u, v, ζ, w, we assume that a choice of $\mu \in [-\mu_*, \mu_*]$ and $\alpha \in [-\alpha_*, \alpha_*]$ has been made, and, when we want to study the dependence on the parameters, we will use superscripts like $\zeta^{(\mu,\alpha)}$ etc.

The purpose of this subsection is to verify the following:

1. that the asymptotic conditions (1.4.4), (1.4.5), (1.4.9) for ζ and w are true;
2. that differentiation of the ε-power series for ζ and w term-by-term in the r variable is justified;
3. that $\zeta^{(\mu,\alpha)}, w^{(\mu,\alpha)}$ are continuous with respect to $\mu \in [-\mu_*, \mu_*]$ and $\alpha \in [-\alpha_*, \alpha_*]$;
4. that $\zeta(r) > 0$ on $[r_0, \infty)$;
5. that $\psi = \psi_\varepsilon = \psi^{(\mu,\alpha)}$ can be solved for in the original system (1.1.13) satisfying the conditions $\psi(r) \geq 0$ for $r \in [r_0, \infty)$, $\lim_{r\to\infty} \psi(r) = 1$, $\lim_{\varepsilon\to 0^+} \psi_\varepsilon(r) = 1$ for all $r \geq r_0$, and that $\psi^{(\mu,\alpha)}$ is continuous in the parameters μ and α.

We tackle them one by one in the order presented above:

1. From the inequalities

$$|u_j(r)| \leq \frac{SR^j}{(j+\delta)^2} e^{-r/2} \quad , \quad |v_j(r)| \leq \frac{SR^j}{(j+\delta)^2} e^{-r/2} \tag{1.4.156}$$

(consequence of (1.4.101) and (1.4.130)), we conclude:

$$|u(r)| = \left| \sum_{j=0}^{\infty} u_j(r) \varepsilon^j \right| \leq S e^{-r/2} \sum_{j=0}^{\infty} \frac{(R\varepsilon)^j}{(j+\delta)^2} < S e^{-r/2} \sum_{j=0}^{\infty} (R\varepsilon)^j \tag{1.4.157}$$

and similarly for $v(r)$. The geometric series above is summable because $\varepsilon < \varepsilon_* = 1/R$. So this proves that u and v decay exponentially to 0 as $r \to \infty$. Given the relation (1.4.57) between (w, w') and (u, v), the same is true for w and w', proving (1.4.5).

The same argument can be made for $\eta(r)$. Now, since

$$\zeta(r) = \zeta_{RWN}(r) + \eta(r) = \left(1 - \frac{2\mu\varepsilon}{r} + \frac{\varepsilon}{r^2}\right)^{-1} + \eta(r) \ , \tag{1.4.158}$$

we conclude (1.4.4) and (1.4.9) too.

2. Term-by-term differentiation (in the r variable) of our ε-power series for ζ, w and w' is justified once we can prove that their corresponding series of r-derivatives $\sum_j \zeta_j'(r)\varepsilon^j$ etc. converge uniformly with respect to $r \in [r_0, \infty)$. Uniformity is not an issue, given how each derivative $\zeta_j'(r)$, $w_j'(r)$ and $w_j''(r)$ can be seen (from their definitions in proposition 1.4.2) to depend on r through functions of the form $r^{-k_1}e^{-k_2 r}$ (where $k_1, k_2 \geq 0$), which are uniformly bounded on $[r_0, \infty)$. But pointwise convergence of the r-derivative ε-series must be proved first.

   So fix an $r \in [r_0, \infty)$. We illustrate the idea for the ζ series. Call

$$g_n(\varepsilon) = \sum_{j=0}^{n} \zeta_j(r)\varepsilon^j \quad , \quad g(\varepsilon) = \lim_{n\to\infty} g_n(\varepsilon) \ . \tag{1.4.159}$$

   We already know that $g(\varepsilon)$ is well-defined when $\varepsilon < \varepsilon_*$, and now we'd like to prove that

$$h(\varepsilon) = \lim_{n\to\infty} g_n'(\varepsilon) \tag{1.4.160}$$

   is too. It's clear that the same technique presented in this section can prove that $h(\varepsilon)$ is well-defined when $\varepsilon < \varepsilon_{**}$, for some $\varepsilon_{**} > 0$ that is potentially smaller than ε_* (after all, the polynomial recursion obtained for the derivative series will not be the exact same). Take ε_{**} as large as it can be, and assume for a contradiction that $\varepsilon_{**} < \varepsilon_*$. Standard theorems on systems of ODE's imply that the main differential system (1.1.13) can be solved around our fixed value of r with a solution that is analytic in ε, defined for parameters ε in a small open interval around ε_{**}. We already know how to write the solution as an ε power series for any $\varepsilon < \varepsilon_{**}$ (because differentiation term-by-term is justified for this range); the corresponding ζ is such that $\zeta'(r) = h(\varepsilon)$. But, since this same ζ, as an ε-series, is necessarily still well-defined when ε is a bit past ε_{**}, the uniqueness of power series representations proves that also h is well-defined there, contradicting the maximality of ε_{**}. This proves our claim.

3. Observe that the coefficients $\zeta_1^{(\mu,\alpha)}$ and $w_1^{(\mu,\alpha)}$ introduced in subsection 1.4.1 are linear expressions of μ and α, while every subsequent ζ_{j+1} and w_{j+1} is defined recursively in terms of integrals of polynomial expressions of previous coefficients ζ_k and w_k. This implies that, for each fixed $r \geq r_0$, there exist polynomial expressions

$$P_j(\mu, \alpha) = \sum_{k+l\leq d_j} p_{jkl}\mu^k\alpha^l \quad , \quad Q_j(\mu, \alpha) = \sum_{k+l\leq d_j} q_{jkl}\mu^k\alpha^l \ , \tag{1.4.161}$$

of some finite degree d_j, such that, for each $j \geq 0$ and each $(\mu, \alpha) \in [-\mu_*, \mu_*] \times [-\alpha_*, \alpha_*]$,

$$\zeta_j^{(\mu,\alpha)}(r) = P_j(\mu, \alpha) \quad , \quad w_j^{(\mu,\alpha)}(r) = Q_j(\mu, \alpha) \ . \tag{1.4.162}$$

This implies, for the ζ power series and for this fixed r,

$$\zeta^{(\mu,\alpha)}(r) = \sum_{j=0}^{\infty} \sum_{k+l \leq d_j} p_{jkl} \mu^k \alpha^l \varepsilon^j = \sum_{k+l \leq d_j} \left(\sum_{j=0}^{\infty} p_{jkl} \varepsilon^j \right) \mu^k \alpha^l \ . \tag{1.4.163}$$

This power series of (μ, α) is absolutely convergent, as we proved, for any values of the parameters μ, α in the allowed range, and in particular is a continuous function of them. Proceed similarly for w.

4. Given the expression (1.4.155) for ε, let $\gamma \in (0, 1/4)$ be such that

$$\varepsilon = \frac{\gamma}{R} = \frac{\gamma r_0^7}{240(15 + 4r_0\mu_* + r_0^4\alpha_*)} < \frac{\gamma r_0^7}{3600} \ . \tag{1.4.164}$$

The same power series estimate as in (1.4.157), but this time for η (which starts at index $j = 1$), implies

$$|\eta(r)| = \left| \sum_{j=1}^{\infty} \eta_j(r) \varepsilon^j \right| \leq S e^{-r/2} \sum_{j=1}^{\infty} \frac{R\varepsilon}{(j+\delta)^2} < \frac{S}{\delta^2} \sum_{j=1}^{\infty} \gamma^j = \frac{2\gamma}{1-\gamma} \ . \tag{1.4.165}$$

Given that

$$\zeta(r) = \zeta_{\mathrm{RWN}}(r) + \eta(r) = \left(1 - \frac{2\mu\varepsilon}{r} + \frac{\varepsilon}{r^2}\right)^{-1} + \eta(r) \ , \tag{1.4.166}$$

we have

$$\zeta(r) > \left(1 + \frac{\varepsilon}{r^2}\right)^{-1} - \frac{2\gamma}{1-\gamma} > \left(1 + \frac{\gamma r_0^7}{3600 r_0^2}\right)^{-1} - \frac{2\gamma}{1-\gamma} = \left(1 + \frac{\gamma r_0^5}{3600}\right)^{-1} - \frac{2\gamma}{1-\gamma} \ . \tag{1.4.167}$$

The condition for this expression to be positive is

$$\frac{\gamma^2 r_0^5}{3600} + 3\gamma - 1 < 0 \ . \tag{1.4.168}$$

The left side increases with r_0 and γ, and is negative with $r_0 = 1$ and $\gamma = 1/4$, so we have $\zeta(r) > 0$ on $r \in [r_0, \infty)$ for any $0 < r_0 < 1$ and $0 < \gamma < 1/4$.

5. Recall the ψ equation in (1.1.13):

$$\psi' = -\frac{\varepsilon\psi}{r^3}(w')^2 \ . \tag{1.4.169}$$

Plug in for w the solution to (1.1.13) that we just proved exists, which is continuous as a function of μ and α and analytic in ε. The following expression solves this equation (and is itself also continuous as a function of μ and α and analytic in ε):

$$\psi(r) = \exp\left(\varepsilon \int_r^\infty \frac{w'(s)^2}{s^3} \mathrm{d}s\right) \ . \tag{1.4.170}$$

Observe that, given the exponential decay of $w'(r)$ as $r \to \infty$, the integral is well-defined and we will have $\psi(r) \to 1$ as $r \to \infty$, as required. Also note that ψ is decreasing in r, so this asymptotic condition also proves that $\psi(r) > 0$ on $[r_0, \infty)$. Finally, expanding the argument of exp in this formula as a power series in ε will yield an expression whose degree-0 term is 1, and this justifies the claim that $\lim_{\varepsilon\to 0} \psi_\varepsilon(r) = \psi_0(r) := 1$ for all $r \geq r_0$.

With this we conclude the study of the main system (1.1.13) in the regime of r away from 0.

1.5 Radial variable close to 0

In this section we prove that solutions to the Maxwell-BLTP-Einstein system (1.1.13) exist over a domain $r \in (0, r_0]$, for small enough r_0, in such a way that finiteness of the integrals (1.3.50) and (1.3.51) (performed over $(0, r_0)$ instead of $(0, \infty)$) is granted. We recall the system here for convenience:

$$\begin{cases} \psi' = -\dfrac{\varepsilon\psi}{r^3}(w')^2 \\[2ex] \zeta' = \dfrac{(1-\zeta)\zeta}{r} + \dfrac{\varepsilon}{r^3}((1-w^2)\zeta^2 - (w')^2\zeta) \\[2ex] w'' = \left(\dfrac{3-\zeta}{r} + \dfrac{\varepsilon\zeta}{r^3}(1-w^2)\right) w' + \zeta w \end{cases} \tag{1.5.1}$$

Again the focus will be for the most part only on the system without the ψ equation. The main results to be proved in this section are:

- the existence of a 1-parameter family (call the parameter σ) of solutions with finite energy close to $r = 0$; and

- a uniform-in-σ quantitative estimate for the pointwise difference between the solution families corresponding to $\varepsilon = 0$ and to $\varepsilon > 0$.

They are described in the next two theorems:

Theorem 1.5.1. *For every $0 \le \varepsilon < 1/60$ and $0 < r_0 < 1/360$, the Maxwell-BLTP-Einstein system (1.1.13) admits a 1-parameter family of solutions ψ, ζ, w in $(0, r_0)$, parametrized by a real number σ such that $|\sigma| < 1/360$, which are continuous in σ at any $r \in (0, r_0]$ and satisfy the following* asymptotic conditions *at $r = 0$:*

$$0 < \lim_{r\to 0^+} \zeta(r) < \infty \quad , \quad 0 < \lim_{r\to 0^+} \left| \frac{w(r) - 1}{r^2} \right| < \infty \quad ,$$
$$0 < \lim_{r\to 0^+} \left| \frac{w'(r)}{r} \right| < \infty \quad , \quad 0 < \lim_{r\to 0^+} r^{\varepsilon Y^2} \psi(r) < \infty \tag{1.5.2}$$

where the constant Y in the last condition is such that $|Y| \le 1$. In particular this implies that the integrals

$$\int_0^{r_0} \frac{\psi(w-1)^2}{r^2} \mathrm{d}r \quad , \quad \int_0^{r_0} \frac{\psi \zeta^{-1} (w')^2}{r^2} \mathrm{d}r \quad , \quad \int_0^{r_0} \frac{\psi(w-1)}{r^2} \mathrm{d}r$$

are all finite.

Theorem 1.5.2. *For $\varepsilon \in [0, 1/60)$, consider*

$$x^{(\varepsilon)}(r,\sigma) = \zeta^{(\varepsilon)}(r,\sigma) \quad , \quad y^{(\varepsilon)}(r,\sigma) = \frac{(w')^{(\varepsilon)}(r,\sigma)}{r} \quad , \quad z^{(\varepsilon)}(r,\sigma) = \frac{w^{(\varepsilon)}(r,\sigma) - 1}{r^2} \tag{1.5.3}$$

*where $\zeta^{(\varepsilon)}(r,\sigma), w^{(\varepsilon)}(r,\sigma)$ are the 1-parameter family of solutions described in the theorem above. Then, for all $r \in (0, 1/360)$ and $\sigma \in (-1/360, 1/360)$, the **perturbation terms** $\widetilde{x}^{(\varepsilon)}, \widetilde{y}^{(\varepsilon)}, \widetilde{z}^{(\varepsilon)}$ defined by*

$$x^{(\varepsilon)}(r,\sigma) = x^{(0)}(r,\sigma) + \varepsilon \widetilde{x}^{(\varepsilon)}(r,\sigma) \quad , \quad \textit{etc.} \tag{1.5.4}$$

satisfy the bound

$$|\widetilde{x}^{(\varepsilon)}(r,\sigma)| \, , \; |\widetilde{y}^{(\varepsilon)}(r,\sigma)| \, , \; |\widetilde{z}^{(\varepsilon)}(r,\sigma)| \; \le \; \frac{60\varepsilon}{(1-\gamma)^2} \tag{1.5.5}$$

where

$$\gamma = \max\{360r, 360\sigma\} \in [0,1) \ . \tag{1.5.6}$$

1.5.1 Desingularization

We will apply a standard technique from the theory of Dynamical Systems to transform the ζ and w equations in system (1.1.13) into an autonomous system with an equilibrium point whose unstable manifold consists of orbits corresponding to solutions that satisfy the desired asymptotic conditions at $r = 0$.

First transform it into a 4D first-order, autonomous system by thinking of both r and $h = w'$ as variables:

$$\begin{cases} \zeta' = \dfrac{\zeta(1-\zeta)}{r} + \dfrac{\varepsilon}{r^3}\left(\zeta^2 - \zeta^2 w^2 - \zeta h^2\right) \\[2ex] h' = \left(\dfrac{3-\zeta}{r} + \varepsilon \dfrac{\zeta}{r^3}(1-w^2)\right) h + \zeta w \\[2ex] w' = h \\[2ex] r' = 1 \end{cases} \tag{1.5.7}$$

Denote the independent variable of this system by t_1. In order to obtain a system with an equilibrium point at $r = 0$, it is enough to introduce a new variable t_2 such that $r\frac{\mathrm{d}}{\mathrm{d}t_1} = \frac{\mathrm{d}}{\mathrm{d}t_2}$; that is, for any function g, if we define $\hat{g}(t_2) = g(t_1(t_2))$, then

$$\frac{\mathrm{d}\hat{g}}{\mathrm{d}t_2}(t_2) = g'(t_1(t_2))r(t_1(t_2)) \ . \tag{1.5.8}$$

We will choose

$$t_2 = \log(t_1) \ . \tag{1.5.9}$$

Letting $\hat{x}, \hat{y}, \hat{z}, \hat{s}$ be functions of t_2 related respectively to ζ, h, w, r by $\hat{x}(t_2) = \zeta(t_1(t_2)) = \zeta(e^{t_2})$ etc., we obtain the dynamical system that they satisfy by multiplying the right-hand side of (1.5.7) by r

and replacing the variable names:

$$\begin{cases} \hat{x}' = \hat{x}(1-\hat{x}) + \dfrac{\varepsilon}{\hat{s}^2}\left(\hat{x}^2 - \hat{x}^2\hat{z}^2 - \hat{x}\hat{y}^2\right) \\ \\ \hat{y}' = \left(3 - \hat{x} + \varepsilon\dfrac{\hat{x}}{\hat{s}^2}(1-\hat{z}^2)\right)\hat{y} + \hat{s}\hat{x}\hat{z} \\ \\ \hat{z}' = \hat{s}\hat{y} \\ \\ \hat{s}' = \hat{s} \end{cases} \tag{1.5.10}$$

Finally, we modify the dependent variables $\hat{y}, \hat{z}$ into new ones y, z whose finiteness at $r = 0$ will imply finiteness of the integrals (1.3.52) from section 1.1, according to (1.3.53) and (1.3.54). For the sake of notational consistency, we also rename $\hat{x}, \hat{s}$ as x, s. So let

$$x = \hat{x} \quad , \quad y = \frac{\hat{y}}{\hat{s}} \quad , \quad z = \frac{\hat{z}-1}{\hat{s}^2} \quad , \quad s = \hat{s} \ . \tag{1.5.11}$$

Then we compute the derivatives:

$$\begin{aligned} x' &= \hat{x}' = x(1-x) + \frac{\varepsilon}{s^2}(x^2 - x^2(s^2z+1)^2 - x(sy)^2) \\ &= x - x^2 - \varepsilon(xy^2 + 2x^2z + s^2x^2z^2) \\ y' &= \frac{\hat{y}'\hat{s} - \hat{y}\hat{s}'}{\hat{s}^2} = \frac{\hat{y}' - \hat{y}}{\hat{s}} = \frac{1}{s}\left[\left(3 - x + \varepsilon\frac{x}{s^2}(1-(s^2z+1)^2)\right)sy + sx(s^2z+1) - sy\right] \\ &= x + 2y - xy + s^2xz - \varepsilon(2xyz + s^2xyz^2) \\ z' &= \frac{\hat{z}'\hat{s}^2 - 2\hat{s}\hat{s}'(\hat{z}-1))}{\hat{s}^4} = \frac{\hat{z}' - 2\hat{z} + 2}{\hat{s}^2} = \frac{\hat{y}}{\hat{s}} - 2\frac{\hat{z}-1}{\hat{s}^2} = y - 2z \\ s' &= \hat{s}' = s \end{aligned}$$

We thus have a non-singular, 4D, first-order, autonomous dynamical system in (x, y, z, s) with a parameter ε:

$$\begin{cases} x' = x - x^2 - \varepsilon(xy^2 + 2x^2z + s^2x^2z^2) \\ y' = x + 2y - xy + s^2xz - \varepsilon(2xyz + s^2xyz^2) \\ z' = y - 2z \\ s' = s \end{cases} \tag{1.5.12}$$

Given that $r(t_1) = t_1$, we have $s(t_2) = r(e^{t_2}) = e^{t_2}$, and in particular

$$\lim_{t_2 \to -\infty} s(t_2) = 0 \ . \tag{1.5.13}$$

Therefore, evolving an orbit backwards in "time" t_2 corresponds to letting its s coordinate decrease to 0, and, in order to obtain orbits corresponding to finite energy solutions to the original system, it will be enough to find orbits whose coordinates converge to finite values at $s = 0$. This can only happen if this orbit belongs to the unstable manifold of an equilibrium point at $s = 0$. So our next task is to find a suitable critical point and study the linearized system around it.

Remark 1.5.3. The solution to the Maxwell-BLTP flat-space equations

$$\zeta \equiv 1 \quad , \quad w(r) = (1+r)e^{-r} \quad , \quad w'(r) = -re^{-r} \tag{1.5.14}$$

is written in the new variables as

$$x(t_2) \equiv 1 \quad , \quad y(t_2) = -e^{-e^{t_2}} \quad , \quad z(t_2) = \frac{(1+e^{t_2})e^{-e^{t_2}} - 1}{e^{2t_2}} \quad , \quad s(t_2) = e^{t_2} \; . \tag{1.5.15}$$

The corresponding orbit, obtained by letting the independent parameter t_2 vary in $\mathbb{R}$, "comes from" the point

$$(X, Y, Z, S) = \left(1, -1, -\frac{1}{2}, 0\right) \; , \tag{1.5.16}$$

that is, this point is its limit as $t_2 \to -\infty$. On the other hand, the RWN solution

$$\zeta(r) = \left(1 - \frac{2\mu\varepsilon}{r} + \frac{\varepsilon}{r^2}\right)^{-1} \quad , \quad w \equiv w' \equiv 0 \tag{1.5.17}$$

becomes

$$x(t_2) = \left(1 - \frac{2\mu\varepsilon}{e^{t_2}} + \frac{\varepsilon}{e^{2t_2}}\right)^{-1} \quad , \quad y \equiv 0 \quad , \quad z(t_2) = -e^{-2t_2} \quad , \quad s(t_2) = e^{t_2} \; , \tag{1.5.18}$$

with the orbit diverging as t_2 approaches $-\infty$ (for $\varepsilon > 0$). Therefore we see that restricting our attention only to solutions of our desingularized system (1.5.12) that come from an equilibrium point at $s = 0$ precludes the scenario that we end up finding the one that corresponds to the RWN solution to the original system.

1.5.2 Critical point analysis

Let $(X^{(\varepsilon)}, Y^{(\varepsilon)}, Z^{(\varepsilon)}, S^{(\varepsilon)})$ denote a critical point of system (1.5.12). When there is no need to specify the ε-dependence, we will omit the superscript (ε).

Due to the 3$^{\text{rd}}$ and 4$^{\text{th}}$ equations, it is clear that

$$Y = 2Z \quad , \quad S = 0 \; . \tag{1.5.19}$$

Plug this into the right-hand side of the 1st and 2nd equations and set them equal to zero:

$$\begin{aligned} 0 &= X - X^2 - \varepsilon(4XZ^2 + 2X^2Z) = X(1 - 4\varepsilon Z^2) - X^2(1 + 2\varepsilon Z) \\ 0 &= X + 4Z - 2XZ - 4\varepsilon XZ^2 \end{aligned} \tag{1.5.20}$$

First of all, when $X = 0$, the second equation gives $Z = 0$ and we obtain the critical point $(0, 0, 0, 0)$, which is always a critical point for any $\varepsilon \geq 0$. So assume $X \neq 0$ in what follows, and divide the first equation by X.

If $\varepsilon = 1$, the first equation can be factored as $(1 + 2Z)(1 - 2Z - X) = 0$. In case the first factor is zero, we obtain the solution $\left(2, -1, -\frac{1}{2}, 0\right)$. In case it's the second factor that is zero, we solve it for X and plug it into the second equation to find $Z = -1/2$, which then yields the same point.

Now assume $\varepsilon \neq 1$. We claim that $1 + 2\varepsilon Z \neq 0$. Indeed, assuming $1 + 2\varepsilon Z = 0$ and looking at the first equation in (1.5.20): since $\varepsilon \neq 1$, we can't have $1 - 4\varepsilon Z^2 = 0$ also; hence $X = 0$, but this plugged into the second equation implies $Z = 0$, which is not the case. Now, given this claim, we can solve for X in the first equation and plug it into the second, obtaining

$$X = \frac{1 - 4\varepsilon Z^2}{1 + 2\varepsilon Z} \quad , \quad 16\varepsilon^2 Z^4 + 8\varepsilon Z^3 + 2Z + 1 = 0 \ . \tag{1.5.21}$$

It will be most convenient to work in terms of Y. We have then

$$X = \frac{1 - \varepsilon Y^2}{1 + \varepsilon Y} \quad , \quad Z = \frac{Y}{2} \quad , \quad \varepsilon^2 Y^4 + \varepsilon Y^3 + Y + 1 = 0 \ . \tag{1.5.22}$$

Lemma 1.5.4. *For all $\varepsilon \geq 0$, consider the polynomial*

$$p(t) = \varepsilon^2 t^4 + \varepsilon t^3 + t + 1 \ . \tag{1.5.23}$$

Then it only has real roots when $\varepsilon \in [0, 1]$, and in that case:

- *there are at most two roots $t_1^{(\varepsilon)} \leq -1 \leq t_2^{(\varepsilon)} < 0$;*
- *these roots are equal to each other (and equal to -1) if and only if $\varepsilon = 0, 1$.*

Proof. When $\varepsilon = 0$ the only root is -1. When $\varepsilon = 1$, the polynomial factors as $p(t) = (t^3 + 1)(t + 1)$ and again only has the real root -1. Now assume $\varepsilon \neq 1$, $\varepsilon > 0$. Compute the derivatives:

$$p'(t) = 4\varepsilon^2 t^3 + 3\varepsilon t^2 + 1 \quad , \quad p''(t) = 12\varepsilon^2 t^2 + 6\varepsilon t \ . \tag{1.5.24}$$

The two critical points of p' are therefore $u = -1/(2\varepsilon)$ and $v = 0$, and since

$$p'(u) = -\frac{4\varepsilon^2}{8\varepsilon^3} + \frac{3\varepsilon}{4\varepsilon^2} + 1 = 1 + \frac{1}{4\varepsilon} > 0 \quad , \quad p'(v) = 1 > 0 \ , \tag{1.5.25}$$

there is only one $z \in \mathbb{R}$ such that $p'(z) = 0$, and it is negative (given that $u < 0$ and $\lim_{t\to-\infty} p'(t) = -\infty$). Hence z is a global minimum point of p, and p can have either 0, 1 or 2 real roots, depending on whether $p(z) > 0$, $p(z) = 0$, $p(z) < 0$ respectively.

Carrying out polynomial long division, we have

$$p(t) = \left(\frac{t}{4} + \frac{1}{16\varepsilon}\right) p'(t) + \frac{1}{16}\left(-3t^2 + 12t + 16 - \frac{1}{\varepsilon}\right) \ ; \tag{1.5.26}$$

in particular the sign of $p(z)$ is the same as that of $q(z)$, where q is the polynomial defined by

$$q(t) = -3t^2 + 12t + 16 - \frac{1}{\varepsilon} \ . \tag{1.5.27}$$

The discriminant of q is

$$\Delta = 12^2 + 12\left(16 - \frac{1}{\varepsilon}\right) = 12\left(28 - \frac{1}{\varepsilon}\right) \ . \tag{1.5.28}$$

If $\varepsilon < 1/28$, this is negative, ensuring $q(t) < 0$ for all $t \in \mathbb{R}$, which means $p(z) < 0$, and so p has 2 real roots. Otherwise, q has at most two real roots given by

$$x_\pm = 2 \pm \frac{1}{3}\sqrt{84 - \frac{3}{\varepsilon}} \ , \tag{1.5.29}$$

and the condition for, say, $q(z) < 0$ is that $z < x_-$ or $z > x_+$. But since $z < 0$ and $x_+ > 0$, this condition can be written as just $z < x_-$. And since z was defined as the only real root of the polynomial p' (which is positive to the right of z and negative to the left), this is the case if and only if $p'(x_-) > 0$. Computing $p'(x_-)$ and simplifying, we get

$$p'(x_-) = 32\varepsilon(1 + 8\varepsilon)\left(1 - \frac{1}{9}\sqrt{84 - \frac{3}{\varepsilon}}\right) \ . \tag{1.5.30}$$

This is positive if and only if

$$\sqrt{84 - \frac{3}{\varepsilon}} < 9 \quad \iff \quad \varepsilon < 1 \ . \tag{1.5.31}$$

□

With this we have finished finding the critical points (X, Y, Z, S) of (1.5.12). There are at most 3 of them:

- For $\varepsilon \in [0,1]$, two critical points $P_1^{(\varepsilon)}, P_2^{(\varepsilon)}$ are given by

$$P_j^{(\varepsilon)} = \left(\frac{1 - 4\varepsilon t_j^{(\varepsilon)2}}{1 + 2\varepsilon t_j^{(\varepsilon)}}, \frac{t_j^{(\varepsilon)}}{2}, t_j^{(\varepsilon)}, 0 \right) \quad , \quad j = 1, 2 \; , \tag{1.5.32}$$

  and they coincide when $\varepsilon = 0, 1$.

- For any $\varepsilon \geq 0$, the point $P_3^{(\varepsilon)} = (0,0,0,0)$ is also a critical point.

Given that the solution of the original system for large r was obtained as a perturbation of the flat-space solution, we shall focus our analysis on the point among these three that converges to the one described in (1.5.16) as $\varepsilon \to 0$, which is $P_2^{(\varepsilon)}$. We will drop the 2 and denote it by just

$$P^{(\varepsilon)} = (X^{(\varepsilon)}, Y^{(\varepsilon)}, Z^{(\varepsilon)}, 0) \; . \tag{1.5.33}$$

We will also omit the (ε) superscript whenever the value of ε is clear. We are interested in its *unstable manifold*, which we call $\mathcal{W}^{(\varepsilon)}$, defined as the collection of orbits of (1.5.12) whose limit as $t_2 \to -\infty$ is $P^{(\varepsilon)}$.

In all that follows, we will use the notations $[*, \cdots, *]^t$ and $(*, \cdots, *)$ interchangeably to denote points (or vectors) in $\mathbb{R}^3$ and $\mathbb{R}^4$, depending on which is more convenient in each case.

The linearization matrix of (1.5.12) at $P^{(\varepsilon)}$, containing the partial derivatives of the right-hand side with respect to x, y, z, s evaluated at P, can be calculated to be

$$M^{(\varepsilon)} = \begin{bmatrix} 1 - 2X - \varepsilon(4Z^2 + 4XZ) & -4\varepsilon XZ & -2\varepsilon X^2 & 0 \\ 1 - 2Z - 4\varepsilon Z^2 & 2 - X - 2\varepsilon XZ & -4\varepsilon XZ & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} . \tag{1.5.34}$$

We see that, for any ε, there is an eigenvalue, which we call $\lambda_1^{(\varepsilon)}$, equal to 1, with a corresponding eigenvector $[0,0,0,1]^t$. We will call $N^{(\varepsilon)}$ the upper-left 3×3 block of $M^{(\varepsilon)}$. Given the relations (1.5.22), it is written in terms of Y as:

$$N^{(\varepsilon)} = \begin{bmatrix} -1 + \varepsilon Y^2 & -2\varepsilon Y \dfrac{1 - \varepsilon Y^2}{1 + \varepsilon Y} & -2\varepsilon \left(\dfrac{1 - \varepsilon Y^2}{1 + \varepsilon Y} \right)^2 \\ 2 - \varepsilon Y^2 + \varepsilon Y^3 + \varepsilon^2 Y^4 & 1 + \varepsilon Y^2 & -2\varepsilon Y \dfrac{1 - \varepsilon Y^2}{1 + \varepsilon Y} \\ 0 & 1 & -2 \end{bmatrix} . \tag{1.5.35}$$

Let $\lambda_2^{(\varepsilon)}, \lambda_3^{(\varepsilon)}, \lambda_4^{(\varepsilon)}$ denote its (potentially complex) eigenvalues. When $\varepsilon = 0$, we have $Y = -1$ and it can be calculated that

$$\lambda_2^{(0)} = 1 \quad , \quad \lambda_3^{(0)} = -1 \quad , \quad \lambda_4^{(0)} = -2 \; . \tag{1.5.36}$$

Hence, when $\varepsilon > 0$ is small, $M^{(\varepsilon)}$ will still have two eigenvalues $\lambda_1^{(\varepsilon)} = 1$ and $\lambda_2^{(\varepsilon)}$ with positive real part and two others with negative real part (in fact they must remain all real, since there is no multiplicity among $\lambda_2^{(0)}, \lambda_3^{(0)}, \lambda_4^{(0)}$). The Hartman-Grobman Theorem states that the unstable manifold $\mathcal{W}^{(\varepsilon)}$ of the equilibrium point $P^{(\varepsilon)}$ is 2-dimensional and tangent at $P^{(\varepsilon)}$ to the plane spanned by eigenvectors corresponding to the positive $\lambda_j^{(\varepsilon)}$'s. Our goal in this section is to find an analytic parametrization for it and prove its convergence in a small enough neighborhood of $P^{(\varepsilon)}$.

But before we do that, we will need to find bounds on the eigenvalues $\lambda_1^{(\varepsilon)}, \lambda_2^{(\varepsilon)}$ and on certain expressions involving $X^{(\varepsilon)}, Y^{(\varepsilon)}, Z^{(\varepsilon)}$. Due to the proof method used, we will have to stay restricted to small values of ε away from 1 (at first $\varepsilon < 1/2$, then $\varepsilon < 1/60$), but these restrictions are more than enough for our purposes.

Lemma 1.5.5. *For all* $\varepsilon \in [0, 1/2)$*, there exist* $\delta_X^{(\varepsilon)}, \delta_Y^{(\varepsilon)}, \delta_Z^{(\varepsilon)} \in [0, 1]$ *such that*

$$\begin{aligned} X^{(\varepsilon)} &= 1 + 4\delta_X^{(\varepsilon)}\varepsilon^2 \\ Y^{(\varepsilon)} &= -1 + 2\delta_Y^{(\varepsilon)}\varepsilon \\ Z^{(\varepsilon)} &= -\frac{1}{2} + \delta_Z^{(\varepsilon)}\varepsilon \end{aligned} \tag{1.5.37}$$

Proof. It is enough to prove (considering that $Y^{(\varepsilon)} = 2Z^{(\varepsilon)}$)

$$-1 \le \; Y^{(\varepsilon)} \le -1 + 2\varepsilon \quad , \quad 1 \le X^{(\varepsilon)} \le 1 + 4\varepsilon^2 \; . \tag{1.5.38}$$

Let us drop the (ε) superscript. From the proof of lemma 1.5.4 we know $p(Y) = 0$ where

$$p(t) = \varepsilon^2 t^4 + \varepsilon t^3 + t + 1 \tag{1.5.39}$$

and furthermore $-1 \le Y < 0$. In particular, due to $Y \ge -1 > -1/(2\varepsilon)$,

$$0 < 1 + 2\varepsilon Y \le 1 \tag{1.5.40}$$

and

$$1 - \varepsilon Y^2 > 1 - \varepsilon > \frac{1}{2} \; . \tag{1.5.41}$$

From implicitly differentiating $p(Y) = 0$ we obtain

$$\frac{\mathrm{d}Y}{\mathrm{d}\varepsilon} = -Y^3 \frac{1 + 2\varepsilon Y}{1 + 3Y^2 + 4\varepsilon^2 Y^3} \ . \tag{1.5.42}$$

The denominator can be simplified using $p(Y) = 0$:

$$1 + 3Y^2 + 4\varepsilon^2 Y^3 = 1 - \varepsilon Y^2 + 4(\varepsilon^2 Y^4 + \varepsilon Y^3) = 1 - \varepsilon Y^2 - \frac{4}{Y}(Y+1) = -3 - \varepsilon Y^2 - \frac{4}{Y} \ , \tag{1.5.43}$$

which is bounded below by $-3 - \varepsilon Y^2 + 4 > 1/2$ (using (1.5.41)). In particular $\frac{\mathrm{d}Y}{\mathrm{d}\varepsilon} > 0$. But using (1.5.40) to bound (1.5.42) above, we have

$$\frac{\mathrm{d}Y}{\mathrm{d}\varepsilon} \leq -(-1)^3 \frac{1}{1/2} = 2 \ . \tag{1.5.44}$$

Now the inequality stated in this lemma is a consequence of the Mean Value Theorem and the fact that $Y^{(0)} = -1$.

To obtain the X bounds, rewrite its formula given in (1.5.22) as

$$X - 1 = -\varepsilon Y \frac{1 + Y}{1 + \varepsilon Y} \ . \tag{1.5.45}$$

The three positive numbers $-\varepsilon Y, 1 + Y, 1 + \varepsilon Y$ can be bounded with the Y bounds just proved, and this yields

$$0 \leq X - 1 \leq \frac{2\varepsilon^2}{1 - \varepsilon + 2\varepsilon^2} < 4\varepsilon^2 \ . \tag{1.5.46}$$

□

Proposition 1.5.6. *For all $\varepsilon \in (0, 1/60)$, the linearization matrix $M^{(\varepsilon)}$ has 2 positive eigenvalues $\lambda_1^{(\varepsilon)}, \lambda_2^{(\varepsilon)}$ satisfying*

$$\lambda_1^{(\varepsilon)} = 1 \quad , \quad 1 < \lambda_2^{(\varepsilon)} < 1 + 60\varepsilon \ . \tag{1.5.47}$$

Proof. We've seen that $\lambda_1^{(\varepsilon)} = 1$ is an eigenvalue. We must show that the eigenvalues $\lambda_2^{(\varepsilon)}, \lambda_3^{(\varepsilon)}, \lambda_4^{(\varepsilon)}$ of $N^{(\varepsilon)}$ are 1 positive and 2 negative, with $\lambda_2^{(\varepsilon)} > 0$ satisfying the bounds given.

Let the characteristic polynomial of $N^{(\varepsilon)}$ be denoted

$$\chi^{(\varepsilon)}(t) = \det\left(N^{(\varepsilon)} - tI\right) = -t^3 + a_2^{(\varepsilon)} t^2 + a_1^{(\varepsilon)} t + a_0^{(\varepsilon)} \ . \tag{1.5.48}$$

We have $\chi^{(0)}(t) = -t^3 - 2t^2 + t + 2$. Write each coefficient of $\chi^{(\varepsilon)}$ as a perturbation of the $\varepsilon = 0$ coefficients:

$$a_2^{(\varepsilon)} = -2 + \varepsilon\delta_2^{(\varepsilon)} \quad , \quad a_1^{(\varepsilon)} = 1 + \varepsilon\delta_1^{(\varepsilon)} \quad , \quad a_0^{(\varepsilon)} = 2 + \varepsilon\delta_0^{(\varepsilon)} \; , \tag{1.5.49}$$

and use formula (1.5.35) for $N^{(\varepsilon)}$ to compute:

$$\begin{aligned} \delta_2^{(\varepsilon)} &= 2Y^2 \\ \delta_1^{(\varepsilon)} &= (-3\varepsilon^3 Y^6 - 6\varepsilon^2 Y^5 + (10\varepsilon^2 - 3\varepsilon)Y^4 + 16\varepsilon Y^3 - (4\varepsilon - 6)Y^2 - 4Y)/(1 + \varepsilon Y)^2 \\ \delta_0^{(\varepsilon)} &= (-6\varepsilon^3 Y^6 - 12\varepsilon^2 Y^5 + 6\varepsilon(\varepsilon - 1)Y^4 + 12\varepsilon Y^3 + 4Y^2 - 4Y - 2)/(1 + \varepsilon Y)^2 \end{aligned} \tag{1.5.50}$$

Using $\varepsilon^2 Y^4 + \varepsilon Y^3 + Y + 1 = 0$, the polynomials of Y that appear in these formulas can be made simpler. One of the factors $1 + \varepsilon Y$ in the denominator of $\delta_1^{(\varepsilon)}$ can also be cancelled. The end result is

$$\begin{aligned} \delta_2^{(\varepsilon)} &= 2Y^2 \\ \delta_1^{(\varepsilon)} &= Y(10\varepsilon Y^2 + 9Y - 1)/(1 + \varepsilon Y) \\ \delta_0^{(\varepsilon)} &= 2(6\varepsilon Y^3 + (3\varepsilon + 5)Y^2 - 2Y - 4)/(1 + \varepsilon Y)^2 \end{aligned} \tag{1.5.51}$$

Using the Y bounds (1.5.38) (and remembering that those bounds are negative), we can see

$$1 - \varepsilon \leq 1 + \varepsilon Y \leq 1 + \varepsilon(-1 + 2\varepsilon) = 1 - \varepsilon + 2\varepsilon^2 \tag{1.5.52}$$

$$40\varepsilon^3 - 40\varepsilon^2 + 10\varepsilon - 10 = 10\varepsilon(-1 + 2\varepsilon)^2 - 9 - 1 \leq 10\varepsilon Y^2 + 9Y - 1 \leq 10\varepsilon + 9(-1 + 2\varepsilon) - 1 = 28\varepsilon - 10 \tag{1.5.53}$$

$$\begin{aligned} 12\varepsilon^3 + 8\varepsilon^2 - 27\varepsilon + 3 = -6\varepsilon + (3\varepsilon + 5)(-1 + 2\varepsilon)^2 - 2(-1 + 2\varepsilon) - 4 &\leq 6\varepsilon Y^3 + (3\varepsilon + 5)Y^2 - 2Y - 4 \\ &\leq 6\varepsilon(-1 + 2\varepsilon)^3 + (3\varepsilon + 5) + 2 - 4 = 48\varepsilon^4 - 72\varepsilon^3 + 36\varepsilon^2 - 3\varepsilon + 3 \end{aligned} \tag{1.5.54}$$

In order to correctly multiply these expressions to get bounds on $\delta_1^{(\varepsilon)}$ and $\delta_0^{(\varepsilon)}$, we need to know their sign. For ε small enough ($\varepsilon < 1/60$ works) we can see that the left- and right-side bounds in (1.5.52), (1.5.53) and (1.5.54) are > 0, < 0 and > 0 respectively. Hence we can say

$$1.28 \leq 2(-1 + 2\varepsilon)^2 \leq \delta_2^{(\varepsilon)} \leq 2 \tag{1.5.55}$$

$$6.26 \leq (-1 + 2\varepsilon)\frac{28\varepsilon - 10}{1 - \varepsilon + 2\varepsilon^2} \leq \delta_1^{(\varepsilon)} \leq (-1)\frac{40\varepsilon^3 - 40\varepsilon^2 + 10\varepsilon - 10}{1 - \varepsilon} \leq 10.4 \tag{1.5.56}$$

$$0.92 \leq 2\frac{12\varepsilon^3 + 8\varepsilon^2 - 27\varepsilon + 3}{(1 - \varepsilon + 2\varepsilon^2)^2} \leq \delta_0^{(\varepsilon)} \leq 2\frac{48\varepsilon^4 - 72\varepsilon^3 + 36\varepsilon^2 - 3\varepsilon + 3}{(1 - \varepsilon)^2} \leq 7.39 \tag{1.5.57}$$

(the numeric bounds are true for the range considered for ε). This implies

$$\sup_{-3<t<2} |\delta_2^{(\varepsilon)} t^2 + \delta_1^{(\varepsilon)} t + \delta_0^{(\varepsilon)}| \le 18 + 33 + 8 = 59 \ . \tag{1.5.58}$$

Hence, for any $t \in (-3, 2)$, if $|\chi^{(0)}(t)| \ge 120\varepsilon$, then $\chi^{(0)}(t)$ and $\chi^{(\varepsilon)}(t)$ have the same sign, because, by the definition of $\delta_j^{(\varepsilon)}$,

$$|\chi^{(\varepsilon)}(t) - \chi^{(0)}(t)| = \varepsilon |\delta_2^{(\varepsilon)} t^2 + \delta_1^{(\varepsilon)} t + \delta_0^{(\varepsilon)}| \le 59\varepsilon < \frac{120\varepsilon}{2} \le \frac{|\chi^{(0)}(t)|}{2} \ . \tag{1.5.59}$$

Now let x stand for any of the 3 roots $-2, -1, 1$ of $\chi^{(0)}(t) = -t^3 - 2t^2 + t + 2$. The derivative at these values can be calculated to be

$$\frac{\mathrm{d}\chi^{(0)}}{\mathrm{d}t}(-2) = 21 \quad , \quad \frac{\mathrm{d}\chi^{(0)}}{\mathrm{d}t}(-1) = 2 \quad , \quad \frac{\mathrm{d}\chi^{(0)}}{\mathrm{d}t}(1) = -6 \ . \tag{1.5.60}$$

Note that $60\varepsilon < 1$ is smaller than the minimum distance between any of the 3 roots of $\chi^{(0)}$, hence the two points $x \pm 60\varepsilon \in (-3, 2)$ have precisely one root (x) between them, and in particular the two values $\chi^{(0)}(x \pm 60\varepsilon)$ have opposite signs. These two values can be computed as:

$$\begin{aligned} \chi^{(0)}(x \pm 60\varepsilon) &= -(x \pm 60\varepsilon)^3 - 2(x \pm 60\varepsilon)^2 + (x \pm 60\varepsilon) + 2 \\ &= \chi^{(0)}(x) \pm 60\varepsilon \frac{\mathrm{d}\chi^{(0)}}{\mathrm{d}t}(x) + (60\varepsilon)^2(-3x - 2) \mp (60\varepsilon)^3 \\ &= 60\varepsilon \bigg(\pm \frac{\mathrm{d}\chi^{(0)}}{\mathrm{d}t}(x) - 60\varepsilon(3x + 2 \pm 60\varepsilon) \bigg) \ . \end{aligned} \tag{1.5.61}$$

Direct verification of every possibility for x and the $\pm$ sign, using (1.5.60), gives

$$|\chi^{(0)}(x \pm 60\varepsilon)| \ge 60\varepsilon \cdot 2 = 120\varepsilon \ , \tag{1.5.62}$$

and, due to what we observed above, this implies that $\chi^{(0)}(x+60\varepsilon)$ and $\chi^{(\varepsilon)}(x+60\varepsilon)$ have the same sign, and that also $\chi^{(0)}(x - 60\varepsilon)$ and $\chi^{(\varepsilon)}(x - 60\varepsilon)$ have the same sign. But we also noted that the later sign is opposite to the former; in particular, there exists a root of $\chi^{(\varepsilon)}$ between $x - 60\varepsilon$ and $x + 60\varepsilon$. Since $x = -2, -1, 1$, this is enough to prove that 2 of the roots of $\chi^{(\varepsilon)}$ are still negative and 1 is positive (call the positive root $\lambda_2^{(\varepsilon)}$), while also proving the bound

$$1 - 60\varepsilon \le \lambda_2^{(\varepsilon)} \le 1 + 60\varepsilon \ . \tag{1.5.63}$$

In order to improve the lower bound on $\lambda_2^{(\varepsilon)}$ as stated in the proposition statement, it suffices to show that $\chi^{(\varepsilon)}(1) > 0$ (indeed, $\chi^{(\varepsilon)}(t)$ is a cubic polynomial with leading coefficient $-t^3$, and so the fact that it is positive at 1 will mean that there must be a root to the right of 1; this root can only be the only positive root $\lambda_2^{(\varepsilon)}$ that we proved exists). Just compute:

$$\chi^{(\varepsilon)}(1) = \frac{-2 - 8Y + (12 - 4\varepsilon)Y^2 + 32\varepsilon Y^3 + 9\varepsilon(2\varepsilon - 1)Y^4 - 18\varepsilon^2 Y^5 - 9\varepsilon^3 Y^6}{(1 + \varepsilon Y)^2} \; . \tag{1.5.64}$$

Using (1.5.38), the numerator can be seen to be positive too, just like what we did when bounding $\delta_j^{(\varepsilon)}$. □

Proposition 1.5.7. *For all $\varepsilon \in [0, 1/60)$, the eigenvalue $\lambda_2^{(\varepsilon)}$ of $M^{(\varepsilon)}$ has a corresponding eigenvector that can be written in the form*

$$v^{(\varepsilon)} = \begin{bmatrix} p^{(\varepsilon)}\varepsilon \\ 3 + q^{(\varepsilon)}\varepsilon \\ 1 \\ 0 \end{bmatrix} \quad \textit{for} \quad \begin{cases} 0 < p^{(\varepsilon)} < 4 \\ 0 < q^{(\varepsilon)} < 60 \end{cases} . \tag{1.5.65}$$

Proof. $\lambda_2^{(\varepsilon)}$ is the only positive eigenvalue of the matrix $N^{(\varepsilon)}$ defined in (1.5.35). If we find a corresponding eigenvector for this matrix, then we get one for $M^{(\varepsilon)}$ by adjoining a 0 in the fourth coordinate.

Let the matrix $\Delta_N^{(\varepsilon)}$ be defined by

$$N^{(\varepsilon)} = N^{(0)} + \varepsilon \Delta_N^{(\varepsilon)} \; , \tag{1.5.66}$$

which means

$$\Delta_N^{(\varepsilon)} = \begin{bmatrix} Y^2 & -2XY & -2X^2 \\ -Y^2 + Y^3 + \varepsilon Y^4 & Y^2 & -2XY \\ 0 & 0 & 0 \end{bmatrix} =: \begin{bmatrix} a & b & -c \\ -d & a & b \\ 0 & 0 & 0 \end{bmatrix} . \tag{1.5.67}$$

The positive numbers a, b, c, d defined by this equation also depend on ϵ, but we omit the superscript (ε) to unclutter the notation. Using the bounds we found on X, Y in lemma 1.5.5, we can find bounds for a, b, c (we will not need to know bounds for d):

$$\begin{aligned} 1 - 4\varepsilon + 4\varepsilon^2 \leq a \leq 1 \; , \\ 2 - 4\varepsilon \leq b \leq 2 + 8\varepsilon^2 \; , \\ 2 \leq c \leq 2 + 16\varepsilon^2 + 32\varepsilon^4 \; . \end{aligned} \tag{1.5.68}$$

Let $\lambda^{(\varepsilon)}$ be written in the form

$$\lambda^{(\varepsilon)} = 1 + \varepsilon\delta_\lambda^{(\varepsilon)} \quad , \quad \delta_\lambda^{(\varepsilon)} \in [0, 60) \tag{1.5.69}$$

(as per proposition 1.5.6). We know that the corresponding eigenspace is 1-dimensional. First we claim that it is spanned by a vector whose 3rd coordinate is nonzero. Indeed, assume for a contradiction that there exists a nonzero eigenvector of the form $[v_x, v_y, 0]^t$. Then

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = (N^{(\varepsilon)} - \lambda^{(\varepsilon)} I) \begin{bmatrix} v_x \\ v_y \\ 0 \end{bmatrix} = \begin{bmatrix} -1 + \varepsilon a - \lambda^{(\varepsilon)} & \varepsilon b & -\varepsilon c \\ 2 - \varepsilon d & 1 + \varepsilon a - \lambda^{(\varepsilon)} & \varepsilon b \\ 0 & 1 & -2 - \lambda^{(\varepsilon)} \end{bmatrix} \begin{bmatrix} v_x \\ v_y \\ 0 \end{bmatrix} . \tag{1.5.70}$$

The third row implies $v_y = 0$, and then the first row gives $(-1 + \varepsilon a - \lambda^{(\varepsilon)})v_x = 0$. But note that

$$-1 + \varepsilon a - \lambda^{(\varepsilon)} = -1 + \varepsilon a - 1 - \varepsilon\delta_\lambda^{(\varepsilon)} < -2 + \frac{1}{60} < 0 \ , \tag{1.5.71}$$

(using $a \leq 1$), giving $v_x = 0$, a contradiction.

Hence, by rescaling, we can find an eigenvector $v^{(\varepsilon)}$ for $\lambda^{(\varepsilon)}$ with the third coordinate equal to 1. Write it in the form

$$v^{(\varepsilon)} = v^{(0)} + \varepsilon\delta_v^{(\varepsilon)} = \begin{bmatrix} \varepsilon p^{(\varepsilon)} \\ 3 + \varepsilon q^{(\varepsilon)} \\ 1 \end{bmatrix} \quad , \quad \delta_v^{(\varepsilon)} = \begin{bmatrix} p^{(\varepsilon)} \\ q^{(\varepsilon)} \\ 0 \end{bmatrix} , \tag{1.5.72}$$

where $v^{(0)} = [0, 3, 1]^t$ is a corresponding eigenvector when $\varepsilon = 0$. Expanding out the equation

$$(N^{(0)} + \varepsilon\Delta_N^{(\varepsilon)})(v^{(0)} + \varepsilon\delta_v^{(\varepsilon)}) = (1 + \varepsilon\delta_\lambda^{(\varepsilon)})(v^{(0)} + \varepsilon\delta_v^{(\varepsilon)}) \ , \tag{1.5.73}$$

subtracting $N^{(0)}v^{(0)} = v^{(0)}$, and dividing by ε, we get

$$\begin{aligned} \begin{bmatrix} -2 + \varepsilon(a - \delta_\lambda^{(\varepsilon)}) & \varepsilon b & -\varepsilon c \\ 2 - \varepsilon d & \varepsilon(a - \delta_\lambda^{(\varepsilon)}) & \varepsilon b \\ 0 & 1 & -3 - \varepsilon\delta_\lambda^{(\varepsilon)} \end{bmatrix} \begin{bmatrix} p^{(\varepsilon)} \\ q^{(\varepsilon)} \\ 0 \end{bmatrix} &= (N^{(\varepsilon)} - \lambda^{(\varepsilon)} I)\delta_v^{(\varepsilon)} \\ &= (-\Delta_N^{(\varepsilon)} + \delta_\lambda^{(\varepsilon)} I)v^{(0)} = \begin{bmatrix} -3b + c \\ -3a - b + 3\delta_\lambda^{(\varepsilon)} \\ \delta_\lambda^{(\varepsilon)} \end{bmatrix} . \end{aligned} \tag{1.5.74}$$

This is a linear system for $p^{(\varepsilon)}, q^{(\varepsilon)}$ consisting of 3 equations. Since $\lambda^{(\varepsilon)}$ is an eigenvalue of $N^{(\varepsilon)}$ (whose 3 eigenvalues are all distinct), the matrix on the left has rank 2, but we also know that the system must be consistent, given that it came from the equation that establishes $v^{(\varepsilon)}$ as a corresponding eigenvector. Hence, if we manage to solve 2 independent equations out of these 3, the remaining one is automatically true.

The $p^{(\varepsilon)}$ coefficient in the first equation is nonzero:

$$-2+\varepsilon(a-\delta_\lambda^{(\varepsilon)}) = -2+\varepsilon a-\varepsilon-\delta_\lambda^{(\varepsilon)}\varepsilon^2 < -2+\varepsilon(1-0) < -2+\frac{1}{60} = -\frac{119}{60}\ . \tag{1.5.75}$$

Therefore the 1st and 3rd equations are independent. The 3rd one is immediately solved: $q^{(\varepsilon)} = \delta_\lambda^{(\varepsilon)}$ (in particular we have $0 < q^{(\varepsilon)} < 60$ as claimed). Plugging that into the 1st gives

$$p^{(\varepsilon)} = \frac{3b-c+\varepsilon b\delta_\lambda^{(\varepsilon)}}{2-\varepsilon(a-\delta_\lambda^{(\varepsilon)})}\ . \tag{1.5.76}$$

Using the bounds on b, c that we deduced, we conclude that $3b-c+\varepsilon b\delta_\lambda^{(\varepsilon)}$ is positive and

$$3b-c+\varepsilon b\delta_\lambda^{(\varepsilon)} < 6+24\varepsilon^2-2+\frac{(2+8\varepsilon^2)60}{60} = 6+32\varepsilon^2 < 7\ . \tag{1.5.77}$$

This and (1.5.75) then imply that $p^{(\varepsilon)}$ is positive and

$$p^{(\varepsilon)} < \frac{7\cdot 60}{119} < 4 \tag{1.5.78}$$

as claimed. $\square$

1.5.3 Analytic parametrization of the unstable manifold

Suppose $\varepsilon \in [0, 1/60)$ is fixed. We will omit the ε dependence from the notation of most symbols from now on.

Denote an arbitrary orbit of system (1.5.12) by $\boldsymbol{x} = \boldsymbol{x}(t) = (x(t), y(t), z(t), s(t))$, and let $\boldsymbol{F}$ denote its right-hand side, viewed as a multinomial in the variables x, y, z, s:

$$\boldsymbol{F}(x,y,z,s) = \begin{bmatrix} x-x^2-\varepsilon(xy^2+2x^2z+s^2x^2z^2) \\ x+2y-xy+s^2xz-\varepsilon(2xyz+s^2xyz^2) \\ y-2z \\ s \end{bmatrix}\ . \tag{1.5.79}$$

Let $v_1 = [0,0,0,1]^t$ and v_2 as in (1.5.65) be eigenvectors of the linearization matrix $\boldsymbol{DF}(P)$ at $P = (X,Y,Z,0)$ with corresponding eigenvalues $\lambda_1 = 1$ and $\lambda_2 \geq 1$. By the Hartman-Grobman Theorem, there exist open sets $U \ni P$ and $V \ni 0$ of $\mathbb{R}^4$ and a diffeomorphism $G : U \to V$ taking orbits of (1.5.12) to orbits of the linearized system $\boldsymbol{x}' = \boldsymbol{DF}(P)\boldsymbol{x}$, and this implies that the unstable manifold $\mathcal{W}$ associated to the equilibrium point P is a 2D manifold. We are going to find a parametrization for it. Let a differentiable map

$$W : U_0 \to \mathbb{R}^4 \quad , \quad W(\tau,\sigma) = (x(\tau,\sigma), y(\tau,\sigma), z(\tau,\sigma), s(\tau,\sigma)) \ , \ (\tau,\sigma) \in U_0 \tag{1.5.80}$$

(where $0 \in U_0 \subseteq \mathbb{R}^2$) be given, and assume that it satisfies

$$W(0) = P \quad , \quad \frac{\partial W}{\partial \tau}(0) = \xi_1 v_1 \quad , \quad \frac{\partial W}{\partial \sigma}(0) = \xi_2 v_2 \tag{1.5.81}$$

where $\xi_1, \xi_2 \in \mathbb{R}$ are arbitrary (we define $\xi_1 = 1$ and $\xi_2 = 1/4$). It can be proved (see [BM16]) that W is a parametrization of $\mathcal{W}$ if and only if it satisfies the **invariance equation**

$$DW(\tau,\sigma) \begin{bmatrix} \lambda_1 \tau \\ \lambda_2 \sigma \end{bmatrix} = \boldsymbol{F}(W(\tau,\sigma)) \ . \tag{1.5.82}$$

Furthermore, the fact that $\boldsymbol{F}$ is analytic in its variables means that we will be able to obtain an analytic W:

$$W(\tau,\sigma) = \sum_{i,j=0}^{\infty} \boldsymbol{w}_{ij} \tau^i \sigma^j \ , \tag{1.5.83}$$

for coefficients $\boldsymbol{w}_{ij} = (x_{ij}, y_{ij}, z_{ij}, s_{ij}) \in \mathbb{R}^4$. The conditions (1.5.81) then imply that:

- The zeroth coefficient $\boldsymbol{w}_{00} = W(0,0)$ must be the equilibrium point:

  $$\boldsymbol{w}_{00} = (x_{00}, y_{00}, z_{00}, s_{00}) = (X,Y,Z,0) \ . \tag{1.5.84}$$

  In particular note for future use

  $$|x_{00}|, |y_{00}|, |z_{00}| \leq 2 \ . \tag{1.5.85}$$

- The first-degree coefficients $\boldsymbol{w}_{10}, \boldsymbol{w}_{01}$ must be the chosen multiples v_1 and $v_2/4$ of the eigenvectors. We've seen in proposition 1.5.7 that

  $$v_2 = \begin{bmatrix} \varepsilon p \\ 3 + \varepsilon q \\ 1 \end{bmatrix} \quad , \quad \text{where} \begin{cases} 0 < p < 4 \\ 0 < q < 60 \end{cases} . \tag{1.5.86}$$

Note that the components of this vector are bounded by 4 in absolute value, given that $\varepsilon < 1/60$. Hence

$$\boldsymbol{w}_{10} = (x_{10}, y_{10}, z_{10}, s_{10}) = (0,0,0,1) \quad , \quad \boldsymbol{w}_{01} = (x_{01}, y_{01}, z_{01}, s_{01}) = \frac{v_2}{4} \tag{1.5.87}$$

and in particular

$$|x_\alpha|, |y_\alpha|, |z_\alpha| \leq 1 \quad \text{for } |\alpha| = 1 \ . \tag{1.5.88}$$

It's worth mentioning that choosing different values for the scaling parameters ξ_1, ξ_2 in front of the eigenvectors v_1, v_2 doesn't aid in obtaining a larger radius of convergence, because both the series coefficients and the independent variables τ, σ get scaled in an inversely proportional manner. But it can be useful to choose appropriate ξ_1, ξ_2 if we want to perform numerical calculations, where they help deal with precision errors.

Higher-degree coefficients can be found recursively. Let $(i,j) \in \mathbb{N}^2$ with $i + j \geq 2$. Computing the coefficient of $\tau^i \sigma^j$ on both sides of the invariance equation (1.5.82) gives

$$(i\lambda_1^{(\varepsilon)} + j\lambda_2^{(\varepsilon)})\boldsymbol{w}_{ij}^{(\varepsilon)} = \boldsymbol{F}(W^{(\varepsilon)}(\tau, \sigma))_{ij} \tag{1.5.89}$$

The right-hand side of this equation represents the coefficient of $\tau^i \sigma^j$ after we expand out the polynomial $\boldsymbol{F}$ applied to the parametrization of $x_{ij}, y_{ij}, z_{ij}, s_{ij}$ as functions of τ, σ. Let us now see how this gives a recursion relation that permits us to uniquely find all $\boldsymbol{w}_{ij} = (x_{ij}, y_{ij}, z_{ij}, s_{ij})$.

We employ *multi-index* notation, using Greek letters to represent 2-dimensional indices $(k,l) \in \mathbb{N}^2$. The parametrization is written in this notation as

$$W(\tau, \sigma) = \sum_{\alpha \in \mathbb{N}^2} \boldsymbol{w}_\alpha \tau^{\alpha_1} \sigma^{\alpha_2} = \sum_\alpha \boldsymbol{w}_\alpha \tau^{\alpha_1} \sigma^{\alpha_2} \ . \tag{1.5.90}$$

Multi-indices are summed componentwise, and, by definition, two arbitrary multi-indices $\beta = (\beta_1, \beta_2)$, $\gamma = (\gamma_1, \gamma_2)$ satisfy $\beta \leq \gamma$ when $\beta_1 \leq \gamma_1$ and $\beta_2 \leq \gamma_2$. This notion of a partial order is necessary when writing down the coefficients of a polynomial expression involving the unknowns $x_\alpha, y_\alpha, z_\alpha, s_\alpha$; for example

$$xy = \sum_\alpha [xy]_\alpha \tau^{\alpha_1} \sigma^{\alpha_2} \quad \text{where} \quad [xy]_\alpha = \sum_{\beta \leq \alpha} x_\beta y_{\alpha - \beta} \ . \tag{1.5.91}$$

The notation $|\beta|$ will be used to mean the **degree** $\beta_1 + \beta_2$. Note that $|\beta + \gamma| = |\beta| + |\gamma|$ for any $\beta, \gamma \in \mathbb{N}^2$.

So let $\alpha \in \mathbb{N}^2$ with $|\alpha| \geq 2$ be fixed, and assume for recursion that we already uniquely determined all coefficients $\boldsymbol{w}_\beta$ for $|\beta| < |\alpha|$. We will denote by α' the specific multi-index

$$\alpha' = (\alpha_1 - 2, \alpha_2) \ , \tag{1.5.92}$$

which will appear shortly in some formulas. For convenience, we stipulate that the coefficient of a variable corresponding to a multi-index with a negative entry is defined as 0; so for example, when $\alpha_1 < 2$, we have

$$\sum_{\beta \leq \alpha'} x_\beta y_{\alpha' - \beta} = 0 \ . \tag{1.5.93}$$

Start by looking at the 4th coefficient of (1.5.89). The equation reads

$$(\lambda_1 \alpha_1 + \lambda_2 \alpha_2) s_\alpha = s_\alpha \ . \tag{1.5.94}$$

Since $\lambda_1 = 1$ and $\lambda_2 \geq 1$, the left-hand side is different from s_α, so the solution can only be $s_\alpha = 0$. With this and the value of the initial coefficients s_{00}, s_{01}, s_{10}, we have determined all s coefficients:

$$s_{10} = 1 \quad , \quad s_{kl} = 0 \text{ for all other } k, l \ , \tag{1.5.95}$$

implying that the τ parameter is the same as the variable s:

$$s = \sum_\alpha s_\alpha \tau^{\alpha_1} \sigma^{\alpha_2} = \tau \ . \tag{1.5.96}$$

The 3rd equation of (1.5.89) reads

$$(\lambda_1 \alpha_1 + \lambda_2 \alpha_2) z_\alpha = [y - 2z]_\alpha = y_\alpha - 2 z_\alpha \tag{1.5.97}$$

and, once we find y_α, it can be solved as

$$z_\alpha = \frac{y_\alpha}{2 + \lambda_1 \alpha_1 + \lambda_2 \alpha_2} \tag{1.5.98}$$

since the denominator in this expression is not zero.

Now consider the 1st equation in (1.5.89). When expanding out the right-hand side, we use the fact that the $\alpha = (\alpha_1, \alpha_2)$ coefficient of the term containing s^2 $(= \tau^2)$ is the same as the $\alpha' = (\alpha_1 - 2, \alpha_2)$ coefficient of the remaining parts of that term. Other than this, everything else is straightforward:

$$\begin{aligned}(\lambda_1\alpha_1+\lambda_2\alpha_2)x_\alpha &= x_\alpha - [x^2]_\alpha - \varepsilon([xy^2]_\alpha + 2[x^2z]_\alpha + [s^2x^2z^2]_\alpha)\\ &= x_\alpha - [x^2]_\alpha - \varepsilon([xy^2]_\alpha + 2[x^2z]_\alpha + [x^2z^2]_{\alpha'})\\ &= x_\alpha - \sum_{\beta\le\alpha} x_\beta x_{\alpha-\beta} - \varepsilon\bigg(\sum_{\beta\le\alpha}\sum_{\gamma\le\beta}(x_{\alpha-\beta}y_\gamma y_{\beta-\gamma} + 2z_{\alpha-\beta}x_\gamma x_{\beta-\gamma})\\ &\qquad + \sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\delta\le\alpha'-\beta} x_\gamma x_{\beta-\gamma} z_\delta z_{\alpha'-\beta-\delta}\bigg)\ .\end{aligned} \tag{1.5.99}$$

The sums on the right-hand side involve coefficients with degree at most $|\alpha|$, but those with this maximal degree must be of index precisely α, since they are also constrained to be $\le \alpha$. Hence, maximal-degree coefficients can only appear as factors in a product all of whose other coefficients are of index $0 = (0,0)$. Note that the triple sum, where all indices are restricted to be $\le \alpha'$, will not contribute any terms like this. So we see that the terms on the right-hand side involving any α indices are only the following ones:

$$x_\alpha\ ,\ -2Xx_\alpha\ ,\ -\varepsilon(Y^2x_\alpha + 2XYy_\alpha + 4XZx_\alpha + 2X^2z_\alpha)\ .$$

Moving them to the left, we have

$$\begin{aligned}(\lambda_1\alpha_1+\lambda_2\alpha_2 - 1 + 2X + \varepsilon Y^2 + 4\varepsilon XZ)x_\alpha + 2\varepsilon XYy_\alpha + 2\varepsilon X^2 z_\alpha = -\sum_{\substack{\beta\le\alpha\\ \beta\ne 0,\alpha}} x_\beta x_{\alpha-\beta}\\ -\varepsilon\bigg(\sum_{\substack{\beta\le\alpha\\ \beta\ne0\ ,}}\sum_{\substack{\gamma\le\beta\\ \gamma\ne\alpha\\ \beta-\gamma\ne\alpha}}(x_{\alpha-\beta}y_\gamma y_{\beta-\gamma} + 2z_{\alpha-\beta}x_\gamma x_{\beta-\gamma}) + \sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\delta\le\alpha'-\beta} x_\gamma x_{\beta-\gamma}z_\delta z_{\alpha'-\beta-\delta}\bigg)\end{aligned} \tag{1.5.100}$$

Finally, use (1.5.98) on the left to write z_α in terms of y_α. We obtain thus a linear equation for x_α and y_α:

$$a_\alpha x_\alpha + b_\alpha y_\alpha = e_\alpha\ , \tag{1.5.101}$$

where

$$\begin{aligned}a_\alpha &= \lambda_1\alpha_1+\lambda_2\alpha_2 - 1 + 2X + \varepsilon Y^2 + 4\varepsilon XZ = \lambda_1\alpha_1+\lambda_2\alpha_2 + 1 - \varepsilon Y^2\\ b_\alpha &= 2\varepsilon X\left(Y + \frac{X}{2+\lambda_1\alpha_1+\lambda_2\alpha_2}\right)\\ e_\alpha &= -\sum_{\substack{\beta\le\alpha\\ \beta\ne0,\alpha}} x_\beta x_{\alpha-\beta} - \varepsilon\bigg(\sum_{\substack{\beta\le\alpha\\ \beta\ne0\ ,}}\sum_{\substack{\gamma\le\beta\\ \gamma\ne\alpha\\ \beta-\gamma\ne\alpha}}(x_{\alpha-\beta}y_\gamma y_{\beta-\gamma} + 2z_{\alpha-\beta}x_\gamma x_{\beta-\gamma}) + \sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\delta\le\alpha'-\beta} x_\gamma x_{\beta-\gamma}z_\delta z_{\alpha'-\beta-\delta}\bigg)\end{aligned} \tag{1.5.102}$$

(we used equations (1.5.22), which give X, Z in terms of Y, to rewrite a_α in terms of just Y).

Next we do the same for the 2nd equation in (1.5.89). Initially it reads

$$\begin{aligned}(\lambda_1\alpha_1+\lambda_2\alpha_2)y_\alpha &= x_\alpha + 2y_\alpha - [xy]_\alpha - 2\varepsilon[xyz]_\alpha + [xz]_{\alpha'} - \varepsilon[xyz^2]_{\alpha'} \\ &= x_\alpha + 2y_\alpha - \sum_{\beta\le\alpha} x_\beta y_{\alpha-\beta} - 2\varepsilon \sum_{\beta\le\alpha}\sum_{\gamma\le\beta} x_{\alpha-\beta}y_\gamma z_{\beta-\gamma} + \sum_{\beta\le\alpha'} x_\beta z_{\alpha'-\beta} \\ &\quad - \varepsilon \sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\delta\le\alpha'-\beta} x_\delta y_{\alpha'-\beta-\delta} z_\gamma z_{\beta-\gamma}\end{aligned} \tag{1.5.103}$$

Move to the left the terms on the right that involve α indices:

$$x_\alpha \ , \ 2y_\alpha \ , \ -Xy_\alpha - Yx_\alpha \ , \ -2\varepsilon(XYz_\alpha + XZy_\alpha + YZx_\alpha) \ .$$

The equation becomes

$$\begin{aligned}&(-1+Y+2\varepsilon YZ)x_\alpha + (\lambda_1\alpha_1+\lambda_2\alpha_2 - 2 + X + 2\varepsilon XZ)y_\alpha + 2\varepsilon XYz_\alpha \\ &= -\sum_{\substack{\beta\le\alpha \\ \beta\ne 0,\alpha}} x_\beta y_{\alpha-\beta} - 2\varepsilon \sum_{\substack{\beta\le\alpha \\ \beta\ne 0}}\sum_{\substack{\gamma\le\beta \\ \gamma\ne\alpha \\ \beta-\gamma\ne\alpha}} x_{\alpha-\beta}y_\gamma z_{\beta-\gamma} + \sum_{\beta\le\alpha'} x_\beta z_{\alpha'-\beta} - \varepsilon \sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\delta\le\alpha'-\beta} x_\delta y_{\alpha'-\beta-\delta} z_\gamma z_{\beta-\gamma}\end{aligned} \tag{1.5.104}$$

and, after replacing z_α according to (1.5.98), it turns into

$$c_\alpha x_\alpha + d_\alpha y_\alpha = f_\alpha \ , \tag{1.5.105}$$

where

$$\begin{aligned}c_\alpha &= -1 + Y + 2\varepsilon YZ = \varepsilon Y^2 + Y - 1 \\ d_\alpha &= -2 + \lambda_1\alpha_1 + \lambda_2\alpha_2 + X + 2\varepsilon XZ + \frac{2\varepsilon XY}{2+\lambda_1\alpha_1+\lambda_2\alpha_2} = \lambda_1\alpha_1 + \lambda_2\alpha_2 - 1 - \varepsilon Y^2 + \frac{2\varepsilon Y(1-\varepsilon Y)}{2+\lambda_1\alpha_1+\lambda_2\alpha_2} \\ f_\alpha &= -\sum_{\substack{\beta\le\alpha \\ \beta\ne 0,\alpha}} x_\beta y_{\alpha-\beta} - 2\varepsilon \sum_{\substack{\beta\le\alpha \\ \beta\ne 0}}\sum_{\substack{\gamma\le\beta \\ \gamma\ne\alpha \\ \beta-\gamma\ne\alpha}} x_{\alpha-\beta}y_\gamma z_{\beta-\gamma} + \sum_{\beta\le\alpha'} x_\beta z_{\alpha'-\beta} - \varepsilon \sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\delta\le\alpha'-\beta} x_\delta y_{\alpha'-\beta-\delta} z_\gamma z_{\beta-\gamma}\end{aligned} \tag{1.5.106}$$

We can uniquely solve the system comprised of (1.5.101) and (1.5.105) as long as the determinant

$$D_\alpha := a_\alpha d_\alpha - b_\alpha c_\alpha \tag{1.5.107}$$

is nonzero. Then the solution is

$$x_\alpha = \frac{d_\alpha e_\alpha - b_\alpha f_\alpha}{D_\alpha} \quad , \quad y_\alpha = \frac{-c_\alpha e_\alpha + a_\alpha f_\alpha}{D_\alpha} \ . \tag{1.5.108}$$

The following proposition deals with this and shows a uniform-in-α bound involving the coefficients of the linear system above:

Proposition 1.5.8. *For all $\alpha \in \mathbb{N}^2$ with $|\alpha| \geq 2$, we have $D_\alpha \neq 0$ and*

$$\frac{|a_\alpha|}{D_\alpha}\ ,\ \frac{|b_\alpha|}{D_\alpha}\ ,\ \frac{|c_\alpha|}{D_\alpha}\ ,\ \frac{|d_\alpha|}{D_\alpha} \leq 2\ . \tag{1.5.109}$$

In particular formulas (1.5.108) are well-posed and

$$|x_\alpha|, |y_\alpha|, |z_\alpha| \leq 2(|e_\alpha| + |f_\alpha|)\ . \tag{1.5.110}$$

Proof. Let the symbol $\boldsymbol{\lambda} \cdot \boldsymbol{\alpha}$ be used to abbreviate the number $\lambda_1\alpha_1 + \lambda_2\alpha_2$ (which is at least $\alpha_1 + \alpha_2 \geq 2$). We use (1.5.38) to say

$$|X| \leq 1 + 4\left(\frac{1}{2}\right)^2 = 2 \quad , \quad |Y| \leq 1\ . \tag{1.5.111}$$

Now use these to bound the first-order perturbation terms of $a_\alpha, \ldots, d_\alpha$, denoted as $\delta_a \ldots, \delta_d$:

$$\begin{aligned}
a_\alpha &= \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} + 1 - \varepsilon Y^2 =: \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} + 1 + \delta_a \varepsilon \\
b_\alpha &= \varepsilon\left(2XY + \frac{2X^2}{2 + \boldsymbol{\lambda} \cdot \boldsymbol{\alpha}}\right) =: \delta_b \varepsilon \\
c_\alpha &= -1 + Y + \varepsilon Y^2 = -2 + \varepsilon(Y^2 - Y^3 - Y^4) =: -2 + \delta_c \varepsilon \\
d_\alpha &= \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} - 1 + \varepsilon\left(-Y^2 + \frac{2Y(1 - \varepsilon Y)}{2 + \boldsymbol{\lambda} \cdot \boldsymbol{\alpha}}\right) =: \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} - 1 + \delta_d \varepsilon
\end{aligned} \tag{1.5.112}$$

where

$$\begin{aligned}
|\delta_a| &= |Y^2| \leq 1 \\
|\delta_b| &= \left|2XY + \frac{2X^2}{2 + \boldsymbol{\lambda} \cdot \boldsymbol{\alpha}}\right| \leq 4 + \frac{8}{4} = 6 \\
|\delta_c| &= |Y^2 - Y^3 - Y^4| \leq 3 \\
|\delta_d| &= \left|-Y^2 + \frac{2Y(1 - \varepsilon Y)}{2 + \boldsymbol{\lambda} \cdot \boldsymbol{\alpha}}\right| \leq 1 + \frac{2}{4} = \frac{3}{2}
\end{aligned} \tag{1.5.113}$$

In particular

$$\begin{aligned}
|a_\alpha| &\leq \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} + 1 + \varepsilon < \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} + \frac{3}{2} \\
|b_\alpha| &\leq 6\varepsilon < 3 \\
|c_\alpha| &\leq 2 + 3\varepsilon < \frac{7}{2} \\
|d_\alpha| &\leq \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} - 1 + \frac{3}{2}\varepsilon < \boldsymbol{\lambda} \cdot \boldsymbol{\alpha} - \frac{1}{4}
\end{aligned} \tag{1.5.114}$$

and the determinant D_α is

$$\begin{aligned} D_\alpha &= (\boldsymbol{\lambda}\cdot\boldsymbol{\alpha}+1+\delta_a\varepsilon)(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha}-1+\delta_d\varepsilon)-(\delta_b\varepsilon)(-2+\delta_c\varepsilon) \\ &= (\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})^2-1+\big((\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})(\delta_a+\delta_d)+\delta_d-\delta_a+2\delta_b\big)\varepsilon-\delta_b\delta_c\varepsilon^2 \\ &=: (\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})^2-1+\delta_D\varepsilon \end{aligned} \tag{1.5.115}$$

for δ_D satisfying

$$|\delta_D| \le (\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})|\delta_a+\delta_d|+|\delta_a|+2|\delta_b|+|\delta_d|+|\delta_b\delta_c|\varepsilon \le \frac{5}{2}(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})+\frac{47}{2}\ . \tag{1.5.116}$$

Therefore, the fractions $|a_\alpha|/D_\alpha,\dots,|d_\alpha|/D_\alpha$ decay with $1/\boldsymbol{\lambda}\cdot\boldsymbol{\alpha}$, but we shall only need to find a constant upper bound for them: we have

$$D_\alpha \ge (\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})^2-1-\frac{\varepsilon}{2}(5(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})+47) \ge 2(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})-1-\frac{5(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})+47}{4} = \frac{3(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})+43}{4} > \frac{3(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})}{4} > 0\ , \tag{1.5.117}$$

and therefore

$$\begin{aligned} \frac{|a_\alpha|}{D_\alpha} &\le \frac{2(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})+3}{2}\frac{4}{3(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})} = \frac{8+\frac{12}{\boldsymbol{\lambda}\cdot\boldsymbol{\alpha}}}{6} \le \frac{8+6}{6} = \frac{7}{3} \\ \frac{|b_\alpha|}{D_\alpha} &\le 3\frac{4}{3(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})} \le \frac{4}{2} = 2 \\ \frac{|c_\alpha|}{D_\alpha} &\le \frac{7}{2}\frac{4}{3(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})} \le \frac{28}{12} = \frac{7}{3} \\ \frac{|d_\alpha|}{D_\alpha} &\le \frac{4(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})-1}{4}\frac{4}{3(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})} = \frac{16-\frac{4}{(\boldsymbol{\lambda}\cdot\boldsymbol{\alpha})}}{12} < \frac{16}{12} = \frac{4}{3} \end{aligned} \tag{1.5.118}$$

proving the bound claimed.

Finally, inequality (1.5.110) is a consequence of formulas (1.5.108) for x_α, y_α and (1.5.98) for z_α. □

Remark 1.5.9. We shall also need bounds for $|x_\alpha|, |y_\alpha|, |z_\alpha|$ when $|\alpha| = 2$, for future use during the proof of convergence of the power series W. Expanding the formulas for e_α, f_α when $|\alpha| = 2$

(recall (1.5.86) for the definition of p, q) gives:

$$\begin{aligned}
e_{20} &= \varepsilon X^2 Z^2 \\
e_{11} &= 0 \\
e_{02} &= -\frac{1}{16}\Big((\varepsilon p)^2 - \varepsilon\big(X(3+\varepsilon q)^2 + 2Y\varepsilon p(3+\varepsilon q) + 2Z(\varepsilon p)^2 + 4X\varepsilon p\big)\Big) \\
f_{20} &= XZ - \varepsilon XYZ^2 \\
f_{11} &= 0 \\
f_{02} &= -\frac{1}{16}\Big(\varepsilon p(3+\varepsilon q) + 2\varepsilon\big(X(3+\varepsilon q) + Y\varepsilon p + Z\varepsilon p(3+\varepsilon q)\big)\Big)
\end{aligned} \tag{1.5.119}$$

Using

$$\varepsilon \le \frac{1}{60} \quad , \quad |X| \le 2\ ,\ |Y| \le 1\ ,\ |Z| \le \frac{1}{2} \quad , \quad 0 < p < 4\ ,\ 0 < q < 60\ , \tag{1.5.120}$$

we get:

$$|e_{20}| \le \varepsilon < \frac{1}{60} \quad , \quad |f_{20}| \le 1 + \frac{1/2}{60} = \frac{121}{120}\ , \tag{1.5.121}$$

$$|e_{02}| \le \frac{1}{16}\left(\left(\frac{4}{60}\right)^2 + \frac{1}{60}\left(2(3+1)^2 + 2\frac{4}{60}(3+1) + \left(\frac{4}{60}\right)^2 + 8\frac{4}{60}\right)\right) = \frac{7501}{216000}\ , \tag{1.5.122}$$

$$|f_{02}| \le \frac{1}{16}\left(\frac{4}{60}(3+1) + \frac{2}{60}\left(2(3+1) + \frac{4}{60} + \frac{1}{2}\frac{4}{60}(3+1)\right)\right) = \frac{27}{800}\ , \tag{1.5.123}$$

implying

$$|x_{20}|, |y_{20}|, |z_{20}| \le 2(|e_{20}| + |f_{20}|) \le \frac{41}{20} \tag{1.5.124}$$

and

$$|x_{02}|, |y_{02}|, |z_{02}| \le 2(|e_{02}| + |f_{02}|) \le \frac{14791}{108000} < \frac{41}{20}\ . \tag{1.5.125}$$

This number $41/20$ is the one that we will use in the next subsection, when proving that W converges.

Also note that the e_α and f_α coefficients above are null when $\varepsilon = 0$, except for f_{20} which contains a factor XZ that yields $-1/2$ when $\varepsilon = 0$. By keeping track of ε factors in the calculations above and using

$$1 \le X < 1 + \frac{\varepsilon}{15} \quad , \quad -\frac{1}{2} \le Z < -\frac{1}{2} + \varepsilon \tag{1.5.126}$$

to deal with the XZ term in f_{20}, we find bounds for the ε-perturbations of these coefficients, by which we mean the following:

$$\begin{gathered}
|e_{20}| < \varepsilon \quad , \quad e_{11} = 0 \quad , \quad |e_{02}| < \frac{7501\varepsilon}{3600}\ , \\
\left|f_{20} + \frac{1}{2}\right| < \frac{1831\varepsilon}{900} \quad , \quad f_{11} = 0 \quad , \quad |f_{02}| < \frac{81\varepsilon}{40}\ .
\end{gathered} \tag{1.5.127}$$

These inequalities will only be needed in subsection 1.5.6, when studying how far from $\mathcal{W}^{(0)}$ the manifold $\mathcal{W}^{(\varepsilon)}$ is.

1.5.4 Series convergence

Here we employ a technique similar to what we did in lemma 1.4.11 and theorem 1.4.13 in section 1.4, this time in order to estimate the various sums in e_α, f_α recursively. As it turns out, we need a new lemma suitable for multi-index sums of dimension 2, and a power 2 in the denominator is not enough — we will need a power 3.

Lemma 1.5.10. *For every $\delta_1, \delta_2 > 0$,*

$$\sum_{\beta\le\alpha} \frac{1}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3} \le \frac{35+2\left(\dfrac{1}{\delta_1}+\dfrac{1}{\delta_2}\right)^3}{(|\alpha|+\delta_1+\delta_2)^3} \quad , \quad |\alpha| \ge 0 \tag{1.5.128}$$

and

$$\sum_{\substack{\beta\le\alpha\\ \beta\ne 0,\alpha}} \frac{1}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3} \le \frac{35}{(|\alpha|+\delta_1+\delta_2)^3} \quad , \quad |\alpha| \ge 2\ . \tag{1.5.129}$$

Proof. Denote $|\alpha|$ by j. Note that $|\alpha-\beta| = |\alpha| - |\beta| = j - |\beta|$ for all $\beta \in \mathbb{N}^2$, $\beta \le \alpha$. We begin by proving (1.5.129), so let $j \ge 2$. By partial fractions in $|\beta|$:

$$\begin{aligned}\frac{1}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3} = \frac{1}{(j+\delta_1+\delta_2)^3}\Bigg(&\frac{6/(j+\delta_1+\delta_2)^2}{|\beta|+\delta_1} + \frac{3/(j+\delta_1+\delta_2)}{(|\beta|+\delta_1)^2} + \frac{1}{(|\beta|+\delta_1)^3}\\ &+ \frac{6/(j+\delta_1+\delta_2)^2}{|\alpha-\beta|+\delta_2} + \frac{3/(j+\delta_1+\delta_2)}{(|\alpha-\beta|+\delta_2)^2} + \frac{1}{(|\alpha-\beta|+\delta_2)^3}\Bigg)\ .\end{aligned} \tag{1.5.130}$$

As β sweeps the range between $(0,0)$ and α, the expression $\alpha-\beta$ also does. Hence

$$\begin{aligned}\sum_{\beta\le\alpha} \frac{1}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3} &= \frac{1}{(j+\delta_1+\delta_2)^3}\sum_{\beta\le\alpha}\Bigg(\frac{6/(j+\delta_1+\delta_2)^2}{|\beta|+\delta_1} + \frac{3/(j+\delta_1+\delta_2)}{(|\beta|+\delta_1)^2}\\ &\quad + \frac{1}{(|\beta|+\delta_1)^3} + \frac{6/(j+\delta_1+\delta_2)^2}{|\beta|+\delta_2} + \frac{3/(j+\delta_1+\delta_2)}{(|\beta|+\delta_2)^2} + \frac{1}{(|\beta|+\delta_2)^3}\Bigg)\\ &< \frac{1}{(j+\delta_1+\delta_2)^3}\sum_{\beta\le\alpha}\left(\frac{12/j^2}{|\beta|} + \frac{6/j}{|\beta|^2} + \frac{2}{|\beta|^3}\right)\ .\end{aligned} \tag{1.5.131}$$

We perform this sum by grouping together all β of an equal degree. For each $k = 1, \ldots, j$, there are $k+1$ multi-indices β with degree k: $(0,k), (1,k-1), \ldots, (k,0)$ (there may be fewer also satisfying

$\beta \le \alpha$, but we won't need to consider this). Hence we can estimate

$$\sum_{\beta \le \alpha} \frac{1}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3} < \frac{1}{(j+\delta_1+\delta_2)^3} \sum_{k=1}^{j} (k+1)\left(\frac{12/j^2}{k} + \frac{6/j}{k^2} + \frac{2}{k^3}\right)$$
$$= \frac{1}{(j+\delta_1+\delta_2)^3} \sum_{k=1}^{j} \left[\frac{12}{j^2} + \left(\frac{12}{j^2}+\frac{6}{j}\right)\frac{1}{k} + \left(\frac{6}{j}+2\right)\frac{1}{k^2} + \frac{2}{k^3}\right] \tag{1.5.132}$$

Now just bound each separate sum above uniformly over $j \ge 2$:

$$\sum_{k=1}^{j} \frac{12}{j^2} = \frac{12}{j} < 6 \ , \tag{1.5.133}$$

$$\left(\frac{12}{j^2}+\frac{6}{j}\right)\sum_{k=1}^{j}\frac{1}{k} < \left(\frac{12}{j^2}+\frac{6}{j}\right)(1+\log j) < \left(\frac{12}{j^2}+\frac{6}{j}\right)(1+j) = \frac{12}{j^2} + \frac{18}{j} + 6 < 18 \ , \tag{1.5.134}$$

$$\left(\frac{6}{j}+2\right)\sum_{k=1}^{j}\frac{1}{k^2} < \left(\frac{6}{2}+2\right)\sum_{k=1}^{\infty}\frac{1}{k^2} = \frac{5\pi^2}{6} \ , \tag{1.5.135}$$

$$\sum_{k=1}^{j}\frac{2}{k^3} < \sum_{k=1}^{\infty}\frac{2}{k^3} = 2\zeta(3) \ \text{ where } \zeta(p) \text{ gives the sum of a } p\text{-series} \ , \tag{1.5.136}$$

(we bounded the Harmonic Series in (1.5.134) using an integral, similarly to (1.4.128)), yielding

$$\sum_{\beta \le \alpha} \frac{1}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3} < \frac{6+18+\frac{5\pi^2}{6}+2\zeta(3)}{(j+\delta_1+\delta_2)^3} < \frac{35}{(j+\delta_1+\delta_2)^3} \ . \tag{1.5.137}$$

As a side remark, note how, had we tried to prove a similar lemma with a power 2 instead of 3 in the denominator, the second-to-last sum would have looked similar except that it would include $1/k$ instead of $1/k^2$, and would not have a uniform-in-j upper bound.

To prove (1.5.128), we must add to this bound the 2 terms obtained from (1.5.130) by plugging in $\beta = 0$ and $\beta = \alpha$ (even though $|\alpha|$ is now not restricted to be ≥ 2, the bound above remains valid for the sum over all $\beta \ne 0, \alpha$ because these terms are only present if $|\alpha| \ge 2$). By substituting 0 for $|\alpha|$ in the denominators, the sum of these 2 terms can be bounded above by

$$\frac{2}{(|\beta|+\delta_1)^3(|\alpha-\beta|+\delta_2)^3}\left[\frac{1}{\delta_1^3}+\frac{1}{\delta_2^3}+\frac{3}{\delta_1+\delta_2}\left(\frac{1}{\delta_1^2}+\frac{1}{\delta_2^2}\right)+\frac{6}{(\delta_1+\delta_2)^2}\left(\frac{1}{\delta_1}+\frac{1}{\delta_2}\right)\right] \ , \tag{1.5.138}$$

and the expression between brackets simplifies to $\left(\dfrac{1}{\delta_1}+\dfrac{1}{\delta_2}\right)^3$. □

Theorem 1.5.11. *Let $\varepsilon \in [0, 1/60)$ and consider the sequences $(x_\alpha), (y_\alpha), (z_\alpha)$ defined as above. Then there exist $R, S, \delta > 0$ such that, for all $\alpha \in \mathbb{N}^2$,*

$$|x_\alpha|, |y_\alpha|, |z_\alpha| \leq \frac{SR^{|\alpha|}}{(|\alpha| + \delta)^3} \ . \tag{1.5.139}$$

Furthermore, it is possible to have

$$R = 360 \quad , \quad \delta < \frac{1}{7} \quad , \quad S = 2\delta^3 \ . \tag{1.5.140}$$

Proof. Fix a small $\delta > 0$ (to be specified later). Define

$$X_\alpha = \max\{|x_\alpha|, |y_\alpha|, |z_\alpha|\} \geq 0 \ . \tag{1.5.141}$$

We have bounds for X_α when $|\alpha| \leq 2$, given by (1.5.85), (1.5.88), (1.5.124) and (1.5.125):

$$X_{00} \leq 2 \quad , \quad X_{01}, X_{10} \leq 1 \quad , \quad X_{02}, X_{11}, X_{20} \leq \frac{41}{20} \ , \tag{1.5.142}$$

To make the claimed inequality work when $|\alpha| \leq 2$, we take

$$S = 2\delta^3 \quad , \quad R \geq \frac{(1+\delta)^3}{2\delta^3} \quad , \quad R^2 \geq \frac{41(2+\delta)^3}{20\delta^3} \ . \tag{1.5.143}$$

One can check that, for $\delta < 0.4$, the first of these two inequalities for R implies the second. So impose $\delta < 0.4$ *a priori* and define

$$R = \frac{(1+\delta)^3}{2\delta^3} \ . \tag{1.5.144}$$

In particular, note the following inequality (to be used later in this proof):

$$\frac{1}{R^2} = \frac{4\delta^6}{(1+\delta)^6} < 4\delta^6 \ . \tag{1.5.145}$$

Now let $j \geq 2$ and suppose for induction that the claimed inequality (1.5.139) is true for multi-indices of degree j or smaller. Let $\alpha \in \mathbb{N}^2$ with $|\alpha| = j + 1$. We will prove that it is true for X_α, noting that

$$|x_\alpha|, |y_\alpha|, |z_\alpha| \leq 2(|e_\alpha| + |f_\alpha|) \quad \Longrightarrow \quad X_\alpha \leq 2(|e_\alpha| + |f_\alpha|) \ . \tag{1.5.146}$$

We estimate $2(|e_\alpha|+|f_\alpha|)$ by taking the absolute value of all terms in the formulas (1.5.102), (1.5.106) for e_α, f_α and substituting all x, y, z terms with X:

$$2(|e_\alpha| + |f_\alpha|) \le 2\Bigg[2 \sum_{\substack{\beta<\alpha \\ \beta\neq 0,\alpha}} X_\beta X_{\alpha-\beta} + 5\varepsilon \sum_{\substack{\beta\le\alpha \\ \beta\neq 0}} \sum_{\substack{\gamma\le\beta \\ \gamma\neq\alpha \\ \beta-\gamma\neq\alpha}} X_{\alpha-\beta} X_\gamma X_{\beta-\gamma}$$
$$+ \sum_{\beta\le\alpha'} X_\beta X_{\alpha'-\beta} + 2\varepsilon \sum_{\beta\le\alpha'} \sum_{\gamma\le\beta} \sum_{\theta\le\alpha'-\beta} X_\theta X_{\alpha'-\beta-\theta} X_\gamma X_{\beta-\gamma}\Bigg] . \quad (1.5.147)$$

First let us rewrite the second of these sums, separating out the terms from it that include an X_{00} factor (this is just so that lemma 1.5.10 can be applied to what will be left). Note that the sum of the indices in this term is α, while the conditions in the summation are the same as saying that the term X_α does not occur. Hence only one of the three $X_{\alpha-\beta}, X_\gamma, X_{\beta-\gamma}$ can be equal to X_{00}, and we have (changing β to $\alpha-\beta$)

$$\sum_{\substack{\beta\le\alpha \\ \beta\neq 0}} \sum_{\substack{\gamma\le\beta \\ \gamma\neq\alpha \\ \beta-\gamma\neq\alpha}} X_{\alpha-\beta} X_\gamma X_{\beta-\gamma} = 3X_{00} \sum_{\substack{\beta\le\alpha \\ \beta\neq 0,\alpha}} X_\beta X_{\alpha-\beta} + \sum_{\substack{\beta\le\alpha \\ \beta\neq 0,\alpha}} X_\beta \sum_{\substack{\gamma\le\alpha-\beta \\ \gamma\neq 0,\alpha-\beta}} X_\gamma X_{\alpha-\beta-\gamma} . \quad (1.5.148)$$

By then bounding X_{00} with 2 and combining the first term in (1.5.148) above with that in (1.5.147), we have

$$2(|e_\alpha| + |f_\alpha|) \le 2\Bigg[(2+30\varepsilon) \sum_{\substack{\beta<\alpha \\ \beta\neq 0,\alpha}} X_\beta X_{\alpha-\beta} + 5\varepsilon \sum_{\substack{\beta\le\alpha \\ \beta\neq 0,\alpha}} X_\beta \sum_{\substack{\gamma\le\alpha-\beta \\ \gamma\neq 0,\alpha-\beta}} X_\gamma X_{\alpha-\beta-\gamma}$$
$$+ \sum_{\beta\le\alpha'} X_\beta X_{\alpha'-\beta} + 2\varepsilon \sum_{\beta\le\alpha'} \sum_{\gamma\le\beta} \sum_{\theta\le\alpha'-\beta} X_\theta X_{\alpha'-\beta-\theta} X_\gamma X_{\beta-\gamma}\Bigg] . \quad (1.5.149)$$

This recursive inequality, once the induction hypothesis is applied to its right side, is in a form amenable to application of lemma 1.5.10. In the first two of its terms, we will use inequality (1.5.129) with its δ-independent numerator, 35, because the sums in these terms exclude the smallest and largest indices. We also remark that $|\alpha-\beta| = |\alpha| - |\beta| = j+1-|\beta|$ and that, to complete the induction, we want to make the term $SR^{j+1}/(j+1+\delta)^3$ appear.

- For the first term,

$$\sum_{\substack{\beta\le\alpha \\ \beta\neq 0,\alpha}} X_\beta X_{\alpha-\beta} \le S^2 \sum_{\substack{\beta\le\alpha \\ \beta\neq 0,\alpha}} \frac{R^{|\beta|} R^{j+1-|\beta|}}{(|\beta|+\delta)^3 (j+1-|\beta|+\delta)^3}$$
$$\le S^2 R^{j+1} \frac{35}{(j+1+2\delta)^3} < \frac{SR^{j+1}}{(j+1+\delta)^3} 70\delta^3 . \quad (1.5.150)$$

- The inequality above applies to half of the second term, and the rest is similar:

$$\sum_{\substack{\beta\le\alpha\\ \beta\ne 0,\alpha}} X_\beta \sum_{\substack{\gamma\le\alpha-\beta\\ \gamma\ne 0,\alpha-\beta}} X_\gamma X_{\alpha-\beta-\gamma} \le S^3 \sum_{\substack{\beta\le\alpha\\ \beta\ne 0,\alpha}} \frac{R^{|\beta|}}{(|\beta|+\delta)^3}\frac{35R^{j+1-|\beta|}}{(j+1-|\beta|+2\delta)^3}$$
$$< S^3R^{j+1}\frac{35^2}{(j+1+3\delta)^3} < \frac{SR^{j+1}}{(j+1+\delta)^3}4900\delta^6 \ . \quad (1.5.151)$$

- In the third term we need inequality (1.5.128). Also note that the indices add up to α', whose degree is $j-1$.

$$\sum_{\beta\le\alpha'} X_\beta X_{\alpha'-\beta} \le S^2R^{j-1}\frac{35+16/\delta^3}{(j-1+2\delta)^3} < \frac{SR^{j+1}}{(j+1+\delta)^3}\frac{27}{R^2}(70\delta^3+32) \ , \quad (1.5.152)$$

where we used

$$\frac{1}{(j-1+2\delta)^3} = \frac{1}{(j+1+\delta)^3}\left(\frac{j+1+\delta}{j-1+2\delta}\right)^3 = \frac{1}{(j+1+\delta)^3}\left(1+\frac{2-\delta}{j-1+2\delta}\right)^3$$
$$< \frac{1}{(j+1+\delta)^3}\left(1+\frac{2-\delta}{1+2\delta}\right)^3 = \frac{1}{(j+1+\delta)^3}\left(3-\frac{5\delta}{1+2\delta}\right)^3 < \frac{27}{(j+1+\delta)^3} \ , \quad (1.5.153)$$

which is similar to (1.4.138) and requires $j\ge 2$, as we assumed before starting the inductive step.

- In the last term, lemma 1.5.10 is needed three times:

$$\sum_{\beta\le\alpha'}\sum_{\gamma\le\beta}\sum_{\theta\le\alpha'-\beta} X_\theta X_{\alpha'-\beta-\theta}X_\gamma X_{\beta-\gamma} \le S^4R^{j-1}\sum_{\beta\le\alpha'}\frac{35+16/\delta^3}{(j-1-|\beta|+2\delta)^3}\frac{35+16/\delta^3}{(|\beta|+2\delta)^3}$$
$$\le \frac{S^4R^{j-1}}{(j-1+4\delta)^3}\left(35+\frac{16}{\delta^3}\right)^2\left(35+\frac{2}{\delta^3}\right) < \frac{SR^{j+1}}{(j+1+\delta)^3}\frac{27}{R^2}(70\delta^3+32)^2(70\delta^3+4) \ . \quad (1.5.154)$$

All together, we have proved that

$$X_\alpha \le \frac{SR^{j+1}}{(j+1+\delta)^3}b_{R,\delta} \ , \quad (1.5.155)$$

with the expression $b_{R,\delta}$ (which we must prove is less than 1) equal to

$$b_{R,\delta} = 2\left[(2+30\varepsilon)70\delta^3 + 5\varepsilon\cdot 4900\delta^6 + \frac{27}{R^2}\Big((70\delta^3+32) + 2\varepsilon(70\delta^3+32)^2(70\delta^3+4)\Big)\right] \ . \quad (1.5.156)$$

Using (1.5.145) to bound $1/R^2$:

$$b_{R,\delta} \le 4\delta^3\left[70 + 1050\varepsilon + 12250\varepsilon\delta^3 + 54\delta^3\Big((70\delta^3+32) + 2\varepsilon(70\delta^3+32)^2(70\delta^3+4)\Big)\right] \ . \quad (1.5.157)$$

Using $\varepsilon < 1/60$:

$$b_{R,\delta} < \delta^3 \left[350 + \delta^3 \left(45828 + 3780\delta^3 + \frac{9}{5}(70\delta^3 + 32)^2(70\delta^3 + 4)\right)\right] \ . \tag{1.5.158}$$

In particular, it will be necessary to choose δ such that

$$\delta^3 < \frac{1}{350} \ . \tag{1.5.159}$$

So we can assume this *a priori* to bound all occurrences of δ^3 inside the square brackets and conclude

$$b_{R,\delta} < \delta^3 \left[350 + \frac{1}{350}\left(45828 + \frac{3780}{350} + \frac{9}{5}\left(\frac{70}{350} + 32\right)^2 \left(\frac{70}{350} + 4\right)\right)\right] = \frac{15730117}{31250}\delta^3 < 504\delta^3 \ . \tag{1.5.160}$$

Therefore, if

$$\delta = (504)^{-1/3} \approx 0.126 < \frac{1}{7} \ , \tag{1.5.161}$$

the induction is complete. Plugging this into the definition of R, we get

$$R = \frac{(1+\delta)^3}{2\delta^3} \approx 359.43 < 360 \ , \tag{1.5.162}$$

and again, just like in the proof of theorem 1.4.13, we are allowed to redefine R to be exactly 360. $\square$

Corollary 1.5.12. *For $\varepsilon \in [0, 1/60)$, the radius of convergence of*

$$W(\tau,\sigma) = \sum_\alpha (x_\alpha, y_\alpha, z_\alpha, s_\alpha)\tau^{\alpha_1}\sigma^{\alpha_2} \tag{1.5.163}$$

is at least $1/360$*.*

Proof. Let $R = 360$. For any $\sigma, \tau \in \mathbb{R}$ with $|\sigma|, |\tau| < 1/R$, we have

$$\left|\sum_\alpha x_\alpha \tau^{\alpha_1}\sigma^{\alpha_2}\right| \leq \sum_\alpha \frac{SR^{|\alpha|}}{(|\alpha|+\delta)^3}\tau^{\alpha_1}\sigma^{\alpha_2} < \frac{S}{\delta^3}\sum_{\alpha_1=0}^{\infty}\sum_{\alpha_2=0}^{\infty}(R\tau)^{\alpha_1}(R\sigma)^{\alpha_2} \ , \tag{1.5.164}$$

and the 2 geometric series are convergent. The same is valid for y, z, while we already remarked that the series for $s = \tau$ is a finite sum, hence of infinite radius. $\square$

1.5.5 The ψ equation and finiteness of the energy

In the introductory section 1.1 we've seen how finiteness of the integrals (1.3.50) and (1.3.51), that is,

$$\int_0^\infty \frac{\psi\zeta^{-1}(w')^2}{r^2}\mathrm{d}r \quad , \quad \int_0^\infty \frac{\psi(w-1)}{r^2}\mathrm{d}r \ ,$$

implies a finite electric field energy as well as a finite value for the electric potential at $r = 0$. We also mentioned that, after we prove that one of the solutions we found in section 1.4 for large r intersects one of the ones we found here for small r, the only problematic endpoint in these integrals is $r = 0$, given the asymptotics of the solutions for large r. We will now verify the finiteness of these integrals along any solutions (ψ, ζ, w) that correspond to orbits of the unstable manifold $\mathcal{W}$ that we just proved exists.

The equilibrium point $P = (X, Y, Z, 0)$ that we found in the above work satisfies

$$0 < |X| < \infty \quad , \quad 0 < |Y| < \infty \quad , \quad 0 < |Z| < \infty \ . \tag{1.5.165}$$

Going back through the desingularization steps in (1.5.1), we realize that these inequalities can be written in the form

$$0 < \lim_{r\to 0}\zeta(r) < \infty \quad , \quad 0 < \lim_{r\to 0}\left|\frac{w(r)-1}{r^2}\right| < \infty \quad , \quad 0 < \lim_{r\to 0}\left|\frac{w'(r)}{r}\right| < \infty \ . \tag{1.5.166}$$

We now study the behavior of ψ along solutions on the unstable manifold $\mathcal{W}$. The relevant equation is that in (1.1.13):

$$\frac{\mathrm{d}\psi}{\mathrm{d}r} = -\varepsilon\frac{\psi(r)}{r^3}\left(\frac{\mathrm{d}w}{\mathrm{d}r}\right)^2 \ . \tag{1.5.167}$$

To solve it, we apply to ψ the same steps performed in subsection 1.5.1, with the first one being the only nontrivial step: consider

$$\hat{\chi}(r) = r^{\varepsilon Y^2}\psi(r) \ . \tag{1.5.168}$$

Then, for prime denoting $\mathrm{d}/\mathrm{d}r$,

$$\hat{\chi}'(r) = \varepsilon Y^2 r^{\varepsilon Y^2 - 1}\psi(r) - \varepsilon r^{\varepsilon Y^2}\frac{\psi(r)w'(r)^2}{r^3} = \varepsilon\hat{\chi}(r)\left(Y^2 - \frac{h(r)^2}{r^3}\right) \ . \tag{1.5.169}$$

Now let $\chi(t_2) = \hat{\chi}(t_1(t_2))$ and evaluate the above at $t_1(t_2)$:

$$\frac{\mathrm{d}\chi}{\mathrm{d}t_2} = \varepsilon\chi(t_2)\left(Y^2 - \frac{\hat{y}^2}{\hat{s}^2}\right) = \varepsilon\chi(Y^2 - y^2) \ . \tag{1.5.170}$$

This is solved by

$$\chi(t_2) = \chi_0 \exp\left(\varepsilon \int_{t_0}^{t_2} (Y^2 - y(t)^2)\mathrm{d}t\right) \ . \tag{1.5.171}$$

where t_0, χ_0 are arbitrary with $\chi_0 = \chi(t_0)$. We claim that it is possible to choose $t_0 = -\infty$; that is, we claim that, along any orbit $\boldsymbol{x}(t)$ in the unstable manifold $\mathcal{W}$, the function $Y^2 - y^2$ is integrable around $t = -\infty$. Granted this claim, we will then have

$$\lim_{r\to 0} r^{\varepsilon Y^2}\psi(r) = \lim_{t_2\to-\infty} \chi(t_2) = \chi = \lim_{t_2\to-\infty} \chi(t_2) < \infty \ , \tag{1.5.172}$$

which, together with (1.5.166), implies that the integrands in (1.5.5) blow up like $r^{-\varepsilon Y^2}$ near 0, still within the integrable range when $\varepsilon < 1$ (recall that $|Y| \leq 1$). This implies, as we had claimed, that ψ does not grow fast enough around $r = 0$ to render the energy infinite.

To justify the claim above, first estimate

$$\left|\int_{-\infty}^{t_2} (Y^2 - y(t)^2)\mathrm{d}t\right| \leq \left(Y + \sup_{t\leq t_2} |y(t)|\right) \int_{-\infty}^{t_2} |y(t) - Y|\mathrm{d}t \ . \tag{1.5.173}$$

Since $\lim_{t\to-\infty} y(t) = Y$ exists, the constant outside the integral is finite, and we just need to prove that the integral is too.

Since $\boldsymbol{x}(t)$ is an orbit on $\mathcal{W}$, for every $t < t_2$ there exist parameters $\tau(t), \sigma(t)$ such that

$$\boldsymbol{x}(t) = W(\tau(t), \sigma(t)) \quad , \quad t < t_2 \ , \tag{1.5.174}$$

and in particular

$$\boldsymbol{x}(t) - P = \sum_{|\alpha|\geq 1} \boldsymbol{w}_\alpha \tau(t)^{\alpha_1}\sigma(t)^{\alpha_2} \ . \tag{1.5.175}$$

Differentiating (1.5.174) with respect to t gives

$$\boldsymbol{F}(W(\tau(t), \sigma(t))) = \boldsymbol{F}(\boldsymbol{x}(t)) = \boldsymbol{x}'(t) = DW(\tau(t), \sigma(t)) \begin{bmatrix} \tau'(t) \\ \sigma'(t) \end{bmatrix} \ , \tag{1.5.176}$$

which, given the invariance equation (1.5.82), becomes

$$DW(\tau(t), \sigma(t)) \begin{bmatrix} \lambda_1\tau(t) \\ \lambda_2\sigma(t) \end{bmatrix} = DW(\tau(t), \sigma(t)) \begin{bmatrix} \tau'(t) \\ \sigma'(t) \end{bmatrix} \ . \tag{1.5.177}$$

We can assume $DW(\tau(t), \sigma(t))$ is invertible by bringing t_2 closer to $-\infty$ if necessary, and this becomes a simple ODE system for τ, σ with solution

$$\tau(t) = C_1 e^{\lambda_1 t} \quad , \quad \sigma(t) = C_2 e^{\lambda_2 t} \tag{1.5.178}$$

for some C_1, C_2 which depend on the orbit chosen. Now plug this into (1.5.175) and use the bound (1.5.139) on $|y_\alpha|$:

$$|y(t) - Y| \leq S \sum_{|\alpha|\geq 1} \frac{|C_1|^{\alpha_1}|C_2|^{\alpha_2}R^{|\alpha|}}{(|\alpha|+\delta)^3} e^{(\lambda_1\alpha_1+\lambda_2\alpha_2)t} \leq \frac{2\delta^3}{\delta^3} \sum_{|\alpha|\geq 1} (CR)^{|\alpha|} e^{(\lambda_1\alpha_1+\lambda_2\alpha_2)t} \ , \tag{1.5.179}$$

where $C = \max\{|C_1|, |C_2|\}$. Using the fact that $\lambda_1 = 1, \lambda_2 < 1 + 60\varepsilon < 2$,

$$|y(t) - Y| \leq 2 \sum_{|\alpha|\geq 1} (CRe^{2t})^{|\alpha|} \ . \tag{1.5.180}$$

Decreasing t_2 once again if necessary, we may assume $CRe^{2t} \leq \gamma < 1$ for some constant γ. Then this is summable:

$$\begin{aligned} |y(t) - Y| \leq 2 \left(\sum_{\alpha\in\mathbb{N}^2} (CRe^{2t})^{|\alpha|} - 1 \right) &= \frac{2}{(1-CRe^{2t})^2} - 2 \\ &= \frac{2CRe^{2t}(2 - CRe^{2t})}{(1-CRe^{2t})^2} < \frac{2CRe^{2t}(2-\gamma)}{(1-\gamma)^2} \ . \end{aligned} \tag{1.5.181}$$

This is enough to guarantee that $y(t) - Y$ is integrable from $-\infty$, as claimed.

1.5.6 ε-perturbation of the unstable manifold $\mathcal{W}$

Now that we have a good estimate for the radius of convergence of the power series for the unstable manifold $\mathcal{W}^{(\varepsilon)}$, we want to understand how far from $\mathcal{W}^{(0)}$ it is - that is, we want to find bounds for the ε-perturbation of the coordinates of this manifold in (x, y, z, s)-space, as described by theorem 1.5.2.

We need to start using (ε) superscripts again. For each $\varepsilon \in [0, 1/60)$, denote by

$$\boldsymbol{w}_\alpha^{(\varepsilon)}(\tau,\sigma) = (x_\alpha^{(\varepsilon)}(\tau,\sigma), y_\alpha^{(\varepsilon)}(\tau,\sigma), z_\alpha^{(\varepsilon)}(\tau,\sigma), s_\alpha^{(\varepsilon)}(\tau,\sigma)) \tag{1.5.182}$$

the coefficients of the power series

$$W^{(\varepsilon)}(\tau,\sigma) = \sum_{\alpha\in\mathbb{N}^2} \boldsymbol{w}_\alpha^{(\varepsilon)} \tau^{\alpha_1}\sigma^{\alpha_2} \ , \tag{1.5.183}$$

which we just proved converges with a uniform-in-ε radius of 1/360. Define **perturbation coefficients**, denoted with a tilde:

$$\widetilde{\boldsymbol{w}_\alpha}^{(\varepsilon)}(\tau,\sigma) = (\widetilde{x_\alpha}^{(\varepsilon)}(\tau,\sigma), \widetilde{y_\alpha}^{(\varepsilon)}(\tau,\sigma), \widetilde{z_\alpha}^{(\varepsilon)}(\tau,\sigma), \widetilde{s_\alpha}^{(\varepsilon)}(\tau,\sigma)) \ , \tag{1.5.184}$$

according to

$$\boldsymbol{w}_\alpha^{(\varepsilon)} = \boldsymbol{w}_\alpha^{(0)} + \varepsilon \widetilde{\boldsymbol{w}_\alpha}^{(\varepsilon)} \ . \tag{1.5.185}$$

Each $\widetilde{\boldsymbol{w}}_\alpha^{(\varepsilon)}$ term itself depends on ε in an analytic way that we shall not need to consider. We are interested in obtaining bounds for them which are ε-independent over the domain $\varepsilon \in [0, 1/60)$, so we are going to omit the (ε) superscript from them to clean up the notation.

We repeat here the relevant information about the $\boldsymbol{w}_\alpha$ coefficients to see how $\widetilde{\boldsymbol{w}_\alpha}$ can be obtained. First of all, the s coefficients contain no perturbation terms: given that $s_\alpha^{(\varepsilon)}$ is 1 if $\alpha = (1,0)$ and 0 otherwise, we have

$$\widetilde{s_\alpha} = 0 \quad , \quad \alpha \in \mathbb{N}^2 \ . \tag{1.5.186}$$

Next, the initial values of the x, y, z coefficients for $|\alpha| \leq 1$ are given in equations (1.5.84), (1.5.86), (1.5.87) as

$$\left\{ \begin{array}{rcl} x_{00}^{(\varepsilon)} &=& X^{(\varepsilon)} \\ y_{00}^{(\varepsilon)} &=& Y^{(\varepsilon)} \\ z_{00}^{(\varepsilon)} &=& Z^{(\varepsilon)} \end{array} \right. \quad , \quad \left\{ \begin{array}{rcl} x_{10}^{(\varepsilon)} &=& 0 \\ y_{10}^{(\varepsilon)} &=& 0 \\ z_{10}^{(\varepsilon)} &=& 0 \end{array} \right. \quad , \quad \left\{ \begin{array}{rcl} x_{01}^{(\varepsilon)} &=& \dfrac{\varepsilon p^{(\varepsilon)}}{4} \\ y_{01}^{(\varepsilon)} &=& \dfrac{3 + \varepsilon q^{(\varepsilon)}}{4} \\ z_{01}^{(\varepsilon)} &=& \dfrac{1}{4} \end{array} \right. \quad , \tag{1.5.187}$$

and we have proven in lemmas 1.5.5 and 1.5.7 that

$$\left\{ \begin{array}{rcll} X^{(\varepsilon)} &=& 1 + 4\delta_X^{(\varepsilon)}\varepsilon^2 & \text{with } 0 \leq \delta_X^{(\varepsilon)} \leq 1 \\ Y^{(\varepsilon)} &=& -1 + 2\delta_Y^{(\varepsilon)}\varepsilon & \text{with } 0 \leq \delta_Y^{(\varepsilon)} \leq 1 \\ Z^{(\varepsilon)} &=& -1/2 + \delta_Z^{(\varepsilon)}\varepsilon & \text{with } 0 \leq \delta_Z^{(\varepsilon)} \leq 1 \end{array} \right. \quad , \quad \left\{ \begin{array}{l} 0 \leq p^{(\varepsilon)} \leq 4 \\ 0 \leq q^{(\varepsilon)} \leq 60 \end{array} \right. \ . \tag{1.5.188}$$

This implies that

$$\left\{ \begin{array}{rcl} |\widetilde{x_{00}}| &\leq& 4\varepsilon < 1/15 \\ |\widetilde{y_{00}}| &\leq& 2 \\ |\widetilde{z_{00}}| &\leq& 1 \end{array} \right. \quad , \quad \left\{ \begin{array}{rcl} |\widetilde{x_{01}}| &\leq& 1 \\ |\widetilde{y_{01}}| &\leq& 15 \\ \widetilde{z_{01}} &=& 0 \end{array} \right. \quad , \quad \left\{ \begin{array}{rcl} \widetilde{x_{10}} &=& 0 \\ \widetilde{y_{10}} &=& 0 \\ \widetilde{z_{10}} &=& 0 \end{array} \right. \tag{1.5.189}$$

Finally the recursion for x, y, z coefficients when $|\alpha| \geq 2$ is given in (1.5.101), (1.5.105) and (1.5.98) as

$$\left\{ \begin{array}{rcl} a_\alpha^{(\varepsilon)} x_\alpha^{(\varepsilon)} + b_\alpha^{(\varepsilon)} y_\alpha^{(\varepsilon)} &=& e_\alpha^{(\varepsilon)} \\ c_\alpha^{(\varepsilon)} x_\alpha^{(\varepsilon)} + d_\alpha^{(\varepsilon)} y_\alpha^{(\varepsilon)} &=& f_\alpha^{(\varepsilon)} \end{array} \right. \quad , \quad z_\alpha^{(\varepsilon)} = \frac{y_\alpha^{(\varepsilon)}}{2 + \lambda_1^{(\varepsilon)}\alpha_1 + \lambda_2^{(\varepsilon)}\alpha_2} \ , \tag{1.5.190}$$

where

$$e_\alpha^{(\varepsilon)} = -\sum_{\substack{\beta\le\alpha\\ \beta\neq 0,\alpha}} x_\beta^{(\varepsilon)} x_{\alpha-\beta}^{(\varepsilon)}$$
$$-\varepsilon\Bigg(\sum_{\substack{\beta\le\alpha\\ \beta\neq 0}} \sum_{\substack{\gamma\le\beta\\ \gamma\neq\alpha\\ \beta-\gamma\neq\alpha}} (x_{\alpha-\beta}^{(\varepsilon)} y_\gamma^{(\varepsilon)} y_{\beta-\gamma}^{(\varepsilon)} + 2z_{\alpha-\beta}^{(\varepsilon)} x_\gamma^{(\varepsilon)} x_{\beta-\gamma}^{(\varepsilon)}) + \sum_{\beta\le\alpha'} \sum_{\gamma\le\beta} \sum_{\delta\le\alpha'-\beta} x_\gamma^{(\varepsilon)} x_{\beta-\gamma}^{(\varepsilon)} z_\delta^{(\varepsilon)} z_{\alpha'-\beta-\delta}^{(\varepsilon)} \Bigg) \tag{1.5.191}$$

$$f_\alpha^{(\varepsilon)} = -\sum_{\substack{\beta\le\alpha\\ \beta\neq 0,\alpha}} x_\beta^{(\varepsilon)} y_{\alpha-\beta}^{(\varepsilon)} - 2\varepsilon \sum_{\substack{\beta\le\alpha\\ \beta\neq 0}} \sum_{\substack{\gamma\le\beta\\ \gamma\neq\alpha\\ \beta-\gamma\neq\alpha}} x_{\alpha-\beta}^{(\varepsilon)} y_\gamma^{(\varepsilon)} z_{\beta-\gamma}^{(\varepsilon)}$$
$$+ \sum_{\beta\le\alpha'} x_\beta^{(\varepsilon)} z_{\alpha'-\beta}^{(\varepsilon)} - \varepsilon \sum_{\beta\le\alpha'} \sum_{\gamma\le\beta} \sum_{\delta\le\alpha'-\beta} x_\delta^{(\varepsilon)} y_{\alpha'-\beta-\delta}^{(\varepsilon)} z_\gamma^{(\varepsilon)} z_{\beta-\gamma}^{(\varepsilon)} \tag{1.5.192}$$

We must use these equations to write a recursion for $\widetilde{\boldsymbol{w}_\alpha}$, $|\alpha| \geq 2$. For any such α, define perturbations coefficients corresponding to a_α through f_α above:

$$a_\alpha^{(\varepsilon)} = a_\alpha^{(0)} + \varepsilon\widetilde{a_\alpha} \quad , \quad \text{etc.} \tag{1.5.193}$$

Also here the terms with a tilde depend on ε, but we don't write (ε) over them. In the linear system found in (1.5.190) for $x_\alpha^{(\varepsilon)}$ and $y_\alpha^{(\varepsilon)}$, write each coefficient as a (0) term plus ε times the perturbation term, distribute out and cancel those terms containing only (0) superscripts (this can be done because, by definition of the (0) superscript, the equations

$$\begin{cases} a_\alpha^{(0)} x_\alpha^{(0)} + b_\alpha^{(0)} y_\alpha^{(0)} &= e_\alpha^{(0)} \\ c_\alpha^{(0)} x_\alpha^{(0)} + d_\alpha^{(0)} y_\alpha^{(0)} &= f_\alpha^{(0)} \end{cases} \tag{1.5.194}$$

are true). Finally, divide by a common factor of ε. What is obtained can then be put in the form

$$\begin{cases} a_\alpha^{(\varepsilon)} \widetilde{x_\alpha} + b_\alpha^{(\varepsilon)} \widetilde{y_\alpha} &= -\widetilde{a_\alpha} x_\alpha^{(0)} - \widetilde{b_\alpha} y_\alpha^{(0)} + \widetilde{e_\alpha} =: \widetilde{E_\alpha} \\ c_\alpha^{(\varepsilon)} \widetilde{x_\alpha} + d_\alpha^{(\varepsilon)} \widetilde{y_\alpha} &= -\widetilde{c_\alpha} x_\alpha^{(0)} - \widetilde{d_\alpha} y_\alpha^{(0)} + \widetilde{f_\alpha} =: \widetilde{F_\alpha} \end{cases} . \tag{1.5.195}$$

We've already proved in proposition 1.5.8 that the solution to this system is unique and satisfies

$$|\widetilde{x_\alpha}|, |\widetilde{y_\alpha}| \leq 2(|\widetilde{E_\alpha}| + |\widetilde{F_\alpha}|) \ . \tag{1.5.196}$$

Having obtained these solutions, we get $\widetilde{z_\alpha}$ using the equation for $z_\alpha^{(\varepsilon)}$ shown above in (1.5.190), and it satisfies

$$|\widetilde{z_\alpha}| \leq \frac{|\widetilde{y_\alpha}|}{2} \tag{1.5.197}$$

because $z_\alpha^{(0)} = y_\alpha^{(0)}/2$. This and equation (1.5.196) together imply

$$|\widetilde{x_\alpha}|, |\widetilde{y_\alpha}|, |\widetilde{z_\alpha}| \leq 2(|\widetilde{E_\alpha}| + |\widetilde{F_\alpha}|) \quad \Longrightarrow \quad \widetilde{X_\alpha} \leq 2(|\widetilde{E_\alpha}| + |\widetilde{F_\alpha}|) \ . \tag{1.5.198}$$

where

$$\widetilde{X_\alpha} = \max\{|\widetilde{x_\alpha}|, |\widetilde{y_\alpha}|, |\widetilde{z_\alpha}|\} \geq 0 \quad , \quad \alpha \in \mathbb{N}^2 \ . \tag{1.5.199}$$

Hence we need to estimate $|\widetilde{E_\alpha}|$ and $|\widetilde{F_\alpha}|$ by a workable expression involving sums of the coefficients $\widetilde{X_\beta}$ for $\beta < \alpha$. It will also involve coefficients X_β for $\beta \leq \alpha$, where

$$X_\alpha = \max\{|x_\alpha^{(0)}|, |y_\alpha^{(0)}|, |z_\alpha^{(0)}|\} \geq 0 \quad , \quad \alpha \in \mathbb{N}^2 \ . \tag{1.5.200}$$

The two initial terms in the system (1.5.195) defining both $\widetilde{E_\alpha}$ and $\widetilde{F_\alpha}$ are easily bounded:

$$\begin{cases} |-\widetilde{a_\alpha} x_\alpha^{(0)} - \widetilde{b_\alpha} y_\alpha^{(0)}| \leq X_\alpha + 6X_\alpha = 7X_\alpha \\ |-\widetilde{c_\alpha} x_\alpha^{(0)} - \widetilde{d_\alpha} y_\alpha^{(0)}| \leq 3X_\alpha + (3/2)X_\alpha = (9/2)X_\alpha \end{cases} . \tag{1.5.201}$$

For this, we've used equations (1.5.112) and (1.5.113), which contain bounds for the perturbations of the a_α through d_α coefficients that can be paraphrased as:

$$|\widetilde{a_\alpha}| \leq 1 \quad , \quad |\widetilde{b_\alpha}| \leq 6 \quad , \quad |\widetilde{c_\alpha}| \leq 3 \quad , \quad |\widetilde{d_\alpha}| \leq \frac{3}{2} \ . \tag{1.5.202}$$

Remark 1.5.13. As was the case in subsection 1.5.4, we need to obtain the bound for $\widetilde{X_\alpha}$ for $|\alpha| = 2$ directly, before letting the recursion kick in at $|\alpha| \geq 3$. So let $|\alpha| = 2$. The inequalities (1.5.127) in remark 1.5.9 already provide bounds for $\widetilde{e_\alpha}, \widetilde{f_\alpha}$. It will be enough to write all of them as

$$|\widetilde{e_\alpha}|, |\widetilde{f_\alpha}| < \frac{21}{10} \quad , \quad |\alpha| = 2 \ . \tag{1.5.203}$$

Plugging these and (1.5.201) into (1.5.195) gives bounds for $\widetilde{E_\alpha}, \widetilde{F_\alpha}$ when $|\alpha| = 2$:

$$|\widetilde{E_\alpha}| < 7X_\alpha + \frac{21}{10} \quad , \quad |\widetilde{F_\alpha}| < \frac{9X_\alpha}{2} + \frac{21}{10} \quad , \quad |\alpha| = 2 \ . \tag{1.5.204}$$

Considering also the bound $41/20$ given in (1.5.124) and (1.5.125) for X_α, and inequality (1.5.198) for $\widetilde{X_\alpha}$, we obtain

$$\widetilde{X_\alpha} \leq 2\left(\left(7 + \frac{9}{2}\right)\frac{41}{20} + \frac{21}{10}\right) = \frac{1027}{20} \quad , \quad |\alpha| = 2 \ . \tag{1.5.205}$$

Now consider $|\alpha| \geq 3$. Bounding the $\widetilde{e_\alpha}$ and $\widetilde{f_\alpha}$ terms inside $\widetilde{E_\alpha}$ and $\widetilde{F_\alpha}$ by induction requires first writing them out by expanding the (1.5.191) and (1.5.192) expressions for $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$, replacing every term $*^{(\varepsilon)}$ with $*^{(0)} + \varepsilon\widetilde{*}$, distributing out, disregarding the expressions that contain no ε factor, and dividing through by ε. After this, we bound them by using absolute values on each separate sum and replacing every $| *^{(0)} |$ by X and every $|\widetilde{*}|$ by $\widetilde{X}$. To display this process, it's better if we show it separately for each sum, double sum etc. appearing in the expressions (1.5.191) and (1.5.192) for $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$:

- Both $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$ contain a sum of the form

$$\sum_{\substack{\beta \leq \alpha \\ \beta \neq 0, \alpha}} *_\beta^{(\varepsilon)} *_{\alpha-\beta}^{(\varepsilon)}$$

Under the process described above, the term $*_\beta^{(0)} *_{\alpha-\beta}^{(0)}$ goes away and the remaining terms lose one factor of ε, producing:

$$\sum_{\substack{\beta \leq \alpha \\ \beta \neq 0, \alpha}} \left(X_\beta \widetilde{X_{\alpha-\beta}} + \widetilde{X_\beta} X_{\alpha-\beta} + \varepsilon \widetilde{X_\beta} \widetilde{X_{\alpha-\beta}} \right) = \sum_{\substack{\beta \leq \alpha \\ \beta \neq 0, \alpha}} \left(2X_\beta \widetilde{X_{\alpha-\beta}} + \varepsilon \widetilde{X_\beta} \widetilde{X_{\alpha-\beta}} \right) \tag{1.5.206}$$

- The $f_\alpha^{(\varepsilon)}$ term also contains the sum

$$\sum_{\beta \leq \alpha'} x_\beta^{(\varepsilon)} z_{\alpha'-\beta}^{(\varepsilon)}$$

The process works similarly to the previous item, giving:

$$\sum_{\beta \leq \alpha'} \left(X_\beta \widetilde{X_{\alpha'-\beta}} + \widetilde{X_\beta} X_{\alpha'-\beta} + \varepsilon \widetilde{X_\beta} \widetilde{X_{\alpha'-\beta}} \right) = \sum_{\beta \leq \alpha'} \left(2X_\beta \widetilde{X_{\alpha'-\beta}} + \varepsilon \widetilde{X_\beta} \widetilde{X_{\alpha'-\beta}} \right) \tag{1.5.207}$$

- Both $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$ also contain sums of the form

$$\sum_{\substack{\beta \leq \alpha \\ \beta \neq 0 \\ \beta-\gamma \neq \alpha}} \sum_{\substack{\gamma \leq \beta \\ , \gamma \neq \alpha}} *_{\alpha-\beta}^{(\varepsilon)} *_\gamma^{(\varepsilon)} *_{\beta-\gamma}^{(\varepsilon)}$$

This time, these sums already appear multiplied by ε in both of the $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$ expressions, so the process described above amounts to simply canceling this overall ε factor from the final result, while the terms inside these sums themselves don't lose an ϵ:

$$\sum_{\substack{\beta+\gamma+\theta=\alpha\\ \beta,\gamma,\theta\neq\alpha}} \left(X_\beta X_\gamma X_\delta + 3\varepsilon X_\beta X_\gamma \widetilde{X_\theta} + 3\varepsilon^2 X_\beta \widetilde{X_\gamma}\widetilde{X_\theta} + \varepsilon^3 \widetilde{X_\beta}\widetilde{X_\gamma}\widetilde{X_\theta} \right)$$
$$= \sum_{\substack{\beta\leq\alpha\\ \beta\neq 0}} \sum_{\substack{\gamma\leq\beta\\ \gamma\neq\alpha\\ \beta-\gamma\neq\alpha}} \left(X_{\alpha-\beta} X_\gamma X_{\beta-\gamma} + 3\varepsilon X_{\alpha-\beta} X_\gamma \widetilde{X_{\beta-\gamma}} + 3\varepsilon^2 X_{\alpha-\beta}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} + \varepsilon^3 \widetilde{X_{\alpha-\beta}}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} \right) \tag{1.5.208}$$

- Finally, both $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$ contain a sum of the form

$$\sum_{\beta\leq\alpha'} \sum_{\gamma\leq\beta} \sum_{\delta\leq\alpha'-\beta} *_\delta^{(\varepsilon)} *_{\alpha'-\beta-\delta}^{(\varepsilon)} *_\gamma^{(\varepsilon)} *_{\beta-\gamma}^{(\varepsilon)}$$

which also appears multiplied by ε. Similarly to the item above, the process makes:

$$\sum_{\beta+\gamma+\theta+\iota=\alpha'} \left(X_\beta X_\gamma X_\theta X_\iota + 4\varepsilon X_\beta X_\gamma X_\theta \widetilde{X_\iota} + 6\varepsilon^2 X_\beta X_\gamma \widetilde{X_\theta}\widetilde{X_\iota} + 4\varepsilon^3 X_\beta \widetilde{X_\gamma}\widetilde{X_\theta}\widetilde{X_\iota} + \varepsilon^4 \widetilde{X_\beta}\widetilde{X_\gamma}\widetilde{X_\theta}\widetilde{X_\iota} \right)$$
$$= \sum_{\beta\leq\alpha'} \sum_{\gamma\leq\beta} \sum_{\delta\leq\alpha'-\beta} \Big(X_\delta X_{\alpha'-\beta-\delta} X_\gamma X_{\beta-\gamma} + 4\varepsilon X_\delta X_{\alpha'-\beta-\delta} X_\gamma \widetilde{X_{\beta-\gamma}} + 6\varepsilon^2 X_\delta X_{\alpha'-\beta-\delta}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}}$$
$$+ 4\varepsilon^3 X_\delta \widetilde{X_{\alpha'-\beta-\delta}}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} + \varepsilon^4 \widetilde{X_\delta}\widetilde{X_{\alpha'-\beta-\delta}}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} \Big) \tag{1.5.209}$$

To bound $\widetilde{E_\alpha}$ and $\widetilde{F_\alpha}$, add all the sums obtained in the items above multiplied by their corresponding coefficients in the equations (1.5.191) and (1.5.192) for $e_\alpha^{(\varepsilon)}$ and $f_\alpha^{(\varepsilon)}$. Also include the initial terms (1.5.201). Then plug all this into (1.5.198), where $|\widetilde{E_\alpha}|$ and $|\widetilde{F_\alpha}|$ appear summed together. The conclusion is that

$$\widetilde{X_\alpha} \leq 23 X_\alpha + 4 \sum_{\substack{\beta\leq\alpha\\ \beta\neq 0,\alpha}} \left(2X_\beta \widetilde{X_{\alpha-\beta}} + \varepsilon \widetilde{X_\beta}\widetilde{X_{\alpha-\beta}} \right) + 2 \sum_{\beta\leq\alpha'} \left(2X_\beta \widetilde{X_{\alpha'-\beta}} + \varepsilon \widetilde{X_\beta}\widetilde{X_{\alpha'-\beta}} \right)$$
$$+ 10 \sum_{\substack{\beta\leq\alpha\\ \beta\neq 0}} \sum_{\substack{\gamma\leq\beta\\ \gamma\neq\alpha\\ \beta-\gamma\neq\alpha}} \left(X_{\alpha-\beta} X_\gamma X_{\beta-\gamma} + 3\varepsilon X_{\alpha-\beta} X_\gamma \widetilde{X_{\beta-\gamma}} + 3\varepsilon^2 X_{\alpha-\beta}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} + \varepsilon^3 \widetilde{X_{\alpha-\beta}}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} \right)$$
$$+ 4 \sum_{\beta\leq\alpha'} \sum_{\gamma\leq\beta} \sum_{\delta\leq\alpha'-\beta} \Big(X_\delta X_{\alpha'-\beta-\delta} X_\gamma X_{\beta-\gamma} + 4\varepsilon X_\delta X_{\alpha'-\beta-\delta} X_\gamma \widetilde{X_{\beta-\gamma}} + 6\varepsilon^2 X_\delta X_{\alpha'-\beta-\delta}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}}$$
$$+ 4\varepsilon^3 X_\delta \widetilde{X_{\alpha'-\beta-\delta}}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} + \varepsilon^4 \widetilde{X_\delta}\widetilde{X_{\alpha'-\beta-\delta}}\widetilde{X_\gamma}\widetilde{X_{\beta-\gamma}} \Big) \tag{1.5.210}$$

Our summation technique can now be applied to prove a bound for $\widetilde{X_\alpha}$ by recursion. It utilizes the same values of R, S, δ as in theorem 1.5.1 (it has to, otherwise the technique is not helpful), but with an extra constant $K = 30$:

Theorem 1.5.14. *For R, S, δ being the same constants as in theorem 1.5.1, we have*

$$\widetilde{X_\alpha} \leq \frac{30SR^{|\alpha|}}{(|\alpha|+\delta)^3} \quad , \quad \alpha \in \mathbb{N}^2 \ . \tag{1.5.211}$$

Proof. The numbers

$$R = 360 \quad , \quad \delta < \frac{1}{7} \quad , \quad S = 2\delta^3 \tag{1.5.212}$$

in theorem 1.5.1 are such that such that

$$X_\alpha \leq \frac{SR^{|\alpha|}}{(|\alpha|+\delta)^3} \quad , \quad \alpha \in \mathbb{N}^2 \ . \tag{1.5.213}$$

Suppose that we seek $K > 0$ such that the inequality

$$\widetilde{X_\alpha} \leq \frac{KSR^{|\alpha|}}{(|\alpha|+\delta)^3} \quad , \quad \alpha \in \mathbb{N}^2 \tag{1.5.214}$$

is true. We want to prove that $K = 30$ is enough.

First note that the desired inequality is true for $|\alpha| \leq 2$. Indeed, we've seen in equations (1.5.189) and (1.5.205) that

$$\widetilde{X_{00}} \leq 2 \quad , \quad \widetilde{X_{01}}, \widetilde{X_{10}} \leq 15 \quad , \quad \widetilde{X_{02}}, \widetilde{X_{11}}, \widetilde{X_{20}} \leq \frac{1027}{20} \ . \tag{1.5.215}$$

Compare to the bounds (1.5.142) for the X_α coefficients when $|\alpha| \leq 2$:

$$X_{00} \leq 2 \quad , \quad X_{01}, X_{10} \leq 1 \quad , \quad X_{02}, X_{11}, X_{20} \leq \frac{41}{20} \ . \tag{1.5.216}$$

The difference between each is by a factor not larger than 30, so, because R, S, δ were enough to ensure (1.5.213) when $|\alpha| \leq 2$, they are also enough to ensure (1.5.214) when $|\alpha| \leq 2$ if $K = 30$.

Now let $j \geq 2$ and assume that (1.5.214) has been proven when $|\alpha| \leq j$. Let $\alpha \in \mathbb{N}^2$ be such that $|\alpha| = j + 1$. We will use equation (1.5.210) to establish (1.5.214) also for α. In what follows, let's abbreviate

$$R_\beta := \frac{SR^{|\beta|}}{(|\beta|+\delta)^3} \tag{1.5.217}$$

Bound each X_β with R_β and each $\widetilde{X_\beta}$ with KR_β. Then the distinction between terms inside each sum containing a different number of factors with a tilde becomes just the number of factors of K that appear, and note how terms inside the last two sums become perfect powers of $1+\varepsilon K$:

$$\widetilde{X_\alpha} \leq 23R_\alpha + 4(2K+\varepsilon K^2) \sum_{\substack{\beta\leq\alpha \\ \beta\neq 0,\alpha}} R_\beta R_{\alpha-\beta} + 2(2K+\varepsilon K^2) \sum_{\beta\leq\alpha'} R_\beta R_{\alpha'-\beta}$$
$$+ 10(1+\varepsilon K)^3 \sum_{\substack{\beta\leq\alpha \\ \beta\neq 0}} \sum_{\substack{\gamma\leq\beta \\ \gamma\neq\alpha \\ \beta-\gamma\neq\alpha}} R_{\alpha-\beta} R_\gamma R_{\beta-\gamma} + 4(1+\varepsilon K)^4 \sum_{\beta\leq\alpha'} \sum_{\gamma\leq\beta} \sum_{\delta\leq\alpha'-\beta} R_\delta R_{\alpha'-\beta-\delta} R_\gamma R_{\beta-\gamma} \quad (1.5.218)$$

Just like in the proof of theorem 1.5.1, we need to separate out from the second-to-last sum those terms containing a factor R_{00}:

$$\sum_{\substack{\beta\leq\alpha \\ \beta\neq 0}} \sum_{\substack{\gamma\leq\beta \\ \gamma\neq\alpha \\ \beta-\gamma\neq\alpha}} R_{\alpha-\beta} R_\gamma R_{\beta-\gamma} = 3R_{00} \sum_{\substack{\beta\leq\alpha \\ \beta\neq 0,\alpha}} R_\beta R_{\alpha-\beta} + \sum_{\substack{\beta\leq\alpha \\ \beta\neq 0,\alpha}} R_\beta \sum_{\substack{\gamma\leq\alpha \\ \gamma\neq 0,\alpha-\beta}} R_\gamma R_{\alpha-\beta-\gamma}$$

Then bound R_{00} by 2 and combine its term into the other sum of the form $\sum_{\substack{\beta\leq\alpha \\ \beta\neq 0,\alpha}} R_\beta R_{\alpha-\beta}$ in the main estimate (also rearrange its order to become similar to the proof of 1.5.1):

$$\widetilde{X_\alpha} \leq 23R_\alpha + (6+4K(2+\varepsilon K)) \sum_{\substack{\beta\leq\alpha \\ \beta\neq 0,\alpha}} R_\beta R_{\alpha-\beta} + 10(1+\varepsilon K)^3 \sum_{\substack{\beta\leq\alpha \\ \beta\neq 0,\alpha}} R_\beta \sum_{\substack{\gamma\leq\alpha-\beta \\ \gamma\neq 0,\alpha-\beta}} R_\gamma R_{\alpha-\beta-\gamma}$$
$$+ 2K(2+\varepsilon K) \sum_{\beta\leq\alpha'} R_\beta R_{\alpha'-\beta} + 4(1+\varepsilon K)^4 \sum_{\beta\leq\alpha'} \sum_{\gamma\leq\beta} \sum_{\delta\leq\alpha'-\beta} R_\delta R_{\alpha'-\beta-\delta} R_\gamma R_{\beta-\gamma} \quad (1.5.219)$$

The estimate of each sum now proceeds exactly as in that proof, yielding

$$\widetilde{X_\alpha} \leq R_{\alpha+1} b_{R,\delta} \quad (1.5.220)$$

for

$$b_{R,\delta} = 23 + (6+4K(2+\varepsilon K))70\delta^3 + 10(1+\varepsilon K)^2 4900\delta^6$$
$$+ \frac{27}{R^2}\left(2K(2+\varepsilon K)(32+70\delta^3) + 4(1+\varepsilon K)^4(32+70\delta^3)^2(4+70\delta^3)\right) \quad (1.5.221)$$

To close the induction, we need to show that $b_{R,\delta} \leq 30$. One can see that this is the case by using $\varepsilon < 1/60$ and the values of $K = 30$ and R, δ as in theorem 1.5.1.

$\square$

The next corollary is a rewriting of the second of the main theorems in this section, theorem 1.5.2:

Corollary 1.5.15. *For any fixed $0 \leq \gamma < 1$ and parameters τ, σ such that*

$$|\tau|, |\sigma| \leq \frac{\gamma}{360} \ , \tag{1.5.222}$$

the components $x^{(\varepsilon)}, y^{(\varepsilon)}, z^{(\varepsilon)}$ of the parametrization $\boldsymbol{w}^{(\varepsilon)}$ of $\mathcal{W}^{(\varepsilon)}$ satisfy

$$|x^{(\varepsilon)}(\tau,\sigma) - x^{(0)}(\tau,\sigma)| \leq \frac{60\varepsilon}{(1-\gamma)^2} \ , \ \textit{similarly for } y, z \ . \tag{1.5.223}$$

Proof. Given that $x^{(\varepsilon)}(\tau,\sigma) = x^{(0)}(\tau,\sigma) + \varepsilon\widetilde{x}(\tau,\sigma)$, we have

$$\begin{aligned}
|x^{(\varepsilon)}(\tau,\sigma) - x^{(0)}(\tau,\sigma)| &\leq \varepsilon \sum_{\alpha} |\widetilde{x_\alpha}||\tau|^{\alpha_1}|\sigma|^{\alpha_2} \\
&\leq \frac{30S\varepsilon}{\delta^3} \sum_{\alpha} R^{|\alpha|} \left(\frac{\gamma}{R}\right)^{\alpha_1} \left(\frac{\gamma}{R}\right)^{\alpha_2} \\
&= \frac{30(2\delta^3)\varepsilon}{\delta^3} \sum_{\alpha_1} \gamma^{\alpha_1} \sum_{\alpha_2} \gamma^{\alpha_2} \\
&= \frac{60\varepsilon}{(1-\gamma)^2}
\end{aligned} \tag{1.5.224}$$

□

We end this section with an explicit description of the unstable manifold $\mathcal{W}^{(0)}$:

Proposition 1.5.16. *For $\tau > 0$, the parametrization $W^{(0)}(\tau,\sigma) = (x(\tau,\sigma), y(\tau,\sigma), z(\tau,\sigma), s(\tau,\sigma))$ of the unstable manifold $\mathcal{W}^{(0)}$ corresponding to $\varepsilon = 0$ is given by*

$$\begin{aligned}
x(\tau,\sigma) &= 1 \\
y(\tau,\sigma) &= -e^{-\tau} + V(\tau,\sigma)(e^{-\tau} - e^{\tau}) \\
z(\tau,\sigma) &= \frac{(1+\tau)e^{-\tau} - 1 + V(\tau,\sigma)((1-\tau)e^{\tau} - (1+\tau)e^{-\tau})}{\tau^2} \\
s(\tau,\sigma) &= \tau
\end{aligned} \tag{1.5.225}$$

where

$$V(\tau,\sigma) = \frac{1}{2} - \frac{3\sigma}{8\tau} \ . \tag{1.5.226}$$

Proof. Considering the general ζ solution of the original system (1.1.13) when $\varepsilon = 0$, which is

$$\zeta(r) = \left(1 + \frac{M}{r}\right)^{-1} \ , \tag{1.5.227}$$

where M is an integration constant. When $M \neq 0$, the limit $\lim_{t_2 \to -\infty} x(t_2) = \lim_{r \to 0} \zeta(r) = 0$ is not the value that it needs to be in order for the corresponding orbit (x, y, z, s) of the desingularized system (1.5.12) to converge to the equilibrium point $P^{(0)} = (1, -1, -1/2, 0)$ as "time" t_2 goes to $-\infty$. Therefore, for any orbits on $\mathcal{W}^{(0)}$, the corresponding ζ necessarily has $M = 0$ (that is, $\zeta \equiv 1$ and $x \equiv 1$). This renders the w equation in (1.1.13) easily solvable:

$$w(r) = C_1(1+r)e^{-r} + C_2(1-r)e^{r} \ , \tag{1.5.228}$$

where C_1, C_2 are integration constants. The expansion of this solution around $r = 0$ is

$$w(r) = (C_1 + C_2) - \frac{C_1 + C_2}{2} r^2 + O(r^3) \ . \tag{1.5.229}$$

The corresponding orbits (x, y, z, s) to such w solutions will only converge to $P^{(0)}$ when the expressions that yield the y and z coordinates of their limit behave correctly:

$$\lim_{r \to 0} \frac{w'(r)}{r} = -1 \quad , \quad \lim_{r \to 0} \frac{w(r) - 1}{r^2} = -\frac{1}{2} \ , \tag{1.5.230}$$

and these conditions are true if and only if $C_1 + C_2 = 1$, restricting the freedom in w to just one parameter $C = C_2 = 1 - C_1$:

$$w(r) = (1+r)e^{-r} + C\big((1-r)e^{r} - (1+r)e^{-r}\big) \ . \tag{1.5.231}$$

The value $C = 0$ corresponds to the solution that we have been calling the "flat-space solution" (all of the solutions described above give the Minkowsky spacetime, since they all have $\zeta \equiv 1$, but only the one with $C = 0$ produces a $w(r)$ that goes to 0 at $r = \infty$). Now write the x, y, z, s functions corresponding to the ζ, w just described as functions of "time" t_2 (that is, replace r by e^{t_2}):

$$\begin{aligned} x \equiv 1 \quad , \quad y = -e^{-e^{t_2}} + C\big(e^{-e^{t_2}} - e^{e^{t_2}}\big) \quad , \\ z = \frac{(1+e^{t_2})e^{-e^{t_2}} - 1 + C\big((1-e^{t_2})e^{e^{t_2}} - (1+e^{t_2})e^{-e^{t_2}}\big)}{e^{2t_2}} \quad , \quad s = e^{t_2} \ . \end{aligned} \tag{1.5.232}$$

They span a 2-dimensional manifold as C and t_2 vary, hence we have found $\mathcal{W} = \mathcal{W}^{(0)}$.

To see how the parameter C is related to the parameters (τ, σ), fix τ, σ, with $\tau \neq 0$, small enough that the series W converges. The point

$$W(\tau, \sigma) = (x(\tau, \sigma), y(\tau, \sigma), z(\tau, \sigma), \tau) \tag{1.5.233}$$

belongs to the manifold $\mathcal{W}$ and thus must be of the form (1.5.232) above (with every e^{t_2} replaced by τ). Hence there must exist $C = C(\tau, \sigma)$ such that

$$\begin{aligned} x(\tau,\sigma) &= 1 \\ y(\tau,\sigma) &= -e^{-\tau} + C(\tau,\sigma)(e^{-\tau} - e^{\tau}) \\ z(\tau,\sigma) &= \frac{(1+\tau)e^{-\tau} - 1 + C(\tau,\sigma)((1-\tau)e^{\tau} - (1+\tau)e^{-\tau})}{\tau^2} \end{aligned} \tag{1.5.234}$$

The second component in the invariance equation (1.5.82) reads

$$\tau\frac{\partial y}{\partial \tau} + \sigma\frac{\partial y}{\partial \sigma} = 1 + 2y - xy + s^2 xz = 1 + y + \tau^2 z\ . \tag{1.5.235}$$

Using y and z as in (1.5.234), we check that this becomes

$$\tau\frac{\partial C}{\partial \tau} + \sigma\frac{\partial C}{\partial \sigma} = 0 \implies C(\tau,\sigma) = U\left(\frac{\sigma}{\tau}\right) \tag{1.5.236}$$

for some real-valued function U. But the invariance equation alone does not carry all the information needed to relate U to the parametrization W, because it doesn't know of the choices made for $W(0,0)$ (the equilibrium point) and the first derivatives $W_\tau(0,0), W_\sigma(0,0)$ (the eigenvectors of the linearization). We will bring them in by considering small τ and σ and connecting them to the values $\boldsymbol{w}_{00}, \boldsymbol{w}_{01}, \boldsymbol{w}_{10}$.

Let $u \in \mathbb{R}$ be given; we want to compute $U(u)$. Choose τ small enough that both τ and $\sigma = u\tau$ are within the radius of convergence of W, and solve for $C(\tau, u\tau) = U(u\tau/\tau) = U(u)$ in the y equation in (1.5.234):

$$U(u) = \frac{y(\tau,u\tau) + e^{-\tau}}{e^{-\tau} - e^{\tau}} = \frac{\sum_\alpha y_\alpha u^{\alpha_2}\tau^{|\alpha|} + e^{-\tau}}{e^{-\tau} - e^{\tau}}\ . \tag{1.5.237}$$

This is true for all small $\tau > 0$, so we can take a limit as $\tau \to 0$. We note that the limit is of the indeterminate form $0/0$, due to

$$\lim_{\tau\to 0}\sum_\alpha y_\alpha u^{\alpha_2}\tau^{|\alpha|} + e^{-\tau} = y_{00} + 1 = -1 + 1 = 0\ . \tag{1.5.238}$$

By L'Hôpital's Rule,

$$U(u) = \lim_{\tau\to 0}\frac{\sum_\alpha y_\alpha u^{\alpha_2}|\alpha|\tau^{|\alpha|-1} - e^{-\tau}}{-e^{-\tau} - e^{\tau}} = \frac{y_{10} + y_{01}u - 1}{-1-1} = \frac{1}{2} - \frac{3u}{8}\ . \tag{1.5.239}$$

Plugging this back into (1.5.234) proves the proposition.

□

1.6 Connecting the two radial regimes

In section 1.5 we proved that, for any

$$0 \leq \varepsilon < \frac{1}{60} \ , \tag{1.6.1}$$

there exists a family of solutions to the desingularized Maxwell-BLTP-Einstein system (1.5.12) tracing out a 2D surface $\mathcal{W}^{(\varepsilon)}$ in 4D space (x, y, z, s), which corresponds to a family of solutions to the original system (1.1.13) satisfying the good asymptotic conditions as $r \to 0$ for a finite EM field energy, as described in subsection 1.3.5. We showed that $\mathcal{W}^{(\varepsilon)}$ is parametrized by 2 real numbers τ, σ in the region

$$|\tau|, |\sigma| \leq \frac{1}{360} \ , \tag{1.6.2}$$

with τ being equal to the s coordinate on $\mathcal{W}^{(\varepsilon)}$. We also obtained an estimate, of degree 1 in ε, for the difference between the coordinates of $\mathcal{W}^{(\varepsilon)}$ and $\mathcal{W}^{(0)}$.

In section 1.4 we proved that, for any fixed $0 < r_0 < 1$ and parameters $\mu_*, \alpha_* > 0$ and $\mu, \alpha, \varepsilon \in \mathbb{R}$ under the restrictions

$$|\mu| < \mu_* \quad , \quad |\alpha| \leq \alpha_* \quad , \quad 0 \leq \varepsilon < \frac{r_0^7}{240(15 + 4r_0\mu_* + r_0^4\alpha_*)} \quad , \quad \varepsilon\mu_*^2 < 1 \ , \tag{1.6.3}$$

there exists a solution, continuous on its parameters μ, α, to the Maxwell-BLTP-Einstein system (1.2.78) on $[r_0, \infty)$ satisfying the good asymptotic conditions as $r \to \infty$ for an asymptotically Minkowsky spacetime and asymptotically Coulomb electric field, as described in subsection 1.3.5. We also proved that, when ε is less than 1/4 of the bound given above, the ζ function is positive, as is desired.

In the present section, we prove that the two families meet at some $0 < r_0 < 1$. We will keep working in (x, y, z, s) variables, since it is more convenient to work in these variables when r is small. We know that the intersection exists when $\varepsilon = 0$, yielding the flat-space solution. To prove that this intersection remains when ε is small, a system of coordinates c_1, c_2, c_3 in the 3-dimensional space $\{(x, y, z, r) \ ; \ r = r_0\}$ will be defined based on the linear-in-ε approximation to the 2-parameter family of good solutions on $[r_0, \infty)$. We will show how certain inequalities, involving these coordinates at general points on each of the two families above, ensure that they intersect as a consequence of the *Poincaré-Miranda theorem*.

Once the intersection is proved, the existence and uniqueness theorem for ODE systems applied to the original system in the variables ζ, w at this point (where there are no singularities) implies that the two orbits from each of the families meeting at this point must join smoothly and constitute a solution for $r \in (0, \infty)$, satisfying all the required asymptotics.

1.6.1 Set-up

Let $\mu_*, \alpha_* > 0$ be fixed. Also fix 2 scalars $\gamma_0, \gamma_\infty \in (0, 1)$ to be specified later, and let r_0, ε_* be defined by

$$r_0 = \frac{3}{4} \cdot \frac{\gamma_0}{360} \quad , \quad \varepsilon_* = \frac{\gamma_\infty r_0^7}{240(15 + 4r_0\mu_* + r_0^4\alpha_*)} \ . \tag{1.6.4}$$

The indices $0, \infty$ in the gamma parameters are intended to remind the reader that they are associated with the family of solutions coming from $r = 0$ and $r = \infty$, respectively. They are going to be needed to ensure convergence of the respective power series, and the reason for the factor $3/4$ in the definition of r_0 will become clear in equation (1.6.13) below. We anticipate that γ_∞ will need to be made small so that ε is small (in particular $gamma_\infty < 1/4$ will hold, a condition that is needed to guarantee $\zeta > 0$).

First let's describe the family of solutions coming from $r = 0$. It is clear that $\varepsilon < 1/60$, so that all results from section 1.5 are valid. Also note that the unstable manifold $\mathcal{W} = \mathcal{W}^{(\varepsilon)}$ extends past the hyperplane $s = r_0$ in the s direction, since the $\tau = s$ parameter can be taken as large as $1/360 > \gamma_0/360 > r_0$. So consider the curve traced out by $\mathcal{W}$ in 3D space $\{(x, y, z, r_0)\}$:

$$\mathcal{C}^{(\varepsilon)} = \mathcal{C} = \mathcal{W} \cap \{(x, y, z, s) \in \mathbb{R}^4 \ , \ s = r_0\} \ . \tag{1.6.5}$$

It is parametrized by σ. We only know its existence for σ values small enough that the W series converges; so we only consider the piece of this curve corresponding to $\sigma \in [\gamma_0/360, \gamma_0/360]$. Let its general point be denoted

$$C(\sigma) := (x_C(\sigma), y_C(\sigma), z_C(\sigma), r_0) \quad , \quad |\sigma| \leq \frac{\gamma_0}{360} \ . \tag{1.6.6}$$

Also let x_N, y_N, z_N ("N" for "null") denote the coordinates of the curve $\mathcal{C}_N$ described above for the value $\varepsilon = 0$. Theorem 1.5.2 gives uniform-in-σ estimates for the perturbation coefficients $\widetilde{x}, \widetilde{y}, \widetilde{z}$ defined by

$$x_C(\sigma) = x_N(\sigma) + \widetilde{x}_C(\sigma) \quad , \quad \text{etc.} \tag{1.6.7}$$

Namely, we proved that

$$|\tilde{x}(\sigma)|, |\tilde{y}(\sigma)|, |\tilde{z}(\sigma)| \leq \frac{60\varepsilon}{(1-\max\{\frac{3\gamma_0}{4},\gamma_0\})^2} = \frac{60\varepsilon}{(1-\gamma_0)^2} \ . \tag{1.6.8}$$

Meanwhile, the components x_N, y_N, z_N of the $\mathcal{W}^{(0)}$ manifold split as a sum of a term accompanied by the function $V(\tau,\sigma) = V(r_0,\sigma)$ and another independent of it, given in formulas (1.5.225). We give names for these pieces:

$$x_N(\sigma) = x_N^{(I)} + V(\sigma)x_N^{(II)} \quad , \quad \text{etc. ,} \tag{1.6.9}$$

where

$$x_N^{(I)} = 1 \quad , \quad y_N^{(I)} = -e^{-r_0} \quad , \quad z_N^{(I)} = \frac{(1+r_0)e^{-r_0}-1}{r_0^2} \ , \tag{1.6.10}$$

$$x_N^{(II)} = 0 \quad , \quad y_N^{(II)} = e^{-r_0} - e^{r_0} \quad , \quad z_N^{(II)} = \frac{(1-r_0)e^{r_0}-(1+r_0)e^{-r_0}}{r_0^2} \ , \tag{1.6.11}$$

and where we denoted $V(r_0,\sigma)$ from (1.5.226) by simply $V(\sigma)$:

$$V(\sigma) = \frac{1}{2} - \frac{3\sigma}{8r_0} \ . \tag{1.6.12}$$

We remarked in the proof of proposition 1.5.16 that the flat-space solution corresponds to the value

$$V(\sigma) = 0 \iff \sigma = \frac{4r_0}{3} \ . \tag{1.6.13}$$

Considering the factor 3/4 in the definition (1.6.4) of r_0, we see that this value of σ is within the radius of convergence for the curve $\mathcal{C}$.

Now let's describe the family of solutions coming from $r=\infty$. For any choice of μ,α satisfying

$$|\mu| \leq \mu_* \quad , \quad |\alpha| \leq \alpha_* \ , \tag{1.6.14}$$

consider the functions $\eta^{(\mu,\alpha)}, u^{(\mu,\alpha)}, v^{(\mu,\alpha)}$ of $r \in [r_0,\infty)$ as obtained in section 1.4:

$$\eta^{(\mu,\alpha)}(r) = \sum_{j=0}^{\infty} \eta_j^{(\mu,\alpha)}(r)\varepsilon^j \quad , \quad u^{(\mu,\alpha)}(r) = \sum_{j=0}^{\infty} u_j^{(\mu,\alpha)}(r)\varepsilon^j \quad , \quad v^{(\mu,\alpha)}(r) = \sum_{j=0}^{\infty} v_j^{(\mu,\alpha)}(r)\varepsilon^j \ . \tag{1.6.15}$$

The original functions ζ, w, w' are written in terms of η, u, v as (formulas (1.4.53) and (1.4.57)):

$$\begin{aligned}
\zeta^{(\mu,\alpha)}(r) &= \zeta_{\text{RWN}}^{(\mu)}(r) + \eta^{(\mu,\alpha)}(r) = \sum_{j=0}^{\infty}\left(\left(\frac{2\mu}{r}-\frac{1}{r^2}\right)^j + \eta_j^{(\mu,\alpha)}\right)\varepsilon^j \\
w^{(\alpha,\mu)}(r) &= \frac{1}{2}((r-1)u^{(\mu,\alpha)}(r) - (r+1)v^{(\mu,\alpha)}(r)) = \frac{1}{2}\sum_{j=0}^{\infty}\left((r-1)u_j^{(\mu,\alpha)}(r) - (r+1)v_j^{(\mu,\alpha)}(r)\right)\varepsilon^j \\
w'^{(\alpha,\mu)}(r) &= \frac{r}{2}(u^{(\mu,\alpha)}(r) + v^{(\mu,\alpha)}(r)) = \frac{r}{2}\sum_{j=0}^{\infty}\left(u_j^{(\mu,\alpha)}(r) + v_j^{(\mu,\alpha)}(r)\right)\varepsilon^j
\end{aligned} \tag{1.6.16}$$

The presence of the parameters μ and α is the reason why we call this a 2-parameter family of solutions. But it is only for $\varepsilon > 0$ that a change in either μ or α yields a change in $\zeta^{(\mu,\alpha)}$ and $w^{(\mu,\alpha)}$, because, when $\varepsilon = 0$, these functions reduce to simply $\zeta_0(r) = 1$, $w_0(r) = (1-r)e^{-r}$, $w_0' = -re^{-r}$, which are independent of μ and α. For our strategy in what follows, we will need parameters that also effect a change in these functions when $\varepsilon = 0$, and this is achieved by rescaling μ and α using a factor of ε. Indeed, we have already remarked in (1.4.161) that each coefficient $\zeta_j^{(\mu,\alpha)}(r), w_j^{(\mu,\alpha)}(r), (w')_j^{(\mu,\alpha)}(r)$ is a polynomial in μ and α of degree no more than j in each. Since each of these coefficients appears multiplied by ε^j in the formulas for $\zeta^{(\mu,\alpha)}$ etc., we are allowed to write ζ and w as functions of the new parameters

$$\nu = \varepsilon\mu \quad , \quad \beta = \varepsilon\alpha \; . \tag{1.6.17}$$

That is, the formulas (note the square brackets instead of parentheses to differentiate them from the ones above)

$$\zeta^{[\nu,\beta]}(r) := \zeta^{(\nu/\varepsilon\;,\;\beta/\varepsilon)}(r) \quad , \quad \text{similarly for } w \text{ and } w' \tag{1.6.18}$$

are well-defined even when $\varepsilon = 0$. The range of allowed parameters ν, β is

$$|\nu| \le \nu_* := \varepsilon_*\mu_* \quad , \quad |\beta| \le \beta_* := \varepsilon_*\alpha_* \; . \tag{1.6.19}$$

There will be no possibility of confusion between summation multi-indices $\alpha, \beta \in \mathbb{N}^2$ and the parameters $\alpha, \beta \in \mathbb{R}$, or between the new parameter $\nu \in \mathbb{R}$ and the original metric function $\nu : (0,\infty) \to \mathbb{R}$.

Remark 1.6.1. Contrary to μ_*, α_*, the numbers ν_*, β_* are not free to be chosen as large as desired. Given ν_*, β_*, the original parameters μ_*, α_* are obtained according to

$$\begin{aligned} \mu_* &= \frac{\nu_*}{\varepsilon} = \frac{240(15 + 4r_0\mu_* + r_0^4\alpha_*)\nu_*}{\gamma_\infty r_0^7} \\ \alpha_* &= \frac{\beta_*}{\varepsilon} = \frac{240(15 + 4r_0\mu_* + r_0^4\alpha_*)\beta_*}{\gamma_\infty r_0^7} \end{aligned} \tag{1.6.20}$$

This gives a linear system for μ_*, α_*:

$$\left\{ \begin{array}{rcrcl} (A - C\nu_*)\mu_* & & -(D\nu_*)\alpha_* & = & B\nu_* \\ -(C\beta_*)\mu_* & + & (A - D\beta_*)\alpha_* & = & B\beta_* \end{array} \right. \quad \text{where} \quad \left\{ \begin{array}{l} A = \gamma_\infty r_0^7 \\ B = 3600 \\ C = 960 r_0 \\ D = 240 r_0^4 \end{array} \right. \tag{1.6.21}$$

The solutions

$$\begin{bmatrix} \mu_* \\ \alpha_* \end{bmatrix} = \frac{1}{A - C\nu_* - D\beta_*} \begin{bmatrix} B\nu_* \\ B\beta_* \end{bmatrix} \tag{1.6.22}$$

are only positive when $C\nu_* + D\beta_* < A$. Therefore, a restriction on the parameters ν_*, β_* is that

$$960\nu_* + 240 r_0^3 \beta_* < \gamma_\infty r_0^6 \; . \tag{1.6.23}$$

The other restriction comes from the required $\varepsilon\mu_*^2 < 1$, but one can check, after finding μ_* from (1.6.22) and using the relation (1.6.4) between ε and r_0, that it is a weaker condition than (1.6.23).

Now compute the values of x, y, z corresponding to $\zeta(r), w(r), w'(r)$ at $s = r_0$ (formulas (1.5.11)), thus obtaining a surface $\mathcal{S}$ inside 3D space $\{(x, y, z, r_0)\}$ parametrized by ν, β. We call

$$x_S(\nu, \beta), y_S(\nu, \beta), z_S(\nu, \beta)$$

the first 3 coordinates of this surface, and $S(\nu, \beta)$ its general point:

$$\mathcal{S} = \{S(\nu, \beta) = (x_S(\nu, \beta), y_S(\nu, \beta), z_S(\nu, \beta), r_0) \; , \; |\nu| \le \nu_*, |\beta| \le \beta_*\} \; . \tag{1.6.24}$$

That is,

$$x_S(\nu, \beta) = \zeta^{[\nu,\beta]}(r_0) \quad , \quad y_S(\nu, \beta) = \frac{w'^{[\nu,\beta]}(r_0)}{r_0} \quad , \quad z_S(\nu, \beta) = \frac{w^{[\nu,\beta]}(r_0) - 1}{r_0^2} \; . \tag{1.6.25}$$

Now let x_P, y_P, z_P ("P" for *plane*) denote these functions calculated with the corresponding series for ζ, w, w' truncated at first degree in ε:

$$\begin{aligned} x_P(\nu, \beta) &= \zeta_0^{[\nu,\beta]}(r_0) + \zeta_1^{[\nu,\beta]}(r_0)\varepsilon \\ y_P(\nu, \beta) &= \frac{w_0'^{[\nu,\beta]}(r_0) + w_1'^{[\nu,\beta]}(r_0)\varepsilon}{r_0} \\ z_P(\nu, \beta) &= \frac{w_0{}^{[\nu,\beta]}(r_0) + w_1{}^{[\nu,\beta]}(r_0)\varepsilon - 1}{r_0^2} \; , \end{aligned} \tag{1.6.26}$$

and call P the general point

$$P(\nu, \beta) = (x_P(\nu, \beta), y_P(\nu, \beta), z_P(\nu, \beta), r_0) \; . \tag{1.6.27}$$

These are affine-linear in the original parameters μ, α (which appear multiplied by ε), hence also in the new ones ν, β (which won't have an ε in front of them), and therefore the collection of values of x_P, y_P, z_P as the parameters ν, β vary trace out the interior and boundary of a parallelepiped $\mathcal{P}^{(\varepsilon)} = \mathcal{P}$ (even when $\varepsilon = 0$) contained in a plane $\mathcal{P}_\star$:

$$\begin{aligned} \mathcal{P} &= \{P(\nu,\beta)\ ,\ |\nu| \leq \nu_*, |\beta| \leq \beta_*\}\ , \\ \mathcal{P}_\star &= \{P(\nu,\beta)\ ,\ \nu,\beta \in \mathbb{R}\}\ . \end{aligned} \tag{1.6.28}$$

Remark 1.6.2. The flat-space solution to our differential system with $\varepsilon = 0$ is given by the zeroth-order terms of the ε-power series defining the surface $\mathcal{S}$, which are the only ones that are not multiples of powers of ν, β. Hence, the parallelepiped $\mathcal{P}$ is the same as the surface $\mathcal{S}^{(0)}$ corresponding to $\varepsilon = 0$, and the values of the parameters at the intersection point between $\mathcal{C}^{(0)}$ and $\mathcal{S}^{(0)}$ for $\varepsilon = 0$ are $\nu = 0$, $\beta = 0$, $\sigma = 4r_0/3$ (the last one was found in equation (1.6.13)). It is to be expected that the intersection when $\varepsilon > 0$ will happen at parameter values close to these. The numbers ν_*, β_* control how large $|\nu|, |\beta|$ can be; we will also seek a number σ_* dictating the maximum size for $|4r_0/3 - \sigma|$.

Proposition 1.6.3. *The equation of the plane $\mathcal{P}_\star$ in 3D $\{(x, y, z, r_0)\}$ space can be written*

$$a_P x + b_P y + c_P z = d_P + \varepsilon e_P \tag{1.6.29}$$

with the coefficients given by

$$\begin{aligned} a_P &= \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) e^{-r_0} + \mathrm{Ei}(-2r_0)e^{r_0} \\ b_P &= \frac{1}{r_0} + \frac{1}{r_0^2} \\ c_P &= 1 \\ d_P &= -\frac{1}{r_0^2} + \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) e^{-r_0} + \mathrm{Ei}(-2r_0)e^{r_0} \\ e_P &= -\frac{1}{6}\left(\frac{1}{r_0^3} + \frac{2}{r_0^4}\right) e^{-r_0} + \frac{2e^{-3r_0}}{r_0^2} + \frac{1}{3}\left(\frac{4}{r_0} + \frac{3}{r_0^2}\right) \mathrm{Ei}(-2r_0)e^{r_0} \\ &\quad - \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) \mathrm{Ei}(-2r_0)e^{-r_0} - \frac{6}{r_0}\mathrm{Ei}(-4r_0)e^{r_0} \end{aligned} \tag{1.6.30}$$

Note that ε does not appear in the 5 formulas above, but does appear multiplying e_P in the plane equation; that is, the effect of a change in ε is a small translation of $\mathcal{P}_\star$.

Proof. Recall the expressions for the zeroth and first order coefficients calculated at r_0, which can be read off of formulas (1.4.48), (1.4.49), (1.4.17)). Writing in the x, y, z coordinates, we get

$$x_P(\nu,\beta) = 1 + \varepsilon\left[-\frac{1}{r_0^2} + \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) e^{-2r_0} + \frac{2\mu}{r_0}\right]\ , \tag{1.6.31}$$

$$y_P(\nu,\beta) = -e^{-r_0} + \varepsilon\Bigg[\frac{1}{12}\left(\frac{1}{r_0}+\frac{5}{r_0^2}+\frac{4}{r_0^3}\right)e^{-r_0} + \frac{1}{2}\left(\frac{1}{r_0}-\frac{2}{r_0^2}-\frac{1}{r_0^3}\right)e^{-3r_0}$$
$$+\frac{1}{3}\Big(2\mathrm{Ei}(-2r_0)-9\mathrm{Ei}(-4r_0)\Big)e^{r_0} + \mu\left(-\left(\frac{1}{r_0}+\frac{1}{r_0^2}\right)e^{-r_0}+\mathrm{Ei}(-2r_0)e^{r_0}\right) - \frac{\alpha}{2}e^{-r_0}\Bigg] , \quad (1.6.32)$$

$$z_P(\nu,\beta) = \frac{(1+r_0)e^{-r_0}-1}{r_0^2} + \varepsilon\Bigg[\frac{1}{12}\left(-\frac{9}{r_0^2}+\frac{4}{r_0^3}-\frac{1}{r_0^4}-\frac{4}{r_0^5}\right)e^{-r_0}$$
$$+\frac{1}{2}\left(\frac{1}{r_0^2}-\frac{3}{r_0^3}+\frac{1}{r_0^4}+\frac{1}{r_0^5}\right)e^{-3r_0} + \frac{1}{3}\Big(2\mathrm{Ei}(-2r_0)-9\mathrm{Ei}(-4r_0)\Big)\left(\frac{1}{r_0}-\frac{1}{r_0^2}\right)e^{r_0}$$
$$+\mu\left(\left(-\frac{1}{r_0^2}+\frac{1}{r_0^4}\right)e^{-r_0}+\mathrm{Ei}(-2r_0)\left(\frac{1}{r_0}-\frac{1}{r_0^2}\right)e^{r_0}\right)+\frac{\alpha}{2}\left(\frac{1}{r_0}+\frac{1}{r_0^2}\right)e^{-r_0}\Bigg] . \quad (1.6.33)$$

Consider the following 3 points on $\mathcal{P}_\star$ (they may fall outside of the domain corresponding to the bounds on μ, α, but that is irrelevant for finding the equation of the plane):

$$Q_1 = P(0,0) \quad , \quad Q_2 = P\left(\frac{1}{\varepsilon},0\right) \quad , \quad Q_3 = P\left(0,\frac{1}{\varepsilon}\right) . \quad (1.6.34)$$

Then $\mathcal{P}_\star$ is the translation by Q_1 of the plane spanned by the two vectors

$$\begin{aligned} Q_2 - Q_1 &= \frac{1}{\varepsilon}\Big[\ \partial_\mu x_P(0,0)\ ,\ \partial_\mu y_P(0,0)\ ,\ \partial_\mu z_P(0,0)\ ,\ r_0\ \Big]^t , \\ Q_3 - Q_1 &= \frac{1}{\varepsilon}\Big[\ \partial_\alpha x_P(0,0)\ ,\ \partial_\alpha y_P(0,0)\ ,\ \partial_\alpha z_P(0,0)\ ,\ r_0\ \Big]^t . \end{aligned} \quad (1.6.35)$$

Note that, since μ and α always appear multiplied by ε in the coordinates of P, and since there is a $1/\varepsilon$ in front of $Q_2 - Q_1$ and $Q_3 - Q_1$, these vectors end up being independent of ε. Compute the vector product $(Q_3 - Q_1) \times (Q_2 - Q_1)$ to find a vector $\boldsymbol{n}$ normal to $\mathcal{P}$; then a possible form of the equation of $\mathcal{P}$ is

$$\boldsymbol{n}_x x + \boldsymbol{n}_y y + \boldsymbol{n}_z z = \boldsymbol{n}\cdot Q_1 \quad , \quad s = r_0 , \quad (1.6.36)$$

where we find that

$$\boldsymbol{n}_x = \left(\frac{1}{r_0^2}+\frac{1}{r_0^3}\right)e^{-2r_0} + \frac{\mathrm{Ei}(-2r_0)}{r_0} \quad , \quad \boldsymbol{n}_y = \left(\frac{1}{r_0^2}+\frac{1}{r_0^3}\right)e^{-r_0} \quad , \quad \boldsymbol{n}_z = \frac{e^{-r_0}}{r_0} , \quad (1.6.37)$$

$$\boldsymbol{n}\cdot Q_1 = \frac{1}{6}\Bigg[-\frac{6e^{-r_0}}{r_0^3} + \left(\frac{6}{r_0^2}+\frac{6}{r_0^3}-\frac{\varepsilon}{r_0^4}-\frac{2\varepsilon}{r_0^5}\right)e^{-2r_0} + \frac{12\varepsilon e^{-4r_0}}{r_0^3}$$
$$+\left(+\frac{6}{r_0}+\frac{8\varepsilon}{r_0^2}+\frac{6\varepsilon}{r_0^3}-\left(\frac{6\varepsilon}{r_0^2}+\frac{6\varepsilon}{r_0^3}\right)e^{-2r_0}\right)\mathrm{Ei}(-2r_0) - \frac{36\varepsilon}{r_0^2}\mathrm{Ei}(-4r_0)\Bigg] \quad (1.6.38)$$

Rescaling these coefficients to make the simple z coefficient equal to 1 and separating out the terms depending on ε from $\boldsymbol{n}\cdot Q_1$ gives the formulas as stated. $\square$

Remark 1.6.4. An upper bound for $|a_P + b_P + c_P + e_P|$ will be needed in subsection 1.6.4, so we quickly figure it out here. The fact mentioned in (1.4.45) is needed:

$$\mathrm{Ei}(-r) < \frac{e^{-r}}{r} \ . \tag{1.6.39}$$

We have:

$$|a_P| = a_P < \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) e^{-r_0} + \frac{e^{-2r_0}}{2r_0} e^{r_0} = \left(\frac{3}{2r_0} + \frac{1}{r_0^2}\right) e^{-r_0} < \frac{2+3r_0}{2r_0^2} \ , \tag{1.6.40}$$

and

$$\begin{aligned}
|e_P| &\le \frac{1}{6}\left(\frac{1}{r_0^3} + \frac{2}{r_0^4}\right) e^{-r_0} + \frac{2e^{-r_0}}{r_0^2} + \frac{1}{3}\left(\frac{4}{r_0} + \frac{3}{r_0^2}\right) \frac{e^{-2r_0}}{2r_0} e^{r_0} \\
&\quad + \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) \frac{e^{-2r_0}}{2r_0} e^{-r_0} + \frac{6}{r_0} \frac{e^{-4r_0}}{4r_0} e^{r_0} \\
&< \frac{1}{6}\left(\frac{1}{r_0^3} + \frac{2}{r_0^4}\right) + \frac{2}{r_0^2} + \frac{1}{3}\left(\frac{4}{r_0} + \frac{3}{r_0^2}\right) \frac{1}{2r_0} + \left(\frac{1}{r_0} + \frac{1}{r_0^2}\right) \frac{1}{2r_0} + \frac{6}{r_0} \frac{1}{4r_0} \\
&= \frac{2 + 4/6 + 1/2 + 6/4}{r_0^2} + \frac{1/6 + 1/2 + 1/2}{r_0^3} + \frac{2/6}{r_0^4} \\
&= \frac{2 + 7r_0 + 28r_0^2}{6r_0^4} \ .
\end{aligned} \tag{1.6.41}$$

Note that r_0^4 is the highest power of r_0 appearing in the denominator for the bounds for a_P and $|e_P|$ as well as in the definitions of b_P and c_P. Using these bounds and definitions and also the fact that $r_0 < 1/360$, we can calculate that

$$|a_P + b_P + c_P + e_P| \le \frac{2}{5r_0^4} \ . \tag{1.6.42}$$

Let us use the plane $\mathcal{P}_\star$ to define a global coordinate system in 3D space $\{(x, y, z, r_0)\}$:

Definition 1.6.5. Given $\boldsymbol{x} = (x, y, z, r_0) \in \mathbb{R}^3 \times \{r_0\}$, the $\boldsymbol{\mathcal{P}_\star}$ **coordinates** $c_1(\boldsymbol{x}), c_2(\boldsymbol{x}), c_3(\boldsymbol{x})$ are defined as follows:

- $c_1(\boldsymbol{x})$ and $c_2(\boldsymbol{x})$ are the ν and β values, respectively, corresponding to the orthogonal projection $\Pi_{\mathcal{P}_\star}(\boldsymbol{x})$ of $\boldsymbol{x}$ onto $\mathcal{P}_\star$:

$$\Pi_{\mathcal{P}_\star}(\boldsymbol{x}) = P(c_1(\boldsymbol{x}), c_2(\boldsymbol{x})) \ . \tag{1.6.43}$$

- $c_3(\boldsymbol{x})$ is a certain signed multiple of the distance of $\boldsymbol{x}$ from $\mathcal{P}_\star$, defined by using the equation of $\mathcal{P}_\star$:

$$c_3(\boldsymbol{x}) = a_P x + b_P y + c_P z - (d_P + \varepsilon e_P) \tag{1.6.44}$$

Note that the correspondence $\boldsymbol{x} \in \mathbb{R}^3 \times \{r_0\} \longleftrightarrow (c_1(\boldsymbol{x}), c_2(\boldsymbol{x}), c_3(\boldsymbol{x})) \in \mathbb{R}^3$ is bijective, with $\mathcal{P}_\star$ corresponding to $c_3 = 0$.

The bulk of the work in this section is going to be proving a set of inequalities involving the c_1, c_2, c_3 coordinates of general points on $\mathcal{C}$ and $\mathcal{S}$. Namely, we seek constants $C_1, C_2, C_3 > 0$ and values of parameters $\gamma_0, \gamma_\infty, \sigma_*, \nu_*, \beta_*$ such that, for any $\varepsilon \in [0, \varepsilon_*)$, the following inequalities hold:

$$|c_3(S(\nu,\beta))| \le C_3 \quad \text{for all } |\nu| \le \nu_* \ , \ |\beta| \le \beta_* \tag{1.6.45}$$

$$c_1(S(-\nu_*,\beta)) \le -C_1 \quad , \quad c_1(S(\nu_*,\beta)) \ge C_1 \quad \text{for all } |\beta| \le \beta_* \tag{1.6.46}$$

$$c_2(S(\nu,-\beta_*)) \le -C_2 \quad , \quad c_2(S(\nu,\beta_*)) \ge C_2 \quad \text{for all } |\nu| \le \nu_* \tag{1.6.47}$$

$$|c_1(C(\sigma))| \le C_1 \quad , \quad |c_2(C(\sigma))| \le C_2 \quad \text{for all } \sigma \in \left[\frac{4r_0}{3} - \sigma_*, \frac{4r_0}{3} + \sigma_*\right] \tag{1.6.48}$$

$$c_3\left(C\left(\frac{4r_0}{3} - \sigma_*\right)\right) \le -C_3 \quad , \quad c_3\left(C\left(\frac{4r_0}{3} + \sigma_*\right)\right) \ge C_3 \tag{1.6.49}$$

Thinking of the normal direction to $\mathcal{P}_\star$ as *vertical* and of the directions on $\mathcal{P}_\star$ as *horizontal*, these inequalities can be interpreted in the following manner:

- (1.6.45): the surface $\mathcal{S}$ does not have too much vertical extent;
- (1.6.46), (1.6.47): the surface $\mathcal{S}$ has enough horizontal extent;
- (1.6.48): the relevant piece of the curve $\mathcal{C}$ does not have too much horizontal extent;
- (1.6.49): the relevant piece of the curve $\mathcal{C}$ has enough vertical extent;

These informal interpretations make it reasonable that $\mathcal{S}$ and $\mathcal{C}$ should intersect. To formally prove that this is the case, assuming that (1.6.45) — (1.6.49) are established, consider 3 continuous functions

$$\begin{aligned} &F_1, F_2, F_3 : [-\nu_*, \nu_*] \times [-\beta_*, \beta_*] \times [-\sigma_*, \sigma_*] \to \mathbb{R} \ , \\ &F_j(\nu,\beta,\sigma) = c_j(S(\nu,\beta)) - c_j\left(C\left(\frac{4r_0}{3} + \sigma\right)\right) \ . \end{aligned} \tag{1.6.50}$$

An intersection between $\mathcal{C}$ and $\mathcal{S}$, that is, the equality $S(\nu,\beta) = C(\sigma)$ for some parameters ν, β, σ, is equivalent to $F_j(\nu,\beta,\sigma) = 0$ for $j = 1,2,3$. Given that the 5 inequalities (1.6.45) — (1.6.49) imply

$$F_1(-\nu_*,\beta,\sigma) \le 0 \quad , \quad F_1(\nu_*,\beta,\sigma) \ge 0 \quad \text{for all } \beta, \sigma \ , \tag{1.6.51}$$

$$F_2(\nu, -\beta_*, \sigma) \leq 0 \quad , \quad F_2(\nu, \beta_*, \sigma) \geq 0 \quad \text{for all } \nu, \sigma \ , \tag{1.6.52}$$

$$F_3(\nu, \beta, -\sigma_*) \leq 0 \quad , \quad F_3(\nu, \beta, \sigma_*) \geq 0 \quad \text{for all } \nu, \beta \ , \tag{1.6.53}$$

the existence of a common zero of F_1, F_2, F_3 will follow from the following theorem, paraphrased from [GD03]:

Theorem 1.6.6. (Poincaré-Miranda) *Let $F_i : [a_i, b_i] \to \mathbb{R}$, $i = 1, \ldots, N$, be continuous functions. Suppose that, for each $i = 1, \ldots, N$ and all $x_j \in [a_j, b_j]$ $(j \neq i)$,*

$$F_i(x_1, \ldots, x_{i-1}, a_i, x_{i+1}, \ldots, x_N) \leq 0 \quad , \quad F_i(x_1, \ldots, x_{i-1}, b_i, x_{i+1}, \ldots, x_N) \geq 0 \ . \tag{1.6.54}$$

Then there exists $\boldsymbol{x} \in [a_1, b_1] \times \cdots \times [a_N, b_N]$ such that $F_i(\boldsymbol{x}) = 0$ for all $i = 1, \ldots, N$.

Therefore, all that is left is to prove each one of the 5 sets of inequalities listed above for appropriate parameter values $\gamma_0, \gamma_\infty, \sigma_*, \nu_*, \beta_*$ and constants C_1, C_2, C_3. We also remind the reader that these parameters are not free to be chosen as arbitrary positive numbers: the gammas are constrained by $\gamma_0, \gamma_\infty \in (0, 1)$, while β_*, ν_* are constrained by (1.6.23) and σ_* by the fact that the point $4r_0/3 + \sigma_*$ needs to remain within the radius of convergence of $\mathcal{C}$:

$$\frac{4r_0}{3} + \sigma_* < \frac{1}{360} \ . \tag{1.6.55}$$

Given the definition (1.6.4) of r_0, this is equivalent to

$$\sigma_* < \frac{1 - \gamma_0}{360} \ . \tag{1.6.56}$$

1.6.2 Proof of (1.6.45)

Inequality (1.6.45) concerns the "vertical" separation between the surface $\mathcal{S}$ of the 2-parameter family from $r = \infty$ (given by an ε-power series) and the plane $\mathcal{P}$ (its first degree truncation). Thus it is simply a truncation error estimate of the ε-series. The fact that the coefficients $a_P, \ldots, e_P$ in the equation of $\mathcal{P}_\star$ are ε-independent is helpful in the calculation.

Define $\tilde{x}_S, \tilde{y}_S, \tilde{z}_S$ as the error in approximating $\mathcal{S}$ by $\mathcal{P}$:

$$\tilde{x}_S(\nu, \beta) = x_S(\nu, \beta) - x_P(\nu, \beta) \quad , \quad \text{similarly for } y, z \ . \tag{1.6.57}$$

Given any point $(x_P+\tilde{x}_S, y_P+\tilde{y}_S, z_P+\tilde{z}_S, r_0)\in\mathcal{S}$, since $(x_P, y_P, z_P, r_0)\in\mathcal{P}_\star$ has a null c_3 coordinate, we have

$$\begin{aligned} c_3(S(\nu,\beta)) &= a_P(x_P+\tilde{x}_S)+b_P(y_P+\tilde{y}_S)+c_P(z_P+\tilde{z}_S)-(d_P+\varepsilon e_P) \\ &= a_P\tilde{x}_S+b_P\tilde{y}_S+c_P\tilde{z}_S\ . \end{aligned} \tag{1.6.58}$$

To write an estimate for this, we begin by writing one for $\tilde{x}_S, \tilde{y}_S, \tilde{z}_S$. We must start from the power series for η, u, v. We proved in theorem 1.4.13 that there exist

$$R\le\frac{240(15+4r_0\mu_*+r_0^4\alpha_*)}{r_0^7}\quad,\quad\delta<\frac{1}{\sqrt{48}}\quad,\quad S=2\delta^2 \tag{1.6.59}$$

such that, for all $r\in[r_0,\infty)$,

$$|\eta_j^{(\nu,\beta)}(r)|, |u_j^{(\nu,\beta)}(r)|, |v_j^{(\nu,\beta)}(r)|\le\frac{SR^j}{(j+\delta)^2}e^{-r/2}<\frac{SR^j}{(j+\delta)^2}\ . \tag{1.6.60}$$

Note that our choice of ε in (1.6.4) can be written

$$\varepsilon=\frac{\gamma_\infty}{R}\ . \tag{1.6.61}$$

Therefore (and similarly for u, v):

$$\left|\sum_{j=2}^{\infty}\eta_j^{(\nu,\beta)}(r_0)\varepsilon^j\right|\le S\sum_{j=2}^{\infty}\frac{(R\varepsilon)^j}{(j+\delta)^2}<\frac{S}{2^2}\sum_{j=2}^{\infty}\gamma_\infty^j=\frac{\delta^2}{2}\frac{\gamma_\infty^2}{1-\gamma_\infty}<\frac{\gamma_\infty^2}{96(1-\gamma_\infty)}\ . \tag{1.6.62}$$

We also need a bound for the tail of the ζ_{RWN} series

$$\sum_{j=2}^{\infty}\left(\frac{2M}{r_0}+\frac{1}{r_0^2}\right)^j\varepsilon^j\ , \tag{1.6.63}$$

which is part of the ζ series (and will turn out almost irrelevant compared to the above). Since

$$\left(\frac{2\mu_*}{r_0}+\frac{1}{r_0^2}\right)\varepsilon\le\frac{\gamma_\infty r_0^5}{240}\cdot\frac{2r_0\mu_*+1}{15+4r_0\mu_*+r_0^4\alpha_*}<\frac{\gamma_\infty r_0^5}{240}\cdot\frac{\frac{15}{2}+2r_0\mu_*+\frac{1}{2}r_0^4\alpha_*}{15+4r_0\mu_*+r_0^4\alpha_*}=\frac{\gamma_\infty r_0^5}{480}\ , \tag{1.6.64}$$

we have

$$\left|\sum_{j=2}^{\infty}\left(\frac{2\mu}{r_0}-\frac{1}{r_0^2}\right)^j\varepsilon^j\right|\le\sum_{j=2}^{\infty}\left(\frac{2M}{r_0}+\frac{1}{r_0^2}\right)^j\varepsilon^j\le\frac{\frac{\gamma_\infty^2 r_0^{10}}{480^2}}{1-\frac{\gamma_\infty r_0^5}{480}}=\frac{(1-\gamma_\infty)r_0^{10}}{480(480-\gamma_\infty r_0^5)}\cdot\frac{\gamma_\infty^2}{1-\gamma_\infty}<\frac{1}{480}\frac{\gamma_\infty^2}{1-\gamma_\infty} \tag{1.6.65}$$

(the value of r_0 chosen in (1.6.4) is more than enough to guarantee $480-\gamma_\infty r_0^5>1$). Now let's see what this implies for ζ, w, w'. Start with

$$|\zeta|\le|\zeta_{\mathrm{RWN}}|+|\eta|\quad,\quad|w(r_0)|\le(r_0+1)\frac{|u(r_0)|+|v(r_0)|}{2}\quad,\quad|w'(r_0)|\le r_0\frac{|u(r_0)|+|v(r_0)|}{2}\ , \tag{1.6.66}$$

which come from formulas (1.4.53) and (1.4.57)). Hence

$$\begin{aligned}
\left|\sum_{j=2}^{\infty} \zeta_j^{(\nu,\beta)}(r_0)\varepsilon^j\right| &\le \left|\sum_{j\ge 2}^{\infty}\left(\frac{2\mu}{r}-\frac{1}{r^2}\right)^j \varepsilon^j\right| + \left|\sum_{j=2}^{\infty} \eta_j^{(\nu,\beta)}(r)\varepsilon^j\right| \le \frac{\gamma_\infty^2}{80(1-\gamma_\infty)} ,\\
\left|\sum_{j=2}^{\infty} w_j^{(\nu,\beta)}(r_0)\varepsilon^j\right| &\le \frac{\gamma_\infty^2(r_0+1)}{96(1-\gamma_\infty)} ,\\
\left|\sum_{j=2}^{\infty} {w'}_j^{(\nu,\beta)}(r_0)\varepsilon^j\right| &\le \frac{\gamma_\infty^2 r_0}{96(1-\gamma_\infty)} .
\end{aligned} \tag{1.6.67}$$

Finally, due to formulas (1.5.11) defining the variables x, y, z:

$$|\tilde{x}_S(\nu,\beta)| \le \frac{\gamma_\infty^2}{80(1-\gamma_\infty)} \quad , \quad |\tilde{y}_S(\nu,\beta)| \le \frac{\gamma_\infty^2}{96(1-\gamma_\infty)} \quad , \quad |\tilde{z}_S(\nu,\beta)| \le \frac{1+r_0}{r_0^2}\frac{\gamma_\infty^2}{96(1-\gamma_\infty)} . \tag{1.6.68}$$

Notice how the -1 in the formula $z = (w-1)/r^2$ should not be taken into account when computing these tails, since it does not affect the ε expansion at any degree other than 0. Using these, the values of b_P, c_P given in (1.6.30) and the bound (1.6.40) for a_P, we have

$$\begin{aligned}
|a_P\tilde{x}_S(\nu,\beta) + b_P\tilde{y}_S(\nu,\beta) + c_P\tilde{z}_S(\nu,\beta)| &\le \frac{\gamma_\infty^2}{1-\gamma_\infty}\left(\frac{2+3r_0}{160r_0^2} + \frac{1+r_0}{96r_0^2} + \frac{1+r_0}{96r_0^2}\right) \\
&= \frac{\gamma_\infty^2(16+19r_0)}{480(1-\gamma_\infty)r_0^2} \\
&< \frac{\gamma_\infty^2}{25(1-\gamma_\infty)r_0^2} =: C_3 .
\end{aligned} \tag{1.6.69}$$

The last inequality uses the fact that $r_0 < 1/360$. This establishes a value for C_3 such that (1.6.45) holds for any choice of parameters $\gamma_0, \gamma_\infty, \sigma_*, \nu_*, \beta_*$.

1.6.3 Proof of (1.6.48)

Inequalities (1.6.48) concern the "horizontal" extent of the curve $\mathcal{C}$ around the parameter value $\sigma = 4r_0/3$. Values of C_1 and C_2 quantifying this extent can easily be found when $\varepsilon = 0$ by using the explicit description of the manifold $\mathcal{W}^{(0)}$, while values that still work when $\varepsilon > 0$ will be possible to obtain because of the estimate (1.6.8) that furnishes a small bound for the ε-perturbation of $\mathcal{C}$.

The definition of the c_1, c_2 coordinates involves an orthogonal projection onto the plane $\mathcal{P}_\star$, whose coordinates are the affine-linear functions x_P, y_P, z_P of (ν,β) given in formulas (1.6.31), (1.6.32), (1.6.33). We begin by calculating this orthogonal projection. Let's use superscripts (1),

(ε), (ν), (β) to denote the coefficients appearing in them (which depend on r_0):

$$x_P(\nu,\beta) =: x_P^{(1)} + \varepsilon x_P^{(\varepsilon)} + \nu x_P^{(\nu)} + \beta x_P^{(\beta)} \quad , \quad \text{similarly for } y_P, z_P \ . \tag{1.6.70}$$

Now define

$$A := \begin{bmatrix} x_P^{(\nu)} & x_P^{(\beta)} \\ \\ y_P^{(\nu)} & y_P^{(\beta)} \\ \\ z_P^{(\nu)} & z_P^{(\beta)} \end{bmatrix} \quad , \quad \boldsymbol{x}^{(1,\varepsilon)} := \begin{bmatrix} x_P^{(1)} + \varepsilon x_P^{(\varepsilon)} \\ \\ y_P^{(1)} + \varepsilon y_P^{(\varepsilon)} \\ \\ z_P^{(1)} + \varepsilon z_P^{(\varepsilon)} \end{bmatrix} \ . \tag{1.6.71}$$

The parametrization of $\mathcal{P}_\star$ in terms of ν, β is written in matrix form as

$$A \begin{bmatrix} \nu \\ \beta \end{bmatrix} = P(\nu,\beta) - \boldsymbol{x}^{(1,\varepsilon)} \ . \tag{1.6.72}$$

We remark that A has maximal rank, for example because $x_P^{(\beta)} = 0$, $x_P^{(\nu)} \neq 0$, $y_P^{(\beta)} \neq 0$. Given any $\boldsymbol{x} = (x, y, z, r_0) \in \mathbb{R}^3 \times \{r_0\}$, we can find the coordinates $c_1(\boldsymbol{x})$ and $c_2(\boldsymbol{x})$, that is, the values of ν, β at the projection $\Pi_{\mathcal{P}_\star}(\boldsymbol{x}) \in \mathcal{P}_\star$, by finding the least-squares "solution" to the (possibly inconsistent) linear system

$$A \begin{bmatrix} \nu \\ \beta \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} - \begin{bmatrix} x_P^{(1)} + \varepsilon x_P^{(\varepsilon)} \\ \\ y_P^{(1)} + \varepsilon y_P^{(\varepsilon)} \\ \\ z_P^{(1)} + \varepsilon z_P^{(\varepsilon)} \end{bmatrix} \ . \tag{1.6.73}$$

In fact, we can rewrite this equation by erasing from it the ε-dependent terms $\varepsilon x_P^{(\varepsilon)}$ etc. — since the effect of ε in only a translation of $\mathcal{P}_\star$, the parameter values ν, β corresponding to planes of different ε values are the same. Since A has maximal rank, the least-squares "solution" is given by the well-known formula

$$\begin{bmatrix} \nu \\ \beta \end{bmatrix} = B \begin{bmatrix} x - x_P^{(1)} \\ y - y_P^{(1)} \\ z - z_P^{(1)} \end{bmatrix} \quad , \quad B := (A^* A)^{-1} A^* \ . \tag{1.6.74}$$

We are now ready to project points of $\mathcal{C}$ onto $\mathcal{P}_\star$. Consider an arbitrary point $C(4r_0/3+\sigma) \in \mathcal{C}$. The first 3 components x_C, y_C, z_C of this point split as

$$x_C\left(\frac{4r_0}{3}+\sigma\right) = x_N^{(I)} + V\left(\frac{4r_0}{3}+\sigma\right)x_N^{(II)} + \tilde{x}_C\left(\frac{4r_0}{3}+\sigma\right) \quad , \quad \text{etc. ,} \tag{1.6.75}$$

where we remark that

$$V\left(\frac{4r_0}{3}+\sigma\right) = \frac{1}{2} - \frac{3}{8r_0}\left(\frac{4r_0}{3}+\sigma\right) = -\frac{3\sigma}{8r_0} \; . \tag{1.6.76}$$

Note that $x_N^{(I)}, y_N^{(I)}, z_N^{(I)}$ found in (1.6.10) are exactly the same as $x_P^{(1)}, y_P^{(1)}, z_P^{(1)}$ defined just above, so that, when plugging the point (x, y, z) given in (1.6.75) into equation (1.6.74) for the ν, β coefficients, they get canceled and we end up with only

$$\begin{bmatrix} c_1(C(4r_0/3+\sigma)) \\ c_2(C(4r_0/3+\sigma)) \end{bmatrix} = B \begin{bmatrix} & & \tilde{x}_C(4r_0/3+\sigma) \\ -\frac{3\sigma}{8r_0}(e^{-r_0}-e^{r_0}) & + & \tilde{y}_C(4r_0/3+\sigma) \\ -\frac{3\sigma}{8r_0}\frac{(1-r_0)e^{r_0}-(1+r_0)e^{-r_0}}{r_0^2} & + & \tilde{z}_C(4r_0/3+\sigma) \end{bmatrix} \; . \tag{1.6.77}$$

Due to $r_0 < 1/360$, the factors multiplying $3\sigma/8r_0$ in the vector above are bounded as such:

$$|e^{-r_0} - e^{r_0}| < \frac{1}{100} \quad , \quad \left|\frac{(1-r_0)e^{r_0}-(1+r_0)e^{-r_0}}{r_0^2}\right| < \frac{1}{500} \tag{1.6.78}$$

(the second one may look like it diverges when r_0 is small, due to the r_0^2 denominator, but actually the zeroth and first derivatives of the numerator at $r = 0$ also vanish). Meanwhile, the terms $\tilde{x}_C, \tilde{y}_C, \tilde{z}_C$ in (1.6.8). Then we conclude

$$\begin{aligned} \left|c_j\left(C\left(\frac{4r_0}{3}+\sigma\right)\right)\right| \le |B_{j1}|\frac{60\varepsilon}{(1-\gamma_0)^2} + |B_{j2}|\left(\frac{3|\sigma|}{800r_0}+\frac{60\varepsilon}{(1-\gamma_0)^2}\right) \\ + |B_{j3}|\left(\frac{3|\sigma|}{4000r_0}+\frac{60\varepsilon}{(1-\gamma_0)^2}\right) \quad , \quad j = 1, 2 \; . \end{aligned} \tag{1.6.79}$$

Bounds for $|B_{ij}|$ are needed now. After computing the matrix product defining B in (1.6.74), we see that its first row as well as B_{23} all end up being multiple of r_0, which makes them small, while B_{21} and B_{22} have an r_0 in the denominator making them large:

$$B_{11} = \frac{r_0 e^{2r_0}(1+2r_0+r_0^2+r_0^4)}{2[(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2))]} \tag{1.6.80}$$

$$B_{12} = \frac{r_0(r_0+1)e^{r_0}(\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2-1-r_0)}{2[(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2))]} \tag{1.6.81}$$

$$B_{13} = \frac{r_0^3 e^{r_0}(\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2-1-r_0)}{2[(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2))]} \tag{1.6.82}$$

$$B_{21} = \frac{(1-r_0^2+r_0^4)e^{2r_0}(\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2-1-r_0)}{r_0[(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2))]} \tag{1.6.83}$$

$$B_{22} = \frac{e^{r_0}(1+r_0-r_0^2-r_0^3+r_0^2e^{2r_0}(-2r_0^3+\mathrm{Ei}(-2r_0)[-2+2r_0^2+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2(1-r_0)]))}{r_0[(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2))]} \tag{1.6.84}$$

$$B_{23} = \frac{r_0e^{r_0}((1+r_0)^2+r_0e^{2r_0}(2+2r_0+\mathrm{Ei}(-2r_0)r_0[-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2]))}{[(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2))]} \tag{1.6.85}$$

Bound (away from 0) the common expression that appears in all the denominators. To do this, use (1.6.39) to conclude that the negative term in this expression is small

$$|\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2)| < \frac{e^{-2r_0}}{2r_0}r_0^2(2+2r_0+\frac{e^{-2r_0}}{2r_0}e^{2r_0}r_0^2) < \frac{r_0}{2}(2+\frac{5r_0}{2}) \tag{1.6.86}$$

and in fact is dominated by the positive terms $2r_0+r_0^2+r_0^4$; then throw these away and just leave

$$(r_0+1)^2+e^{2r_0}(1+2r_0+r_0^2+r_0^4+\mathrm{Ei}(-2r_0)r_0^2(-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2)) > (0+1)^2+e^0(1+0) = 2\ . \tag{1.6.87}$$

As for the numerators, we keep the most significant terms in r_0 and use $r_0 < 1/360$ for all others. We obtain:

$$r_0e^{2r_0}(1+2r_0+r_0^2+r_0^4) < r_0e^{2/360}\left(1+\frac{2}{360}+\frac{1}{360^2}+\frac{1}{360^4}\right) < \frac{11r_0}{10}\ , \tag{1.6.88}$$

$$\begin{aligned}|r_0(r_0+1)e^{r_0}(\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2-1-r_0)| &< r_0(r_0+1)e^{r_0}\left(\frac{r_0}{2}+1+r_0\right)\\ &< r_0\left(\frac{1}{360}+1\right)e^{1/360}\left(\frac{1}{720}+1+\frac{1}{360}\right)\\ &< \frac{101r_0}{100}\ ,\end{aligned} \tag{1.6.89}$$

$$|r_0^3e^{r_0}(\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2-1-r_0)| < r_0^3e^{1/360}\left(\frac{1}{720}+1+\frac{1}{360}\right) < \frac{101r_0^3}{100}\ , \tag{1.6.90}$$

$$|(1-r_0^2+r_0^4)e^{2r_0}(\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2-1-r_0)| < \left(1+\frac{1}{360^2}+\frac{1}{360^4}\right)e^{2/360}\left(\frac{1}{720}+1+\frac{1}{360}\right) < \frac{101}{100} \tag{1.6.91}$$

$$\begin{aligned}&|e^{r_0}(1+r_0-r_0^2-r_0^3+r_0^2e^{2r_0}(-2r_0^3+\mathrm{Ei}(-2r_0)[-2+2r_0^2+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2(1-r_0)]))|\\ &\quad< e^{r_0}\left(1+r_0+r_0^2+r_0^3+r_0^2e^{2r_0}\left(2r_0^3+\frac{1}{2r_0}\left[2+2r_0^2+\frac{r_0}{2}(1+r_0)\right]\right)\right)\\ &\quad< e^{3r_0}\left(1+r_0+r_0^2+r_0^3+2r_0^5+r_0+r_0^3+\frac{1}{4}(r_0^2+r_0^3)\right)\\ &\quad= e^{3r_0}\left(1+2r_0+\frac{5r_0^2}{4}+\frac{9r_0^3}{4}+2r_0^5\right)\\ &\quad< e^{3/360}\left(1+\frac{2}{360}+\frac{5}{4\cdot 360^2}+\frac{9}{4\cdot 360^3}+\frac{2}{360^5}\right) < \frac{51}{50}\ ,\end{aligned} \tag{1.6.92}$$

$$
\begin{aligned}
&|r_0e^{r_0}((1+r_0)^2 + r_0e^{2r_0}(2+2r_0+\mathrm{Ei}(-2r_0)r_0[-2-2r_0+\mathrm{Ei}(-2r_0)e^{2r_0}r_0^2]))| \\
&\qquad < r_0e^{r_0}\left(1+2r_0+r_0^2+r_0e^{2r_0}\left(2+2r_0+\frac{1}{2}\left[2+2r_0+\frac{r_0}{2}\right]\right)\right) \\
&\qquad < r_0e^{3r_0}\left(1+2r_0+r_0^2+2r_0+2r_0^2+r_0+r_0^2+\frac{r_0^2}{4}\right) \\
&\qquad = r_0e^{3r_0}\left(1+5r_0+\frac{17r_0^2}{4}\right) \\
&\qquad < r_0e^{3/360}\left(1+\frac{5}{360}+\frac{17}{4\cdot 360^2}\right) < \frac{41r_0}{40}\ .
\end{aligned}
\tag{1.6.93}
$$

Therefore,

$$
\begin{aligned}
&|B_{11}| \le \frac{11r_0}{40} \quad |B_{12}| \le \frac{101r_0}{400} \quad |B_{13}| \le \frac{101r_0^3}{400} \\
&|B_{21}| \le \frac{101}{200r_0} \quad |B_{22}| \le \frac{51}{100r_0} \quad |B_{23}| \le \frac{41r_0}{80}
\end{aligned}
\tag{1.6.94}
$$

Plug back into the estimate (1.6.79) for the c_1, c_2 coordinates of $C(4r_0/3+\sigma)$, cancel powers of r_0 and use $r_0 < 1/360$ on remaining expressions like $1+r_0$ in the numerators. Finally, bound $|\sigma|$ by the parameter σ_* that we wish to find by the end:

$$
\begin{aligned}
\left|c_1\left(C\left(\frac{4r_0}{3}+\sigma\right)\right)\right| &\le \frac{\sigma_*}{1000} + \frac{60\varepsilon r_0}{(1-\gamma_0)^2} \\
\left|c_2\left(C\left(\frac{4r_0}{3}+\sigma\right)\right)\right| &\le \frac{\sigma_*}{500r_0^2} + \frac{120\varepsilon}{r_0(1-\gamma_0)^2}
\end{aligned}
\tag{1.6.95}
$$

We let these expressions define the constants C_1 and C_2, and thus the inequalities (1.6.48) become automatically true for any choice of parameters $\gamma_0, \gamma_\infty, \sigma_*, \nu_*, \beta_*$:

$$
\begin{aligned}
C_1 &:= \frac{\sigma_*}{1000} + \frac{60\varepsilon r_0}{(1-\gamma_0)^2} \\
C_2 &:= \frac{\sigma_*}{500r_0^2} + \frac{120\varepsilon}{r_0(1-\gamma_0)^2} = \frac{2C_1}{r_0^2}
\end{aligned}
\tag{1.6.96}
$$

1.6.4 Proof of (1.6.49)

Inequalities (1.6.49) concern the "vertical" separation between the plane $\mathcal{P}$ and the endpoints of the segment of the curve $\mathcal{C}$ between $4r_0/3-\sigma_*$ and $4r_0/3+\sigma_*$. They stipulate that this separation should be large enough, quantified by the constant C_3 that we already defined in (1.6.69). This will be achieved by allowing σ_* to be large enough.

Let $C(4r_0/3+\sigma) \in \mathcal{C}$ be a general point on $\mathcal{C}$. According to the definition of the c_3 coordinate of a point and the way in which the coordinates of $\mathcal{C}$ split, found in (1.6.75) above, we have (after some rearranging):

$$c_3\left(C\left(\frac{4r_0}{3}+\sigma\right)\right)=\frac{3\sigma}{8r_0}\left(x_N^{(II)}+z_N^{(II)}+y_N^{(II)}\right)$$
$$+\left(a_Px_N^{(I)}+b_Py_N^{(I)}+c_Pz_N^{(I)}-d_P\right)+\left(a_P\tilde{x}_C(\sigma)+b_P\tilde{y}_C(\sigma)+c_P\tilde{z}_C(\sigma)-e_P\right)\ . \qquad (1.6.97)$$

Direct computation reveals

$$x_N^{(II)}+z_N^{(II)}+y_N^{(II)}=-\frac{2e^{r_0}}{r_0}$$
$$a_Px_N^{(I)}+b_Py_N^{(I)}+c_Pz_N^{(I)}-d_P=0 \qquad (1.6.98)$$
$$|a_P\tilde{x}_C(\sigma)+b_P\tilde{y}_C(\sigma)+c_P\tilde{z}_C(\sigma)-e_P|\le\frac{2}{60r_0^4}\frac{5\varepsilon}{(1-\gamma_0^2)}=\frac{24\varepsilon}{r_0^4(1-\gamma_0^2)}$$

For the inequality above, we used the bound (1.6.8) for the tilde terms and the bound (1.6.42) for the sum $|a_P+b_P+c_P-e_P|$. Thus, the maximum and minimum size of (1.6.97) for $|\sigma|\le\sigma_*$, obtained by plugging in $\sigma=\sigma_*$ and $\sigma=-\sigma_*$ respectively into it, have a lower and upper bound respectively:

$$c_3\left(C\left(\frac{4r_0}{3}+\sigma_*\right)\right)>\frac{3\sigma_*e^{r_0}}{4r_0^2}-\frac{24\varepsilon}{r_0^4(1-\gamma_0^2)}\quad,\quad c_3\left(C\left(\frac{4r_0}{3}+\sigma_*\right)\right)<-\frac{3\sigma_*e^{r_0}}{4r_0^2}+\frac{24\varepsilon}{r_0^4(1-\gamma_0^2)}\ . \qquad (1.6.99)$$

We want to ensure the first bound is larger than $-C_3$ and the second one smaller than C_3; hence we want to ensure that

$$\frac{3\sigma_*e^{2r_0}}{4r_0^2}>\frac{24\varepsilon}{r_0^4(1-\gamma_0^2)}+\frac{\gamma_\infty^2}{25(1-\gamma_\infty)r_0^2}\ , \qquad (1.6.100)$$

where we have replaced C_3 by its value given in (1.6.69)). Now multiply through by r_0^2, forget about e^{2r_0} because it is at least 1, and use

$$\varepsilon=\frac{\gamma_\infty r_0^7}{240(15+4r_0\mu_*+r_0^4\alpha_*)}<\frac{\gamma_\infty r_0^7}{3600}\quad,\quad r_0=\frac{3}{4}\cdot\frac{\gamma_0}{360} \qquad (1.6.101)$$

to conclude that the above inequality is weaker than (that is, it follows from) this next one:

$$\frac{2\gamma_\infty\gamma_0^5}{25\cdot 480^5(1-\gamma_0)^2}+\frac{4\gamma_\infty^2}{75(1-\gamma_\infty)}<\sigma_*\ . \qquad (1.6.102)$$

We must also remember the other restriction on σ, given in (1.6.56):

$$\sigma_*<\frac{1-\gamma_0}{360}\ . \qquad (1.6.103)$$

It's clear that these two inequalities are compatible when γ_∞ is small enough. Now let's keep these on hold until we've also analyzed the last set of inequalities to be proven.

1.6.5 Proof of (1.6.46) and (1.6.47)

Inequalities (1.6.46) and (1.6.47) concern the "horizontal" extent of the surface $\mathcal{S}$. They stipulate that this extent should be large, quantified by the constants C_1 and C_2 that we already defined in (1.6.96). By definition, the first-degree truncation of $\mathcal{S}$, which we called $\mathcal{P}$, has horizontal extent described by the maximum magnitudes ν_* and β_* of ν and β. We shall see that the truncation error between P and S is small enough to not change this extent by much.

Consider a fixed point $S(\nu, \beta) \in \mathcal{S}$, where $|\nu| \leq \nu_*$ and $|\beta| \leq \beta_*$. Its first 3 coordinates are written as perturbations of points on $\mathcal{P}_\star$:

$$x_S(\nu, \beta) = x_P(\nu, \beta) + \tilde{x}_S(\nu, \beta) \quad , \quad \text{similarly for } y, z \; , \tag{1.6.104}$$

and the inequalities (1.6.68) provide bounds for the perturbations. Meanwhile, the c_1, c_2 coordinates of a general point $\boldsymbol{x} = (x, y, z, r_0)$ are defined in equation (1.6.74):

$$\begin{bmatrix} c_1(\boldsymbol{x}) \\ c_2(\boldsymbol{x}) \end{bmatrix} = B \begin{bmatrix} x - (x_P^{(1)} + \varepsilon x_P^{(\varepsilon)}) \\ y - (y_P^{(1)} + \varepsilon y_P^{(\varepsilon)}) \\ z - (z_P^{(1)} + \varepsilon z_P^{(\varepsilon)}) \end{bmatrix} . \tag{1.6.105}$$

Applying this to $\boldsymbol{x} = (x_P(\nu, \beta), y_P(\nu, \beta), z_P(\nu, \beta), r_0)$ just yields (ν, β), since in that case $\boldsymbol{x} \in \mathcal{P}_\star$ already. Therefore, applying it to $\boldsymbol{x} = (x_S(\nu, \beta), y_S(\nu, \beta), z_S(\nu, \beta), r_0)$ will return

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = B \begin{bmatrix} x_N(\nu, \beta) - (x_P^{(1)} + \varepsilon x_P^{(\varepsilon)}) \\ y_N(\nu, \beta) - (y_P^{(1)} + \varepsilon y_P^{(\varepsilon)}) \\ z_N(\nu, \beta) - (z_P^{(1)} + \varepsilon z_P^{(\varepsilon)}) \end{bmatrix} + B \begin{bmatrix} \tilde{x_N}(\nu, \beta) \\ \tilde{y_N}(\nu, \beta) \\ \tilde{z_N}(\nu, \beta) \end{bmatrix} = \begin{bmatrix} \nu \\ \beta \end{bmatrix} + B \begin{bmatrix} \tilde{x}_S(\nu, \beta) \\ \tilde{y}_S(\nu, \beta) \\ \tilde{z}_S(\nu, \beta) \end{bmatrix} , \tag{1.6.106}$$

and we conclude

$$\begin{aligned} |c_1 - \nu| &\leq \frac{\gamma_\infty^2}{1 - \gamma_\infty} \left(\frac{|B_{11}|}{80} + \frac{|B_{12}|}{96} + \frac{(1 + r_0)|B_{13}|}{96 r_0^2} \right) \\ |c_2 - \beta| &\leq \frac{\gamma_\infty^2}{1 - \gamma_\infty} \left(\frac{|B_{21}|}{80} + \frac{|B_{22}|}{96} + \frac{(1 + r_0)|B_{23}|}{96 r_0^2} \right) \end{aligned} \tag{1.6.107}$$

Use the estimates found in (1.6.94) for the coefficients of the B matrix, and bound the $1 + r_0$ term appearing in the bound for $\tilde{z}_S(\nu, \beta)$. We conclude:

$$|c_1 - \nu| < \frac{\gamma_\infty^2 r_0}{100(1 - \gamma_\infty)} \quad , \quad |c_2 - \beta| < \frac{\gamma_\infty^2}{50 r_0 (1 - \gamma_\infty)} \; . \tag{1.6.108}$$

In particular,

$$c_1(S(-\nu_*,\beta)) < -\nu_* + \frac{\gamma_\infty^2 r_0}{100(1-\gamma_\infty)} \quad , \quad c_1(S(\nu_*,\beta)) > \nu_* - \frac{\gamma_\infty^2 r_0}{100(1-\gamma_\infty)} \quad , \quad \text{for all } |\beta| \le \beta_* \ , \tag{1.6.109}$$

$$c_2(S(\nu,-\beta_*)) < -\beta_* + \frac{\gamma_\infty^2}{50 r_0(1-\gamma_\infty)} \quad , \quad c_2(S(\nu,\beta_*)) > \beta_* - \frac{\gamma_\infty^2}{50 r_0(1-\gamma_\infty)} \quad , \quad \text{for all } |\nu| \le \nu_* \ . \tag{1.6.110}$$

Now compare to the definitions (1.6.96) of C_1 and C_2. We will be done if we can ensure

$$\frac{\sigma_*}{1000} + \frac{60\varepsilon r_0}{(1-\gamma_0)^2} < \nu_* - \frac{\gamma_\infty^2 r_0}{100(1-\gamma_\infty)} \tag{1.6.111}$$

$$\frac{\sigma_*}{500 r_0^2} + \frac{120\varepsilon}{r_0(1-\gamma_0)^2} < \beta_* - \frac{\gamma_\infty^2}{50 r_0(1-\gamma_\infty)} \tag{1.6.112}$$

Let's rearrange these inequalities by replacing/bounding ε and r_0 as in (1.6.101), simplifying some numbers, and multiplying the second one through by $r_0^2/2$. Then we need

$$\frac{\sigma_*}{1000} + \frac{\gamma_\infty \gamma_0^8}{60 \cdot 480^8 (1-\gamma_0)^2} + \frac{\gamma_\infty^2 \gamma_0}{48000(1-\gamma_\infty)} < \nu_* \tag{1.6.113}$$

$$\frac{\sigma_*}{1000} + \frac{\gamma_\infty \gamma_0^8}{60 \cdot 480^8 (1-\gamma_0)^2} + \frac{\gamma_\infty^2 \gamma_0}{48000(1-\gamma_\infty)} < \frac{r_0^2 \beta_*}{2} \tag{1.6.114}$$

At the same time, condition (1.6.23) cannot be violated: the parameters ν_*, β_* must be such that

$$960\nu_* + 240 r_0^3 \beta_* = 480\left(2\nu_* + r_0\left(\frac{r_0^2\beta_*}{2}\right)\right) < \gamma_\infty r_0^6 = \frac{\gamma_\infty \gamma_0^6}{480^6} \ . \tag{1.6.115}$$

We have now found all inequalities that need to be valid for some choice of parameters γ_0, γ_∞, σ_*, ν_*, β_*. They are the three inequalities (1.6.113), (1.6.114) and (1.6.115) just above, and the two (1.6.102), (1.6.103) repeated here together:

$$\frac{2\gamma_\infty \gamma_0^5}{25 \cdot 480^5 (1-\gamma_0)^2} + \frac{4\gamma_\infty^2}{75(1-\gamma_\infty)} < \sigma_* < \frac{1-\gamma_0}{360} \ . \tag{1.6.116}$$

1.6.6 Choosing the parameters

Instead of showing here the parameter values that will work, we describe the process used to prove that they exist. At this stage, suppose that γ_0, γ_∞ can be found satisfying the following two main inequalities:

$$\frac{2\gamma_\infty \gamma_0^5}{25 \cdot 480^5 (1-\gamma_0)^2} + \frac{4\gamma_\infty^2}{75(1-\gamma_\infty)} < \frac{1-\gamma_0}{360} \tag{1.6.117}$$

and

$$\frac{2\gamma_\infty\gamma_0^5}{25000\cdot 480^5(1-\gamma_0)^2}+\frac{4\gamma_\infty^2}{75000(1-\gamma_\infty)} + \frac{\gamma_\infty\gamma_0^8}{60\cdot 480^8(1-\gamma_0)^2}+\frac{\gamma_\infty^2\gamma_0}{48000(1-\gamma_\infty)} < \frac{\gamma_\infty\gamma_0^6}{480^7(2+r_0)}\ . \tag{1.6.118}$$

Then we can choose some small $\lambda > 0$ such that

$$\frac{2\gamma_\infty\gamma_0^5}{25\cdot 480^5(1-\gamma_0)^2}+\frac{4\gamma_\infty^2}{75(1-\gamma_\infty)}+\lambda < \frac{1-\gamma_0}{360} \tag{1.6.119}$$

and

$$\frac{2\gamma_\infty\gamma_0^5}{25000\cdot 480^5(1-\gamma_0)^2}+\frac{4\gamma_\infty^2}{75000(1-\gamma_\infty)} + \frac{\gamma_\infty\gamma_0^8}{60\cdot 480^8(1-\gamma_0)^2}+\frac{\gamma_\infty^2\gamma_0}{48000(1-\gamma_\infty)}+\frac{\lambda}{1000} < \frac{\gamma_\infty\gamma_0^6}{480^7(2+r_0)}\ . \tag{1.6.120}$$

Granted this, define

$$\sigma_* = \frac{2\gamma_\infty\gamma_0^5}{25\cdot 480^5(1-\gamma_0)^2}+\frac{4\gamma_\infty^2}{75(1-\gamma_\infty)}+\lambda \tag{1.6.121}$$

and both ν_*, β_* according to

$$\nu_* = \frac{r_0^2\beta_*}{2} = \frac{\sigma_*+\lambda}{1000}+\frac{\gamma_\infty\gamma_0^8}{60\cdot 480^8(1-\gamma_0)^2}+\frac{\gamma_\infty^2\gamma_0}{48000(1-\gamma_\infty)}\ . \tag{1.6.122}$$

It's clear that inequalities (1.6.116), (1.6.113) and (1.6.114) are true, while (1.6.115) goes as follows:

$$\begin{aligned}
&480\left(2\nu_*+r_0\left(\frac{r_0^2\beta_*}{2}\right)\right)\\
&= 480(2+r_0)\left[\frac{1}{1000}\left(\frac{2\gamma_\infty\gamma_0^5}{25\cdot 480^5(1-\gamma_0)^2}+\frac{4\gamma_\infty^2}{75(1-\gamma_\infty)}+\lambda\right)\right.\\
&\qquad\left. + \frac{\gamma_\infty\gamma_0^8}{60\cdot 480^8(1-\gamma_0)^2}+\frac{\gamma_\infty^2\gamma_0}{48000(1-\gamma_\infty)}\right]\\
&< 480(2+r_0)\frac{\gamma_\infty\gamma_0^6}{480^7(2+r_0)}\\
&= \frac{\gamma_\infty\gamma_0^6}{480^6}\ .
\end{aligned} \tag{1.6.123}$$

Hence, all that is left is prove that γ_0, γ_∞ can be chosen making (1.6.117) and (1.6.118) true.

Let us now clean up these inequalities to see where the important parts are. An *a priori* upper bound for $1/(1-\gamma_\infty)$ is $4/3$, from the necessary condition $\gamma_\infty < 1/4$. We can also find one for $1/(1-\gamma_0)^2$ coming from the fact that $\gamma_0 < 1$; for example let's impose

$$\gamma_0 < \frac{9}{10} \iff \frac{1}{(1-\gamma_0)^2} < 100\ . \tag{1.6.124}$$

Replacing these terms by their upper bounds in (1.6.117) and (1.6.118) (as well as $2 + r_0$ by 3 and $1 - \gamma_0$ by 1/10 on the right sides) produces stronger inequalities to be proven. We also cancel a factor γ_∞ from (1.6.118):

$$\begin{gathered}\frac{4\gamma_\infty\gamma_0^5}{480^5} + \frac{16\gamma_\infty^2}{225} < \frac{1}{3600} \\ \frac{4\gamma_\infty\gamma_0^5}{1000 \cdot 480^5} + \frac{16\gamma_\infty}{225000} + \frac{5\gamma_0^8}{3 \cdot 480^8} + \frac{\gamma_\infty\gamma_0}{36000} < \frac{\gamma_0^6}{3 \cdot 480^7}\end{gathered} \tag{1.6.125}$$

The first of these can be obtained, once γ_0 is chosen, by making γ_∞ small. Also, noticing that γ_∞ appears in all but one term on the left of the second inequality, we see that making it small enough will also prove that inequality, as long as γ_0 can be chosen such that

$$\frac{5\gamma_0^8}{3 \cdot 480^8} < \frac{\gamma_0^6}{3 \cdot 480^7} \ . \tag{1.6.126}$$

This is equivalent to $\gamma_0 < \sqrt{96}$. Hence we find that the choice of parameters can be made regardless of the value of $\gamma_0 \in (0, 9/10)$.

Chapter 2

Hartree limit of bosonic atom without Born-Oppenheimer approximation

(Supervised by Michael Kiessling)

2.1 Overview

In the context of the *stability of quantum matter* (see [LS09]), there have been several studies of asymptotic properties of the ground state energy and wavefunction of a quantum-mechanical model of a *bosonic atom*: a system comprised of one positively charged nucleus pinned at $0 \in \mathbb{R}^3$ and N negatively charged identical bosons.

More specifically, consider a Hamiltonian defined on wavefunctions of N variables $q_k \in \mathbb{R}^3$ by

$$H^{(N)}(\psi) = -\frac{1}{2}\sum_{j=1}^{N} \Delta_j \psi - N\lambda \sum_{j=1}^{N} \frac{\psi}{|q_j|} + \sum_{\substack{i=1\\ i<j}}^{N} \sum_{j=1}^{N} \frac{\psi}{|q_i - q_j|} \tag{2.1.1}$$

(some physical parameters omitted for clarity), where Δ_j is the Laplacian with respect only to the 3-vector q_j, and $\lambda > 0$ is the absolute value of the ratio of the charge of the nucleus to that of the bosons. The associated energy functional, with domain $\mathcal{D}(Q^{(N)}) = H^1(\mathbb{R}^3)$, is

$$Q^{(N)}(\psi) = \frac{1}{2}\int_{\mathbb{R}^{3N}} |\nabla\psi(\boldsymbol{q})|^2 \mathrm{d}\boldsymbol{q} - N\lambda \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} \frac{|\psi(\boldsymbol{q})|^2}{|q_j|} \mathrm{d}\boldsymbol{q} + \sum_{\substack{i=1\\ i<j}}^{N} \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} \frac{|\psi(\boldsymbol{q})|^2}{|q_i - q_j|} \mathrm{d}\boldsymbol{q} \tag{2.1.2}$$

(where $\boldsymbol{q} = (q_1, \ldots, q_N)$), and the ground-state energy of the system is

$$E(N) = \inf\left\{ Q^{(N)}(\psi) \; ; \; \psi \in \mathcal{D}(Q^{(N)}) \; , \; \|\psi\|_{L^2} = 1 \right\} \; . \tag{2.1.3}$$

There are conditions on λ, assumed throughout this work, that guarantee the existence of a unique minimizer modulo a phase, called the **ground-state** and denoted $\psi_{\mathrm{GS}}^{(N)}$; see [BL83]. It is also known that the minimization can be taken without loss of generality only over those wavefunctions symmetric with respect to permutations of its N variables (which are the only physical ones, due to the fact that the N particles are identical bosons).

One can prove in various ways that the following 1-body functional (*Hartree functional*)

$$\mathcal{H}_\infty(\phi) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla\phi(x)|^2 \mathrm{d}x - \lambda\int_{\mathbb{R}^3} \frac{|\phi(x)|^2}{|x|}\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^6} \frac{|\phi(x)\phi(y)|^2}{|x-y|}\mathrm{d}x\mathrm{d}y \quad , \quad \phi \in H^1(\mathbb{R}^3) \tag{2.1.4}$$

provides a good approximation, when N is large, for the ground state energy of $H^{(N)}$ ([BL83], [Bau84], [Sol90], [BGM00]), and the minimizer of $\mathcal{H}_\infty$ provides a good approximation for marginal probability distributions constructed from the ground state of $H^{(N)}$ ([Kie10]). In particular, we here are picking up on (the proof of) theorem 1 in [Kie10], which states:

- $E(N)/N^3$ grows monotonically as $N \to \infty$, converging to

$$e_\infty := \inf\{\mathcal{H}_\infty(\phi) \ ; \ \phi \in H^1(\mathbb{R}^3) \ , \ \|\phi\|_{L^2} = 1\} \ ;$$

- for N, n given, $n \leq N$, and considering the re-scaled ground-state

$$\tilde{\psi}^{(N)}_{\mathrm{GS}}(\boldsymbol{q}) = N^{-3N/2}\psi^{(N)}_{\mathrm{GS}}(N^{-1}\boldsymbol{q}) \ , \tag{2.1.5}$$

  we have

$$\lim_{N\to\infty}\int_{\mathbb{R}^{3(N-n)}} |\tilde{\psi}^{(N)}_{\mathrm{GS}}|^2(q_1,\ldots,q_n,u_{n+1},\ldots u_N)\mathrm{d}u_{n+1}\cdots\mathrm{d}u_N = |\phi_{\min}(q_1)|^2\cdots|\phi_{\min}(q_n)|^2 \tag{2.1.6}$$

  weakly in $L^1(\mathbb{R}^{3n}) \cap L^{\frac{3n}{3n-2}}(\mathbb{R}^{3n})$, where $\phi_{\min}$ is the unique positive minimizer of $\mathcal{H}_\infty$ with $\|\phi_{\min}\|_{L^2} = 1$.

A crucial part of Kiessling's proof of this result uses the symmetry of ψ and of $Q^{(N)}$ to rewrite $Q^{(N)}(\psi)$ in terms of the 1- and 2-body marginal probability densities associated to the N-body density $|\psi|^2$. Then the Hewitt-Savage theorem on symmetric measures on the space of infinitely many bodies relates those marginals, for large N, to convex combinations of product states $\psi = \phi^{\otimes N}$, which is how the Hartree functional enters the picture.

The significance of the Hartree functional for understanding the asymptotic behavior of many-body boson systems has been well understood for a few decades already, and the proof strategy described above has also been employed to many different problems, both in the classical and the quantum context - see [Rou15] for a good overview on this topic. The main novel contribution by

Kiessling was in being able to recast the statements about the asymptotic behavior of the quantum model (2.1.1) into the language of classical Statistical Mechanics, so that this strategy could be employed. (We also remark that a previous work by Kiessling had established the monotonic increase of $E(N)/(N^2(N-1))$, a slightly weaker result; a simpler strategy was found by Hogreve in [Hog11], and his argument is what is adapted to work in [Kie10]).

2.1.1 Problem description

Problems involving atomic models, like the one described above, will typically assume the so-called *Born-Oppenheimer approximation*. This amounts to setting the mass M of the nucleus equal to ∞, meaning that it is considered to be fixed at the origin and does not have a corresponding position variable in the wavefunction. The present chapter of this thesis is concerned with a first step towards proving a similar result to Kiessling's in [Kie10] without this approximation. Section 2.2 contains the description and proof of the essential uniqueness of a system of coordinates satisfying symmetry properties that are suitable in this study, as well as in any other classical and quantum many-body problems involving identical bodies or groups thereof. Section 2.4 describes what is involved in the study of the many-body problem obtained from the one in [Kie10] after our coordinate transformation is applied.

2.1.2 Summary of results

It is expected (see conjecture 2.4.2 ahead) that a similar result should hold for the more general case of allowing the nucleus to move and to have a corresponding variable q_0 in the wavefunction, a kinetic energy term $-\frac{1}{2M}\Delta_0$ in $H^{(N)}$, and an effect on the potential term ($|q_j|$ is replaced by $|q_j - q_0|$). But this can only be expected to be true after one finds a way to subtract from $Q^{(N)}$ the energy associated to the center-of-mass motion of the system. This can be done by:

1. finding a coordinate change $T : (q_0, q_1, \ldots, q_N) \mapsto (\xi_0, \xi_1, \ldots, \xi_N)$ where

$$\xi_0 = \frac{1}{M+N}(Mq_0 + q_1 + \cdots + q_N) \tag{2.1.7}$$

   is the center-of-mass,

2. defining the transformed Hamiltonian by $\tilde{H}^{(N)}(\chi) = H^{(N)}(\psi)$ where

$$\chi(\xi) = (\det T)^{-3N/2}\psi(T^{-1}(\xi)) \tag{2.1.8}$$

is the transformed wavefunction,

3. subtracting from $\tilde{H}^{(N)}$ the term $-\frac{1}{2(M+N)}\Delta_0$ that corresponds to the kinetic energy of the system, and

4. conditioning the wavefunction on the position ξ_0 of the center-of-mass, in order to be able to consider the problem as an N-body problem for virtual bodies at positions $\xi_1, \ldots, \xi_N$.

The system of coordinates that is by far the most commonly employed for this purpose goes by the name of *Jacobi coordinates*. It consists of recursively defining new coordinates as the separation between one of the bodies' position from the center of mass of a subgroup of the other bodies, which is an inherently asymmetrical procedure. If one is careful about preserving certain orthogonality properties when carrying out this coordinate change, it is possible to obtain a transformed Hamiltonian $\tilde{H}^{(N)}$, as in item 3 above, having a similar structure to $H^{(N)}$ itself; however, the transformed wavefunction χ in (2.1.8) will in general not obey the same symmetry properties that the original ψ did, which renders the techniques that work in the BO approximation case useless in the transformed problem.

Our main contribution in this context is in finding a novel generalization of the system of Jacobi coordinates transformations, suitable for use in problems where permutation symmetry of the bodies' positions plays an important role. We will prove in theorem 2.2.3 that there exists an essentially unique linear coordinate change T as above having the additional properties that

- the transformed Hamiltonian does not include *Hughes-Eckart* terms, that is, terms of the form $\nabla_j \cdot (\nabla_k \chi)$ for $j \neq k$;
- the transformed wavefunction χ in (2.1.8) has permutation symmetry in variables 1 through N whenever ψ also does.

These properties imply that the transformed Hamiltonian has a similar structure as the original and can then be studied by similar techniques and yield similar results. We will also be able to generalize this coordinate change to be applicable to both classical (theorem 2.2.7) and quantum many-body problems involving more than one group of identical particles (theorem 2.2.8), in which case the symmetry of the allowed states only has to be present with respect to permutations of variables within each group. This part of the work has already been published in [Amo19].

Applying this coordinate change to our problem, the transformed Hamiltonian (after some simplification) comes down to

$$\tilde{H}^{(N)}(\chi) = -\frac{1}{2}\sum_{j=1}^{N}\Delta_j\chi - N\lambda\sum_{j=1}^{N}\frac{\chi}{|\xi_j - C\overline{\xi}|} + \sum_{i=1}^{N}\sum_{\substack{j=1 \\ i<j}}^{N}\frac{\chi}{|\xi_i - \xi_j|}\ , \tag{2.1.9}$$

where we abbreviated the *empirical average*

$$\overline{\xi} = \frac{1}{N}(\xi_1 + \cdots + \xi_N) \tag{2.1.10}$$

of the positions of the virtual bodies, and where $C \neq 1$ is a constant. This can be thought of as the Hamiltonian for an N-body problem where the bodies repel each other by the usual Coulomb force and are attracted by this force towards a comoving center $C\overline{\xi}$ (we remark that the problem is not translation-invariant since $C \neq 1$). We will prove that it admits a ground-state energy.

The fact that the potential term in the middle involves all ξ_j variables means that the energy functional cannot be written in terms of n-body marginals anymore (for any $n < N$). So a more careful study of it is needed. We will find in theorem 2.4.6 that, for an absolutely continuous product state with corresponding probability density given in the product form

$$|\chi(\boldsymbol{\xi})|^2\mathrm{d}\boldsymbol{\xi} = u^{\otimes N}(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} = u(\xi_1)\cdots u(\xi_N)\mathrm{d}\boldsymbol{\xi} \tag{2.1.11}$$

(under some natural assumptions on u), the asymptotic behavior of the potential energy is

$$\lim_{N\to\infty}\int_{\mathbb{R}^{3N}}\frac{|\chi(\boldsymbol{\xi})|^2}{|\xi_j - C\overline{\xi}|}\mathrm{d}\boldsymbol{\xi} = \int_{\mathbb{R}^3}\frac{u(x)}{|x|}\mathrm{d}x \quad \text{for all } j = 1, \ldots, N\ . \tag{2.1.12}$$

This result suggests that the problem now at hand should be treatable by employing the same techniques that were successful in the original problem. Namely, on the one hand it immediately implies that e_∞ is an upper bound for $\lim_{N\to\infty}\tilde{E}(N)/N$ (where $\tilde{E}(N)$ is the ground-state energy of the transformed system), because a trial state of the product form plugged into the energy functional recovers the Hartree functional $\mathcal{H}_\infty$. But on the other hand, in order to understand the limit of the ground-state densities and energy as $N \to \infty$, it also suggests that it suffices to study the behavior of the energy functional only on densities arising from product states. The Hewitt-Savage theorem, which relates symmetric probability densities for large N to convex combinations of product states $\chi = \chi^{\otimes N}$, is the tool that realizes this idea.

2.1.3 Future work

The correct adaptation of the strategy employing the Hewitt-Savage theorem to solve the problem described in the above paragraph remains to be found. For completeness, we include the details of this strategy in the last section of the present chapter, pointing out where the difficulty arises.

It would be interesting to extend the study to more general potentials for the interaction between the bodies. As long as they only involve pairwise interactions depending only on the distance between the bodies, the same coordinate change is applicable and yields a Hamiltonian similar to (2.1.9), with the interaction between bosons remaining the same, and that between the bosons and the nucleus involving again the empirical average $\overline{\xi}$. A wider generalization would be to consider Hamiltonians where the kinetic energy terms belong to a wider class - for example the kind of expressions $(-i\nabla + \boldsymbol{A})^2$ or $\sqrt{-\Delta + mc^2}$ that come up, respectively, with an external magnetic field and under special relativity. These would require a new formulation of the coordinate system.

All of this can be applied to improve the scope of theorems in many-body classical and quantum problems involving symmetry and that originally assume the center-of-mass of the system to be fixed at the origin.

2.2 Symmetric center-of-mass coordinate systems

In this section, we describe the useful coordinate transformation that arose from the efforts to solve the problem outlined in the overview above. The contents of this section have been published in *Journal of Mathematical Physics* [Amo19].

2.2.1 Introduction

In non-relativistic classical and quantum N-body problems with a translation-invariant Hamiltonian

$$H = \sum_{1 \le j \le N} \frac{p_j^2}{2m_j} + \sum_{1 \le j < k \le N} V_{jk}(|q_j - q_k|) \ , \qquad (2.2.1)$$

where $q_j \in \mathbb{R}^3$ denotes the position vector of particle j in some arbitrary Galilei frame, p_j its momentum, and m_j its mass, the motion of the center-of-mass has no objective physical significance. Objectively significant are only the intrinsic properties of the N-body system. If $Q \in \mathbb{R}^3$ denotes the position vector of the center-of-mass in the same Galilei frame, and P its momentum:

$$Q = \sum_{1\le j\le N} m_j q_j \quad , \quad P = \sum_{1\le j\le N} p_j \ , \tag{2.2.2}$$

then the Galilei transformation $q_j \mapsto r_j := q_j - Q$ and $p_j \mapsto \pi_j := p_j - \frac{m_j}{M_{\mathrm{Tot}}} P$ (where M_{Tot} is the total mass in the system) separates off the kinetic energy assigned to the center-of-mass, i.e. it accomplishes

$$H = \frac{P^2}{2M_{\mathrm{Tot}}} + \tilde{H} \ , \tag{2.2.3}$$

where

$$\tilde{H} = \sum_{1\le j\le N} \frac{\pi_j^2}{2m_j} + \sum\sum_{1\le j<k\le N} V_{jk}(|r_j - r_k|) \tag{2.2.4}$$

is the “intrinsic Hamiltonian" of the N-body system, encoding all the physically objective features of the N-body system. The N position variables r_j and the N momentum variables π_j are not independent but satisfy the center-of-mass frame constraints

$$\sum_{1\le j\le N} m_j r_j = 0 \quad , \quad \sum_{1\le j\le N} \pi_j = 0 \ . \tag{2.2.5}$$

Thus, in terms of the available degrees of freedom, the intrinsic N-body Hamiltonian is actually equivalent to a non-translation-invariant $(N-1)$-body problem. Therefore it is desirable to find a transformation to new coordinates which expresses $\tilde{H}$ as a function of $N-1$ independent positions and momenta, which can be thought of as pertaining to “virtual bodies”. The so-called *Jacobi coordinates* accomplish this feat (see section 2).

Now, systems whose bodies are identical (or systems involving different groups of identical bodies) enjoy valuable permutation symmetry or anti-symmetry properties in both their Hamiltonian and admissible states, which can play a determining role in their study. But it turns out that, after reducing such systems to $(N-1)$-body systems by employing Jacobi coordinates, one finds that they lose their symmetry properties and can no longer be studied by means of the same techniques. The goal of this paper is to build a center-of-mass coordinate change that preserves symmetry in whatever sense is meaningful for the problem at hand. We will prove that there is an essentially unique coordinate change with this property.

In the next subsection we show how carrying out the Jacobi coordinates change in our bosonic atom system destroys its symmetry. In the one following it we show the construction of our **symmetric center-of-mass system of coordinates** applied to that same problem, proving its uniqueness in the process. Next we show that the same system of coordinates is suitable also for symmetric classical problems, even though they involve fundamentally different notions of configuration space, admissible states and Hamiltonian. The main result is summarized in theorems (2.2.3) and (2.2.7), and the coordinate system in its most compact form in equations (2.2.54) and (2.2.60). Finally in the last subsection we indicate how to generalize the construction to problems involving more than one group of objects of the same type (uniqueness does not hold anymore), culminating in the change of coordinates described in theorem (2.2.8).

2.2.2 Jacobi coordinates: a quantum example

To illustrate the need for a symmetric center-of-mass coordinate system, we start by discussing the model that inspired us to create it, which can be found in [Hog11],[Kie10],[Kie12]. It is a study of the asymptotic properties of the equilibrium configuration energy and ground state of a "bosonic atom" consisting of one positively charged nucleus and N negatively-charged bosons as N goes to infinity, assuming the so-called *Born-Oppenheimer (BO) approximation*, that is, the nucleus is considered to sit immovable at the origin. Our motivation for introducing our system of coordinates was the desire to study the same system, by adapting the same techniques, but without the BO approximation.

But we emphasize that neither the particular type of interaction between the bodies in this model (Coulomb attraction/repulsion) nor the fact that they are bosons instead of fermions is what justifies the need for such a system; the important feature is the symmetry that comes from the fact that all (or all but one) of the bodies are identical.

Consider a quantum-mechanical system consisting of one distinguished particle of mass m_0 and charge $Z > 0$, and N identical particles of mass m and charge $z < 0$, all of which attract or repel each other via the Coulomb potential. The state of the system is given by a $\mathbb{C}$-valued (we ignore spin) wavefunction

$$L^2(\mathbb{R}^{3(1+N)}) \ni \psi = \psi(q_0, q_1, \ldots, q_N) \quad , \quad q_j \in \mathbb{R}^3, j = 0, 1, \ldots, N \tag{2.2.6}$$

where q_0 is the position of the zeroth particle and each q_j, $j \geq 1$, is the position of one of the other particles. Born's Rule says that $|\psi(q_0, q_1, \ldots, q_N)|^2$ is the probability density for the zeroth particle to be at q_0 and for there to exist one of the other particles at each $q_1, \ldots, q_N$. Because of indistinguishability, the only admissible wavefunctions are those that satisfy the *symmetry condition*

$$\psi(q_0, q_1, \ldots, q_N) = \psi(q_0, q_{\sigma(1)}, \ldots, q_{\sigma(N)}) \quad \text{for all permutations } \sigma \in S^N \tag{2.2.7}$$

if particles 1 through N are bosons, or the *anti-symmetry condition* (Pauli exclusion principle)

$$\psi(q_0, q_1, \ldots, q_N) = sgn(\sigma)\psi(q_0, q_{\sigma(1)}, \ldots, q_{\sigma(N)}) \quad \text{for all permutations } \sigma \in S^N \tag{2.2.8}$$

if they are fermions (S^N denotes the symmetric group in N objects). The reason why these conditions must be stated as such, and not in the weaker form $|\psi(q_0, q_1, \ldots, q_N)|^2 = |\psi(q_0, q_{\sigma(1)}, \ldots, q_{\sigma(N)})|^2$ that one might expect from the Born rule, is that it should be true that the expected value of any observable (self-adjoint operator) A, that is, the inner product $\langle \psi, A\psi \rangle_{L^2}$, should be independent of permutations of any but the zeroth variable. Since quantum-mechanical observables are not restricted to simple multiplication operators, but rather can take the form of differential operators as well, it turns out that the condition needed is as given. See [Gir69] for details about this and the Pauli exclusion principle for the case of fermions.

The Hamiltonian operator, defined only for twice-differentiable wavefunctions (but it does admit a self-adjoint extension to a larger domain - see [Lie90], [LS09], [RS75]), is given by summing the kinetic energy differential operators of each particle and the potential energy multiplication operators of each pair of particles:

$$H = -\frac{\hbar^2}{2m_0}\Delta_0 - \frac{\hbar^2}{2m}\sum_{j=1}^{N}\Delta_j - Zz\sum_{j=1}^{N}\frac{1}{|q_j - q_0|} + z^2 \sum_{i=1}^{N}\sum_{\substack{j=1 \\ i<j}}^{N}\frac{1}{|q_i - q_j|} \ . \tag{2.2.9}$$

Here the notation Δ_j indicates the Laplacian operator acting only with respect to $q_j \in \mathbb{R}^3$, that is,

$$\Delta_j = \frac{\partial^2}{\partial x_j^2} + \frac{\partial^2}{\partial y_j^2} + \frac{\partial^2}{\partial z_j^2} \quad , \quad \text{where } q_j = (x_j, y_j, z_j). \tag{2.2.10}$$

Associated to the operator H is the quadratic functional that yields the expected value of the energy in the state ψ, obtained by formally computing the $L^2(\mathbb{R}^{3(1+N)})$ inner product $\langle \psi, H\psi \rangle$ with the help of an integration by parts in the kinetic terms:

$$Q(\psi) = \frac{\hbar^2}{2m_0}\int |\nabla_0\psi|^2 + \frac{\hbar^2}{2m}\sum_{j=1}^{N}\int |\nabla_j\psi|^2 - Zz\sum_{j=1}^{N}\int \frac{|\psi|^2}{|q_j - q_0|} + z^2\sum_{i=1}^{N}\sum_{\substack{j=1 \\ i<j}}^{N}\int \frac{|\psi|^2}{|q_i - q_j|} \tag{2.2.11}$$

with the analogous remark about the notation ∇_j as for the Laplacian above. It turns out that this functional is bounded below when computed on H^1 functions of L^2 norm 1 (for details see [Lie90],[RS75]), and the infimum is interpreted as the equilibrium energy of the system.

Remark 2.2.1. The (anti-)symmetry of ψ permits us to make statements such as

$$\int |\nabla_j \psi|^2 = \int |\nabla_1 \psi|^2 \;,\; \int \frac{|\psi|^2}{|q_j - q_0|} = \int \frac{|\psi|^2}{|q_1 - q_0|} \;,\; \int \frac{|\psi|^2}{|q_i - q_j|} = \int \frac{|\psi|^2}{|q_1 - q_2|} \tag{2.2.12}$$

for all $i \neq j$, which combined with the symmetry of H are useful in Hartree and Hartree-Fock theory for studying asymptotic properties of the equilibrium energy, because they allow the replacement of all indices i and j in Q by 1 and 2, thus re-expressing Q in terms of a conditional two-body functional (depending only on variables q_1, q_2 and conditioned on q_0). For details see [Kie12] or [Rou15].

However, it is easy to argue that there will not exist a *ground-state* having q_0 separated from the other variables; that is, the infimum can never be attained by functions of the form $\psi = \psi_0(q_0)\phi(q_1, \ldots, q_N)$. Indeed, ψ_0 will only contribute to the first term of the energy $Q(\psi)$ (the variable q_0 in the first potential term disappears after a translation change of variables in the integral), which can be made arbitrarily small by reducing $\int |\nabla \psi_0|^2$, but never zero because ψ_0 must have positive L^2 norm. And if this were a classical problem instead, where it *is* possible to reduce the contribution of the zeroth kinetic energy to zero, then it is also easy to see that there would not exist a *unique* minimizer, because the problem is translation-invariant.

On the other hand, the functional Q contains more than the portion of the energy that we are interested in, because contained in the kinetic energy part is the energy of motion of the system as a whole (the kinetic energy of the center-of-mass). But there doesn't exist an operator associated to the kinetic energy of the system that can be subtracted from H in order to isolate the interesting part; the way to achieve this separation is to first change coordinates into a system which includes the center-of-mass as a coordinate:

$$T : (q_0, q_1, \ldots, q_N) \mapsto (\xi_0, \xi_1, \ldots, \xi_N) \quad , \quad \xi_0 = \frac{1}{M_{\text{Tot}}}(m_0 q_0 + m q_1 + \ldots + m q_N) \tag{2.2.13}$$

(we abbreviated the total mass $m_0 + Nm$ with M_{Tot}) and write ψ as an L^2-normalized function of the new ξ coordinates:

$$\chi(\xi_0, \xi_1, \ldots, \xi_N) = |\det T|^{-1/2} \psi(T^{-1}(\xi_0, \xi_1, \ldots, \xi_N)) \;, \tag{2.2.14}$$

then finally express all terms in (2.2.9) using χ instead of ψ, obtaining a new Hamiltonian $\tilde{H}$ such that

$$H\psi = \tilde{H}\chi \tag{2.2.15}$$

whenever ψ and χ are related by (2.2.14). If the coordinate change T is linear, one of the terms in $\tilde{H}$ will involve the Laplacian with respect to ξ_0 (as will become clear in (2.2.25) below), and throwing out this term will leave us with an operator associated to the desired energy of the system.

This process might end up introducing unhelpful *cross-terms*: the Chain Rule applied to (2.2.14) gives (with $\Delta\psi = \nabla \cdot \nabla\psi$)

$$\Delta_j \psi(\boldsymbol{q}) = |\det T|^{1/2} \sum_{k,l=0}^{N} \frac{\partial \xi_k}{\partial q_j} \frac{\partial \xi_l}{\partial q_j} \nabla_k \cdot \nabla_l \chi(T\boldsymbol{q}) \ . \tag{2.2.16}$$

We call *cross-term* an expression of the form k-divergence of l-gradient for $k \neq l$, of which there are none in the original Hamiltonian H. These expressions are known in the literature as *Hughes-Eckart terms* - see [HE30] and [Thi02] for more details.

A commonly employed family of coordinate changes that prevent the appearance of such cross-terms can be found for example in [FO17], [IGM06] and [Pos56], usually referred to by the name *Jacobi coordinates*. It is well-known that the crucial property needed to preclude cross-terms is orthogonality of the matrix $\dfrac{\partial \boldsymbol{q}}{\partial \boldsymbol{\xi}}$ (after suitable rescalings to make all masses equal to 1 - see the next section). It is also well-known that one can construct such matrices even when the objects in the system have different masses - see remark (2.2.2) below. One possible instance of a Jacobi coordinate change consists in starting with the separation between two of the bodies as a new coordinate, then iteratively constructing the others as the separation between the next body and the center-of-mass of the previously used bodies (different normalizing scale factors can be included too). For our problem, then, a Jacobi system of coordinates could look like

$$\begin{cases} \xi_0 & = & (m_0 q_0 + m q_1 + \ldots + m q_N)/M_{\text{Tot}} \\ \xi_1 & = & q_1 - q_2 \\ \xi_2 & = & (q_1 + q_2)/2 - q_3 \\ \vdots & & \vdots \\ \xi_{N-1} & = & (q_1 + q_2 + \cdots + q_{N-1})/(N-1) - q_N \\ \xi_N & = & (q_1 + q_2 + \cdots + q_N)/N - q_0 \end{cases} \tag{2.2.17}$$

Employing this system for $N = 1$ (a two-body problem), what is obtained after (2.2.15) is

$$\tilde{H} = -\frac{\hbar^2}{2(m_0 + m)}\Delta_0 - \frac{\hbar^2}{2\mu}\Delta_1 + \frac{Zz}{|\xi_1|} \tag{2.2.18}$$

where

$$\mu = \frac{M_{\mathrm{Tot}} m}{M_{\mathrm{Tot}} + m} \tag{2.2.19}$$

is called the *reduced mass*. Throwing away the first term of $\tilde{H}$ gives us the Hamiltonian for a one-body problem with mass μ in a central potential, known as the *Kepler problem*. It admits a ground state energy and a unique ground state configuration conditioned on the position ξ_0 of the center-of-mass.

But for $N > 1$ the symmetry of the potential part of the Hamiltonian is hopelessly lost under the change (2.2.17), because one can compute and check that $|\xi_i - \xi_j| \neq |\xi_k - \xi_l|$ if $\{i, j\} \neq \{k, l\}$. Further, the symmetry or anti-symmetry condition on the wavefunction ψ does not translate to anything practical about permutation of the variables $\xi_1, \ldots, \xi_N$ of χ. If we want to study the properties of $\tilde{H}$ using the same techniques as one would for the symmetric H and its (anti-)symmetric wavefunctions, a better change of coordinates is clearly needed.

2.2.3 Symmetric center-of-mass coordinates (quantum case)

Here we describe our coordinate system, illustrated with the same system as in the previous section, and explain in which sense and under which conditions it is unique.

The coordinate change should be an invertible map $T : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)}$ for which we require the following conditions:

1. linearity and independence from Cartesian coordinates;
2. one of the new coordinates is the center-of-mass;
3. the structure of Hamiltonian is preserved and includes $-(\hbar^2/2M_{\mathrm{Tot}})\Delta_0$, the kinetic energy operator of the system in the new coordinates;
4. symmetry of wavefunctions is preserved.

Let us elaborate on each and see how they restrict the possible transformations T further and further.

Condition 1. We demand linearity for simplicity of computation and to avoid singularities. But in order to avoid bringing to the fore such physically meaningless quantities as the scalar coordinates of each particle position, we look for a linear transformation that operates only on the level of the positions of each particle, that is, only on the vectors $q_0, q_1, \ldots, q_N$ as opposed to explicitly referencing the x, y, z coordinates of the particles. So we think of $\mathbb{R}^{3(1+N)}$ in both its domain and range as $(\mathbb{R}^3)^{1+N}$, and we write $T(q_0, q_1, \ldots, q_N) = (\xi_0, \xi_1, \ldots, \xi_N)$, each q_j and ξ_j in $\mathbb{R}^3$. This can be made more formal by saying that T is a tensor product of a $(1+N) \times (1+N)$ matrix $\tilde{T}$ with the 3×3 identity matrix. But to avoid cluttered notation, we denote the elements of $\tilde{T}$ by T_{ij} $(0 \leq i, j \leq N)$, without tildes and hopefully without confusion.

Condition 2. We impose that ξ_0 be the center-of-mass of the system:

$$\xi_0 = \frac{1}{M_{\text{Tot}}}(m_0 q_0 + m q_1 + \cdots + m q_N) \ . \tag{2.2.20}$$

With this the first row of the matrix of $\tilde{T}$ is already determined.

Condition 3. We want T to transform the structure of the Hamiltonian into a form similar to H: kinetic plus potential terms, with the kinetic terms of identical particles appearing with equal weights, the same being true of the potential terms of interaction between similar pairs. Additionally, what should sit in front of the Δ_0 term is the fraction $-\hbar^2/2M_{\text{Tot}}$, so that this term becomes the kinetic energy operator of the whole system. Let us only worry about the kinetic term in (2.2.9) and later study what happens to the potential terms. We stipulate that there should exist some constant $\mu > 0$ (which we call the *reduced mass*) such that

$$-\frac{\hbar^2}{2m_0}\Delta_0\psi(\mathbf{q}) - \frac{\hbar^2}{2m}\sum_{j=1}^{N}\Delta_j\psi(\mathbf{q}) = -\frac{\hbar^2}{2M_{\text{Tot}}}\Delta_0\chi(\boldsymbol{\xi}) - \frac{\hbar^2}{2\mu}\sum_{j=1}^{N}\Delta_j\chi(\boldsymbol{\xi}) \ , \tag{2.2.21}$$

where $\boldsymbol{\xi} = T\mathbf{q}$ and χ is defined by

$$\chi(\boldsymbol{\xi}) = |\det T|^{-1/2}\psi(T^{-1}\boldsymbol{\xi}) \quad , \quad \boldsymbol{\xi} \in \mathbb{R}^{3(1+N)} \ . \tag{2.2.22}$$

By the Chain Rule,

$$\nabla_j\psi(\boldsymbol{q}) = |\det T|^{1/2}\sum_{k=0}^{N} T_{kj}\nabla_k\chi(T\boldsymbol{q}) \tag{2.2.23}$$

and

$$\Delta_j\psi(\boldsymbol{q}) = (\det T)^{1/2}\sum_{k,l=0}^{N} T_{kj}T_{lj}\nabla_k \cdot \nabla_l\chi(T\boldsymbol{q}) \ . \tag{2.2.24}$$

Omitting the $\boldsymbol{q}$ argument of ψ and the $T\boldsymbol{q}$ argument of χ, we then have

$$\begin{aligned}
&-\frac{\hbar^2}{2m_0}\Delta_0\psi - \frac{\hbar^2}{2m}\sum_{j=1}^{N}\Delta_j\psi \\
&\qquad = -|\det T|^{1/2}\left(\frac{\hbar^2}{2m_0}\sum_{k,l=0}^{N}T_{k0}T_{l0}\nabla_k\cdot\nabla_l\chi + \frac{\hbar^2}{2m}\sum_{j=1}^{N}\sum_{k,l=0}^{N}T_{kj}T_{lj}\nabla_k\cdot\nabla_l\chi\right) \\
&\qquad = -|\det T|^{1/2}\frac{\hbar^2}{2}\sum_{k,l=0}^{N}\left(\frac{1}{m_0}T_{k0}T_{l0} + \frac{1}{m}\sum_{j=1}^{N}T_{kj}T_{lj}\right)\nabla_k\cdot\nabla_l\chi\ ,
\end{aligned} \tag{2.2.25}$$

so that we can achieve (2.2.21) by imposing

$$|\det T|^{1/2}\left(\frac{1}{m_0}T_{k0}T_{l0} + \frac{1}{m}\sum_{j=1}^{N}T_{kj}T_{lj}\right) = \begin{cases} 1/M_{\mathrm{Tot}} & ,\quad k=l=0\ , \\ 1/\mu & ,\quad k=l>0\ , \\ 0 & ,\quad k\neq l\ . \end{cases} \tag{2.2.26}$$

Given our choice of ξ_0, the condition for $k=l=0$ holds if and only if

$$\det T = \pm 1\ . \tag{2.2.27}$$

Now rewrite property (2.2.26) as

$$\tilde{T}R^{-1}\tilde{T}^t = S^{-1} \tag{2.2.28}$$

where the $(1+N)\times(1+N)$ matrices R and S are given by

$$R = \mathrm{diag}(m_0, m, \ldots, m) \qquad , \qquad S = \mathrm{diag}(M_{\mathrm{Tot}}, \mu, \ldots, \mu)\ . \tag{2.2.29}$$

Then

$$(\det T)^2 = \frac{\det(R)}{\det(S)} \quad\Longrightarrow\quad \det T = \pm\sqrt{\frac{m_0 m^N}{M_{\mathrm{Tot}}\mu^N}} \tag{2.2.30}$$

and since we need $|\det T| = 1$, we can find μ:

$$\mu = m\left(\frac{m_0}{M_{\mathrm{Tot}}}\right)^{1/N}\ . \tag{2.2.31}$$

Remark 2.2.2. If particles $1,\ldots,N$ in the system were not identical and had potentially different masses $m_1,\ldots,m_N$, as is the case in various examples of many-body problems, then condition 4 (as elaborated below) and the preservation of the symmetry of the potential energy would be meaningless; however it could still be desirable to find a center-of-mass system of coordinates satisfying conditions 1 and 2 that also prevents the appearance of unwieldy cross-terms in the transformed Hamiltonian. In this case one would stipulate the condition

$$-\frac{\hbar^2}{2m_0}\Delta_0\psi(\mathbf{q}) - \frac{\hbar^2}{2}\sum_{j=1}^{N}\frac{1}{m_j}\Delta_j\psi(\mathbf{q}) = -\frac{\hbar^2}{2M_{\text{Tot}}}\Delta_0\chi(\boldsymbol{\xi}) - \frac{\hbar^2}{2}\sum_{j=1}^{N}\frac{1}{\mu_j}\Delta_j\chi(\boldsymbol{\xi}) \ , \tag{2.2.32}$$

for some numbers $\mu_1, \ldots, \mu_N > 0$. Proceeding as in the computations above, one would find

$$\tilde{T} \cdot \operatorname{diag}(m_0, m_1, \ldots, m_N)^{-1} \cdot \tilde{T}^t = \operatorname{diag}(M_{\text{Tot}}, \mu_1, \ldots, \mu_N)^{-1} \ . \tag{2.2.33}$$

This is easily achieved: choose an orthogonal matrix $\mathcal{O}$ whose zeroth row is given by

$$(\mathcal{O}_{0j})_{j=0,1,\ldots,N} = \left(\sqrt{\frac{m_0}{M_{\text{Tot}}}}, \sqrt{\frac{m_1}{M_{\text{Tot}}}}, \ldots, \sqrt{\frac{m_N}{M_{\text{Tot}}}}\right) \tag{2.2.34}$$

so that condition 2 is met, and let

$$\tilde{T} = \operatorname{diag}\left(\frac{1}{\sqrt{M_{\text{Tot}}}}, \frac{1}{\sqrt{\mu_1}}, \ldots, \frac{1}{\sqrt{\mu_N}}\right) \cdot \mathcal{O} \cdot \operatorname{diag}(\sqrt{m_0}, \sqrt{m_1}, \ldots, \sqrt{m_N}) \ . \tag{2.2.35}$$

The only additional constraint comes from $|\det \tilde{T}| = 1$, which, when implemented in (2.2.35) above, produces a restriction on the possible choices of μ_j's:

$$m_0 m_1 \cdots m_N = M_{\text{Tot}}\mu_1 \cdots \mu_N \ . \tag{2.2.36}$$

Condition 4. T must have the property that, if ψ is (anti-)symmetric in the variables $q_1, \ldots, q_N$, then χ defined as in (2.2.22) is (anti-)symmetric in $\xi_1, \ldots, \xi_N$ as well. Let us work out what this implies.

For a given permutation $\sigma \in S^N$ let σ also denote the isomorphism

$$\sigma : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)} \quad , \quad \sigma(x_0, x_1, \ldots, x_N) = (x_0, x_{\sigma(1)}, \ldots, x_{\sigma(N)}) \tag{2.2.37}$$

(each $x_j \in \mathbb{R}^3$). The required equality $\chi = \chi \circ \sigma$ (symmetric case), which translates to

$$|\det T|^{-1/2}\psi(T^{-1}\boldsymbol{\xi}) = \chi(\boldsymbol{\xi}) = \chi(\sigma\boldsymbol{\xi}) = |\det T|^{-1/2}\psi(T^{-1}\sigma\boldsymbol{\xi}) \ , \tag{2.2.38}$$

holds for any wavefunction ψ symmetric in all but the zeroth variables, for all $\sigma \in S^N$ and all $\xi \in \mathbb{R}^{3(1+N)}$, if and only if to every $\sigma \in S^N$ corresponds $\pi \in S^N$ such that

$$\pi T^{-1} = T^{-1}\sigma \tag{2.2.39}$$

(simply compare the arguments of ψ on both ends of (2.2.38) and use symmetry of ψ). In the case of anti-symmetry, for fermionic particles, π must also have the same sign as σ. We remind the reader that $T = \tilde{T} \otimes I_{3\times 3}$ for some $\tilde{T} : \mathbb{R}^{1+N} \to \mathbb{R}^{1+N}$, and of course any $\sigma \in S^N$ acts on $\mathbb{R}^{1+N}$ by permuting coordinates 1 through N with respect to the canonical basis $\{e_0, e_1, \ldots, e_N\} \subseteq \mathbb{R}^{1+N}$. So let

$$\tilde{T}e_1 = \sum_{j=0}^{N} a_j e_j \quad , \quad a_j \in \mathbb{R} \ . \tag{2.2.40}$$

Then condition (2.2.39), after multiplying on left and right by T, means, for any σ, that $\sigma \cdot \tilde{T}e_1$ must be equal to one of the vectors

$$\tilde{T}e_1, \ldots, \tilde{T}e_N \ . \tag{2.2.41}$$

But acting with σ on $\tilde{T}e_1$ has the effect of permuting the coefficients a_j for $j > 0$, and the total number of different permutations that can be formed is

$$\frac{N!}{n_1! \cdots n_m!} \tag{2.2.42}$$

where $n_1, \ldots, n_m$ are the cardinalities of each set of repeated coefficients among the a_j's, $j = 1, \ldots, N$, with $n_1 + \cdots + n_m = N$. Since the number in (2.2.42) must be equal to the number N of different vectors in the list (2.2.41), we need

$$(N-1)! = n_1! \cdots n_m! \tag{2.2.43}$$

which can only happen for all N if $m = 2$ and one of the n_j's is $N-1$ and the other 1 (to see this, consider what happens when $N-1$ is prime). Therefore $\tilde{T}e_1$ written in the basis $\{e_j\}$ must have $N-1$ repeated coefficients among the ones from 1 to N. Analogously the same is true of each $\tilde{T}e_j$ for $j = 2, \ldots, N$, and moreover they all share the same zeroth coefficient. Also note that (2.2.39) implies that performing any permutation on the rows of T (except the zeroth) should yield the same as performing it on the columns instead; hence the coefficients on the zeroth column of $\tilde{T}$ are also all equal, except the zeroth. Finally, by relabeling the nonzero indices (that is, by replacing T with

$T \circ \sigma$ for an appropriate σ), and also remembering (2.2.20), we arrive at a matrix of the form

$$T = \begin{pmatrix} \frac{m_0}{M_{\text{Tot}}} & \frac{m}{M_{\text{Tot}}} & \frac{m}{M_{\text{Tot}}} & \frac{m}{M_{\text{Tot}}} & \cdots & \frac{m}{M_{\text{Tot}}} \\ C & A & B & B & \dots & B \\ C & B & A & B & \dots & B \\ C & B & B & A & \dots & B \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ C & B & B & B & \dots & A \end{pmatrix}_{(1+N)\times(1+N)} \otimes I_{3\times 3} \tag{2.2.44}$$

for some constants A, B, C to be determined.

We refer back to (2.2.26). The cases $k = l > 0$, $0 \neq k \neq l \neq 0$ and $0 = k \neq l$, in that order, give equations for the entries A, B, C in (2.2.44):

$$\frac{C^2}{m_0} + \frac{A^2}{m} + \frac{(N-1)B^2}{m} = \frac{1}{\mu} \quad \Longrightarrow \quad A^2 + (N-1)B^2 = \frac{m}{\mu} - \frac{mC^2}{m_0} \ , \tag{2.2.45}$$

$$\frac{C^2}{m_0} + \frac{2AB}{m} + \frac{(N-2)B^2}{m} = 0 \quad \Longrightarrow \quad 2AB + (N-2)B^2 = -\frac{mC^2}{m_0} \ , \tag{2.2.46}$$

$$C + A + (N-1)B = 0 \quad \Longrightarrow \quad A + (N-1)B = -C \ . \tag{2.2.47}$$

Subtract (2.2.46) from (2.2.45) and write $A^2 - 2AB + B^2$ as $(A-B)^2$ to get an expression for A in terms of B. Plug that into (2.2.47) to find B in terms of C:

$$A = B \overset{(1)}{\pm} \sqrt{\frac{m}{\mu}} \quad , \quad B = -\frac{1}{N}\left(C \overset{(1)}{\pm} \sqrt{\frac{m}{\mu}}\right) \ . \tag{2.2.48}$$

The choice of the $\pm$ sign has to be the same in these two expressions, and that's what the (1) above them signifies. With these, (2.2.45) becomes

$$\frac{C^2}{N} - \frac{m}{N\mu} = -\frac{mC^2}{m_0} \ , \tag{2.2.49}$$

which can be solved to yield

$$C \ = \overset{(2)}{\pm} \sqrt{\frac{m_0 m}{M_{\text{Tot}}\mu}} \ . \tag{2.2.50}$$

This $\pm$ sign has nothing to do with the choice of $\pm$ in (2.2.48), and we keep track of that with the (2) above it. Now it becomes convenient to rewrite A, B, C in terms of only the constant $r = m_0/M_{\text{Tot}} = (\mu/m)^N$:

$$A = B \overset{(1)}{\pm} r^{-\frac{1}{2N}} \quad , \quad B = -\frac{1}{N}(\overset{(2)}{\pm} r^{\frac{1}{2}-\frac{1}{2N}} \overset{(1)}{\pm} r^{-\frac{1}{2N}}) \quad , \quad C = \overset{(2)}{\pm} r^{\frac{1}{2}-\frac{1}{2N}} \ . \tag{2.2.51}$$

We can also write the new coordinates compactly by using the *empirical average*

$$\overline{\boldsymbol{q}} = (q_1 + \cdots + q_N)/N \ . \tag{2.2.52}$$

Computing ξ_1 (a similar computation gives ξ_j), we see how $\overline{\boldsymbol{q}}$ shows up due to the relationship between A and B:

$$\begin{aligned}\xi_1 &= Cq_0 + Aq_1 + B(q_2 + \cdots + q_N) \\ &= Cq_0 + B(q_1 + \cdots + q_N) \overset{(1)}{\pm} r^{-\frac{1}{2N}} q_1 \\ &= Cq_0 + (NB)\overline{\boldsymbol{q}} \overset{(1)}{\pm} r^{-\frac{1}{2N}} q_1 \ .\end{aligned} \tag{2.2.53}$$

Substituting the values of A, B, C, we obtain the final expression of our coordinate change:

$$\begin{cases} \xi_0 &= \quad (m_0 q_0 + m q_1 + \ldots + m q_N)/M_{\text{Tot}} \ , \\ \xi_j &= \quad r^{-\frac{1}{2N}} \left(\overset{(1)}{\pm} (q_j - \overline{\boldsymbol{q}}) \overset{(2)}{\pm} \sqrt{r}(q_0 - \overline{\boldsymbol{q}}) \right) \quad , \quad j = 1, \ldots, N \ . \end{cases} \tag{2.2.54}$$

We have thus proved the following:

Theorem 2.2.3. *For given $m_0, m > 0$ and up to two independent choices of $\pm$ signs and relabeling of nonzero indices, the only family of transformations $T : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)}$ (indexed by N) satisfying the following:*

1. *$T = \tilde{T} \otimes I_{3\times 3}$ for some linear isomorphism $\tilde{T} : \mathbb{R}^{1+N} \to \mathbb{R}^{1+N}$;*

2. *the zeroth component of $T(q_0, q_1, \ldots, q_N)$ in $\mathbb{R}^3$ is given by*

$$\frac{1}{m_0 + Nm}(m_0 q_0 + m q_1 + \cdots + m q_N) \tag{2.2.55}$$

   for all $q_0, q_1, \ldots, q_N \in \mathbb{R}^3$;

3. *there exists $\mu > 0$ such that, for any $\psi : \mathbb{R}^{3(1+N)} \to \mathbb{C}$,*

$$-\frac{\hbar^2}{2m_0}\Delta_0\psi - \frac{\hbar^2}{2m}\sum_{j=1}^{N}\Delta_j\psi = -\frac{\hbar^2}{2(m_0+Nm)}\Delta_0(\psi\circ T) - \frac{\hbar^2}{2\mu}\sum_{j=1}^{N}\Delta_j(\psi\circ T) \ ; \tag{2.2.56}$$

4. *if $\psi : \mathbb{R}^{3(1+N)} \to \mathbb{C}$ is (anti-)symmetric with respect to exchange of any of its $\mathbb{R}^3$ variables 1 through N, then so is $\psi \circ T^{-1}$;*

is the one given by (2.2.54) with the dimensionless constant $r \in (0,1)$ *and the reduced mass* μ *given by*

$$r = \frac{m_0}{m_0 + Nm} \quad , \quad \mu = m r^{1/N} \ . \tag{2.2.57}$$

Remark 2.2.4. When $N = 1$, our T recovers the well-known 2-body system of Jacobi coordinates if we choose $\overset{(2)}{\pm} = -$. Indeed, in this case we have $\overline{\boldsymbol{q}} = q_1$, and equation (2.2.54) shows

$$\xi_1 = r^{-1/2}(0 \overset{(2)}{\pm} r^{1/2}(q_0 - q_1)) = \overset{(2)}{\pm} (q_0 - q_1) \ . \tag{2.2.58}$$

Also (2.2.57) implies that μ is the usual reduced mass (2.2.19) for two bodies.

Remark 2.2.5. It is common in statistical problems to consider a more general space of admissible states, called *density matrices*. This is the set $\mathcal{S} = \mathcal{S}(L^2(\mathbb{R}^{3(1+N)}))$ of self-adjoint, positive, trace-class, unit-trace operators acting on L^2. In this context, a *pure* state ψ as considered above is represented by the projection operator $|\psi\rangle\langle\psi|$, while a mixture of pure states ψ_j with weights $0 < \lambda_j < 1$ (such that $\sum_j \lambda_j = 1$) gets associated to the operator $\sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$. The expected energy in state $\rho \in \mathcal{S}$ is then given by $Q(\rho) = \mathrm{Tr}[H\rho]$, and the state is called *symmetric* with respect to the nonzero variables when $U_\sigma \rho = \rho$ for all $\sigma \in S^N$, where U_σ is the unitary operator $L^2 \ni \psi \mapsto \psi \circ \sigma$ (analogously the concept of *anti-symmetry* involves an additional $sgn(\sigma)$).

We can see that the same conditions as in Theorem (2.2.3) will lead to preservation of symmetry in the energy functional as well as space of states in this context. Indeed, when a change of coordinates T is performed on $\mathbb{R}^{3(1+N)}$, the unitary operator $U_T : L^2 \to L^2$, $U_T(\psi)(\boldsymbol{q}) = |\det T|^{1/2}\psi(T\boldsymbol{q})$ represents the transformation of wavefunctions ψ into the new coordinates. Then a state $|\psi\rangle\langle\psi|$ must become $|U_{T^{-1}}\psi\rangle\langle U_{T^{-1}}\psi|$, and a change of variable in the integral defining the L^2 inner product reveals that this is the same as $|\det T| U_{T^{-1}} |\psi\rangle\langle\psi| U_T$. So we have found the expression of a general state $\rho \in \mathcal{S}$ in the new coordinates $T\boldsymbol{q}$: it is $|\det T| U_{T^{-1}} \rho U_T$. This immediately implies that preservation of (anti-)symmetry of states is satisfied precisely by the same condition (2.2.39) as before. Similarly one can consider pure states $|\psi\rangle\langle\psi|$ in order to understand the transformation of the energy functional and find out that (2.2.26) is the condition that preserves its symmetry.

To finish writing the transformed Hamiltonian, we need to figure out what the potential part becomes, which requires expressing the q_j's in terms of the ξ_k's. The inverse transformation can be computed from (2.2.28): $T^{-1} = R^{-1}T^tS$, yielding

$$T^{-1} = \begin{pmatrix} 1 & \frac{mr^{\frac{1}{N}}}{m_0}C & \frac{mr^{\frac{1}{N}}}{m_0}C & \frac{mr^{\frac{1}{N}}}{m_0}C & \dots & \frac{mr^{\frac{1}{N}}}{m_0}C \\ 1 & r^{1/N}A & r^{1/N}B & r^{1/N}B & \dots & r^{1/N}B \\ 1 & r^{1/N}B & r^{1/N}A & r^{1/N}B & \dots & r^{1/N}B \\ 1 & r^{1/N}B & r^{1/N}B & r^{1/N}A & \dots & r^{1/N}B \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & r^{1/N}B & r^{1/N}B & r^{1/N}B & \dots & r^{1/N}A \end{pmatrix}_{(1+N)\times(1+N)} \otimes I_{3\times 3} \; . \tag{2.2.59}$$

Now plug-in the values of A, B, C given in (2.2.51) to get:

$$\begin{cases} q_0 = \xi_0 \overset{(2)}{\pm} r^{\frac{1}{2}+\frac{1}{2N}}(r^{-1}-1)\overline{\boldsymbol{\xi}} \; , \\ q_j = \xi_0 \overset{(1)}{\pm} r^{\frac{1}{2N}}\xi_j - \left(\overset{(2)}{\pm} r^{\frac{1}{2}+\frac{1}{2N}} \overset{(1)}{\pm} r^{\frac{1}{2N}}\right)\overline{\boldsymbol{\xi}} \quad , \quad j = 1, \dots, N \; , \end{cases} \tag{2.2.60}$$

where $\overline{\boldsymbol{\xi}}$ is defined analogously to how $\overline{\boldsymbol{q}}$ was defined in (2.2.52). In particular, the relevant pairwise distances for our Hamiltonian and for most physically meaningful others become:

$$\begin{cases} |q_j - q_0| = r^{\frac{1}{2N}}\left|\overset{(1)}{\pm}\xi_j - (\overset{(1)}{\pm} 1 \overset{(2)}{\pm} r^{-\frac{1}{2}})\overline{\boldsymbol{\xi}}\right| \quad , \quad j = 1, \dots, N \; , \\ |q_i - q_j| = r^{\frac{1}{2N}}|\xi_i - \xi_j| \quad , \quad i, j = 1, \dots, N \; . \end{cases} \tag{2.2.61}$$

With this, we finally conclude that the potential energy part will transform just like we wished, remaining symmetric with respect to exchanges in the variables other than the zeroth. We conclude that the Hamiltonian that represents the energy intrinsic to the system is given by

$$\tilde{H} = -\frac{\hbar^2}{2mr^{\frac{1}{N}}}\sum_{j=1}^{N}\Delta_j - \frac{zZ}{r^{\frac{1}{2N}}}\sum_{j=1}^{N}\frac{1}{\left|\overset{(1)}{\pm}\xi_j - (\overset{(1)}{\pm} 1 \overset{(2)}{\pm} r^{-\frac{1}{2}})\overline{\boldsymbol{\xi}}\right|} + \frac{z^2}{r^{\frac{1}{2N}}}\sum_{\substack{i=1 \\ i<j}}^{N}\sum_{j=1}^{N}\frac{1}{|\xi_i - \xi_j|} \; . \tag{2.2.62}$$

Remark 2.2.6. Thinking ahead about what this Hamiltonian has to say, first note that the factors of $r^{1/N}$ and $r^{1/2N}$ in front of each term disappear after a suitable rescaling of the argument of the wavefunction, which aids in understanding how the size of the system in its ground-state scales with N. It is also interesting to note that, even after this rescaling, there remains still a dependence on N in the term $\overline{\boldsymbol{\xi}}$, which includes a factor $1/N$. Since the arguments used in Hartree and Hartree-Fock theory to study asymptotic properties of the ground-state and equilibrium energy rely heavily on the fact that the Hamiltonian can be written as a sum of individual terms featuring only 1 or 2 variables ξ_j in them (see [Rou15]), our new transformed problem is not trivial to study. But this is material for future work.

2.2.4 Symmetric center-of-mass coordinates (classical case)

Now we explore a different model given by a classical Hamiltonian to see that the same conditions as in theorem (2.2.3) are still the natural ones to require and the conclusions are still mostly the same, in spite of the different nature of the set of states and the form of the kinetic energy part. This time, in order to even be able to talk about symmetry on the set of admissible states, it is necessary to consider them to be statistical distributions of possible phase space configurations (as opposed to the quantum case, where just a single state ψ already comes with a probabilistic interpretation via the Born rule). The proof follows the same ideas as in the quantum case, but applied to different objects that satisfy different properties, and it turns out that the restrictions imposed by this classical context are not enough to warrant uniqueness. Lest the reader be misled into thinking that the Coulomb potential is necessary in the reasoning, we will give the bodies the possibility to interact pairwise through general potential functions - and everything readily generalizes to threefold, fourfold etc. interactions.

Consider a classical-mechanical system evolving in space $\mathbb{R}^3$ consisting of a distinguished body of mass m_0 and N identical bodies of mass m such that the potential energy of interaction between the first and any of the others is given by a function V, and the one between the identical bodies by a function W, both depending symmetrically on the two interacting bodies. The phase space is

$$\mathcal{D} = \mathbb{R}^{3(1+N)} \times \mathbb{R}^{3(1+N)} = \{(\mathbf{x};\mathbf{p}) = (x_0, x_1, \ldots, x_N; p_0, p_1, \ldots, p_N)\ ;\ x_j, p_j \in \mathbb{R}^3\} \tag{2.2.63}$$

where each x_j and p_j are the position and momentum of particle j (particle 0 being the distinguished one). The Hamiltonian is the function defined on $\mathcal{D}$ given by

$$H(\mathbf{x};\mathbf{p}) = \frac{1}{2m_0}|p_0|^2 + \frac{1}{2m}\sum_{j=1}^{N}|p_j|^2 + \sum_{j=1}^{N} V(x_j, x_0) + \sum_{\substack{i=1 \\ i<j}}^{N}\sum_{j=1}^{N} W(\xi_i, \xi_j) \ . \tag{2.2.64}$$

The set of states of the system is defined as

$$\mathcal{S} = \text{Set of } \{1,\ldots,N\}\text{-permutation-symmetric Borelian probability measures on } \mathcal{D} \tag{2.2.65}$$

where the qualification about permutation symmetry means, as one expects for identical bodies, that any $\nu \in \mathcal{S}$ must satisfy

$$\nu(E) = \nu(U_\sigma(E)) \quad , \quad \sigma \in S^N, E \subseteq \mathcal{D} \text{ Borel-measurable,} \tag{2.2.66}$$

where the isomorphism $U_\sigma : \mathcal{D} \to \mathcal{D}$, for $\sigma \in S^N$, is given by

$$U_\sigma(x_0, x_1, \ldots, x_N; p_0, p_1, \ldots, p_N) = (x_0, x_{\sigma(1)}, \ldots, x_{\sigma(N)}; p_0, p_{\sigma(1)}, \ldots, p_{\sigma(N)}) \ . \tag{2.2.67}$$

(More commonly, H is only defined on the subset of $\mathcal{D}$ of the points $(\mathbf{x};\mathbf{p})$ for which no x_i is equal to an x_j, $i \neq j$, and the admissible states are measures supported away from such points.)

If $T : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)}$ is a bijection onto its image (a coordinate change of the position variables), the question arises of how to extend it to the whole $\mathcal{D}$, that is, how to define the physically meaningful transformation $T' : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)}$ of the momentum coordinates. Note how this consideration only arises in the present context of classical mechanics, because a fundamental difference between it and quantum theory is that in the latter the stipulation of the space of states does not involve momentum variables.

Assuming for a moment that we have found the correct expression for T', we can identify the transformed phase space $\tilde{D}$, set of admissible states $\tilde{\mathcal{S}}$ and Hamiltonian $\tilde{H}$:

$$\tilde{\mathcal{D}} = (T \oplus T')(\mathcal{D}) = \{(T\boldsymbol{x}; T'\boldsymbol{p}) \ ; \ (\boldsymbol{x};\boldsymbol{p}) \in \mathcal{D}\} \ , \tag{2.2.68}$$

$$\tilde{S} = \{(T \oplus T')_* \nu \ ; \ \nu \in \mathcal{S}\} \ , \tag{2.2.69}$$

$$\tilde{H}(\boldsymbol{\xi};\boldsymbol{\pi}) = H(T^{-1}\boldsymbol{\xi}; T'^{-1}\boldsymbol{\pi}) \ , \tag{2.2.70}$$

where the push-forward probability measure $(T \oplus T')_*\nu$ defined by

$$\left((T \oplus T')_*\nu\right)(F) = \nu\left((T \oplus T')^{-1}(F)\right) \quad , \quad F \subseteq \tilde{\mathcal{D}} \text{ Borelian} \tag{2.2.71}$$

is the state in $\tilde{\mathcal{S}}$ corresponding to a state $\nu \in \mathcal{S}$ (no normalization constant is required). The expression for the Hamiltonian must be given as in (2.2.70) due to the property of push-forward measures that says

$$\int_{\mathcal{D}} H \mathrm{d}\nu = \int_{\tilde{\mathcal{D}}} (H \circ (T \oplus T')^{-1}) \mathrm{d}(T \oplus T')_* \nu \ , \tag{2.2.72}$$

that is, the expected value of the energy of the system at the transformed state computed with the transformed Hamiltonian is the same as what it was before the transformation, which is a natural property to desire.

Let us see what kind of conditions are needed for this T to be a symmetric center-of-mass coordinate change for the classical many-body problem at hand. What we called conditions 1 and 2 in theorem (2.2.3) can be stated verbatim here, and in particular they imply that our sought-after T' also satisfies

$$T' = \tilde{T}' \otimes I_{3\times 3} \tag{2.2.73}$$

for some isomorphism $\tilde{T}' : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)}$. Condition 4 now asks that, for all $\nu \in \mathcal{S}$, the transformed state (2.2.71) satisfy $\{1, \ldots, N\}$-symmetry, and there are enough Borelian subsets in Euclidean space to guarantee that this is only possible if the same condition (2.2.39) as before is valid. Hence our T is of the form (2.2.44) (but a similar remark to (2.2.2) applies in case the bodies are not identical and we just wish to avoid cross-terms in the Hamiltonian). Finally condition 3 stipulates that there must exist $\mu > 0$ such that

$$\frac{1}{2m_0}|p_0|^2 + \frac{1}{2m}\sum_{j=1}^{N}|p_j|^2 = \frac{1}{2M_{\mathrm{Tot}}}|\pi_0|^2 + \frac{1}{2\mu}\sum_{j=1}^{N}|\pi_j|^2 \tag{2.2.74}$$

whenever $\boldsymbol{\pi} = T'\boldsymbol{p}$. By computing $|p_0|^2, |p_j|^2$ in terms of $\pi_i \cdot \pi_j$, we see that the components T'^{-1}_{ij} of $\tilde{T}'^{-1}$, rather than the ones of T' or $\tilde{T}'$ like before, are the ones coming into the computation. The required condition will then be

$$\frac{1}{m_0} T'^{-1}_{0k} T'^{-1}_{0l} + \frac{1}{m}\sum_{j=1}^{N} T'^{-1}_{jk} T'^{-1}_{jl} = \begin{cases} 1/M_{\mathrm{Tot}} & , \quad k = l = 0 \ , \\ 1/\mu & , \quad k = l > 0 \ , \\ 0 & , \quad k \neq l \ . \end{cases} \tag{2.2.75}$$

Compare this to (2.2.26). The clear difference is that there is no $|\det T'|^{1/2}$ this time, and the subtle difference is the order of the indices $0k$, $0l$, jk, jl. Using the matrices R and S from (2.2.29), equation (2.2.75) is written as

$$\left(\tilde{T'}^{-1}\right)^t R^{-1}\tilde{T'}^{-1} = S^{-1} \ . \tag{2.2.76}$$

Now we can find T' using the expression (2.2.70) of the transformation of H and the desired new form (2.2.74). The Hamilton equations dictate the law of motion of the system in $(\boldsymbol{x};\boldsymbol{p})$ coordinates and should still hold for the transformed Hamiltonian in $(\boldsymbol{\xi} = T\boldsymbol{x}; \boldsymbol{\pi} = T'\boldsymbol{p})$ coordinates, the possible curves $(\boldsymbol{x}(t);\boldsymbol{p}(t))$ that describe the evolution of a point in phase space satisfy

$$\dot{\boldsymbol{x}} = \frac{\partial H}{\partial \boldsymbol{p}} \qquad , \qquad \dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{x}} \ , \tag{2.2.77}$$

and we would like to also have

$$\dot{\boldsymbol{\xi}} = \frac{\partial \tilde{H}}{\partial \boldsymbol{\pi}} \qquad , \qquad \dot{\boldsymbol{\pi}} = -\frac{\partial \tilde{H}}{\partial \boldsymbol{\xi}} \ . \tag{2.2.78}$$

The zeroth of each of these two systems of equations give

$$p_0 = m_0\dot{x_0} \ , \ p_j = m\dot{x_j} \ , \ \pi_0 = M_{\text{Tot}}\dot{\xi_0} \ , \ \pi_j = \mu\dot{\xi_j} \ , \ j = 1,\ldots,N \ . \tag{2.2.79}$$

Given $\dot{\boldsymbol{\xi}} = T\dot{\boldsymbol{x}}$, we conclude

$$\begin{aligned} \pi_0 &= M_{\text{Tot}}\left(\frac{1}{m_0}T_{00}p_0 + \frac{1}{m}\sum_{k=1}^{N} T_{0k}p_k\right) \ , \\ \pi_j &= \qquad \mu\left(\frac{1}{m_0}T_{j0}p_0 + \frac{1}{m}\sum_{k=1}^{N} T_{jk}p_k\right) \quad , \quad j = 1,\ldots,N \ , \end{aligned} \tag{2.2.80}$$

or

$$\tilde{T'} = S\tilde{T}R^{-1} \ . \tag{2.2.81}$$

Together with (2.2.76), this implies

$$\tilde{T'}^{-1} = R(S\tilde{T}R^{-1})^t S^{-1} = \tilde{T}^t \ . \tag{2.2.82}$$

Plug this into (2.2.75) to finally see that it actually says precisely the same as (2.2.26), except for the $(\det T)^{1/2}$ factor. Hence we may now conclude through the same computations that the transformation (2.2.54) satisfies all constraints. However there is nothing that imposes a value for μ this time. We summarize:

Theorem 2.2.7. *For given $m_0, m, \mu > 0$ and up to two independent choices of $\pm$ signs and relabeling of nonzero indices, the only family of transformations $T : \mathbb{R}^{3(1+N)} \to \mathbb{R}^{3(1+N)}$ (indexed by N) satisfying the following:*

1. *$T = \tilde{T} \otimes I_{3\times 3}$ for some linear isomorphism $\tilde{T} : \mathbb{R}^{1+N} \to \mathbb{R}^{1+N}$;*

2. *the zeroth component of $T(q_0, q_1, \ldots, q_N)$ in $\mathbb{R}^3$ is given by*

$$\frac{1}{m_0 + Nm}(m_0 q_0 + mq_1 + \cdots + mq_N) \tag{2.2.83}$$

   for all $q_0, q_1, \ldots, q_N \in \mathbb{R}^3$;

3. *if $\boldsymbol{\pi} = T'(\boldsymbol{p})$, then (2.2.74) is true;*

4. *if a probability measure ν on $\mathbb{R}^{3(1+N)} \times \mathbb{R}^{3(1+N)}$ is symmetric with respect to exchange of any of its $\mathbb{R}^3$ variables 1 through N in both the first half of its argument (position variables) and the second (momentum variables), then so is the push-forward $(T \oplus T')_* \nu$, where $T' = \tilde{T}' \otimes I_{3\times 3}$ is defined by (2.2.81);*

is the one given by (2.2.44) with A, B, C given as in equations (2.2.48) and (2.2.50).

2.2.5 Many-species problems

Conditions 1 through 4 have analogues that are applicable to problems involving many different groups of identical bodies, which we call *many-species* problems. Here we show that, despite losing uniqueness to the many degrees of freedom afforded by such problems, we can still produce a natural system of center-of-mass coordinates that preserves the symmetries of the Hamiltonian and the permutation symmetry of admissible states with respect to exchange of any two identical bodies. We choose to use quantum-mechanical language again, but it should be clear that the applicability of the result extends to classical physics just like in the above section.

Since the change of coordinates and subsequent dismissal of the center-of-mass coordinate effectively reduce the number of bodies by one, there should be a body that in a sense gets thrown out of consideration. This doesn't mean that it needs to be the most massive one, the "nucleus" or even a different body from all the others, but we will give it a special notation with the index 0. So consider a system containing a distinguished particle of mass m_0 at position $q_0 \in \mathbb{R}^3$, and n groups of identical particles containing $N_1, \ldots, N_n$ particles. We must assume that each N_i is at least 2. Denote by $1 + N$ the total number of particles:

$$1 + N = 1 + N_1 + \cdots + N_n \ . \tag{2.2.84}$$

Suppose that the particles belonging to group i all have mass m_i and are located at $q_1^{(i)}, \dots, q_{N_i}^{(i)}$. Let the energy of interaction between the zeroth particle and a particle of group i be given by a function V_i depending symmetrically on their positions; let the energy of interaction between a particle of group i and another of group j (possibly $i = j$) be given by a function $W_{i,j}$ depending symmetrically on their positions. The Hamiltonian

$$H = -\frac{\hbar^2}{2m_0}\Delta_{q_0} - \frac{\hbar^2}{2}\sum_{i=1}^{n}\frac{1}{m_i}\sum_{k=1}^{N_i}\Delta_{q_k^{(i)}} + \sum_{i=1}^{n}\sum_{k=1}^{N_i} V_i(q_0, q_k^{(i)}) + \\ + \sum_{\substack{i=1 \\ i\le j}}^{n}\sum_{j=1}^{n}\sum_{\substack{k=1 \\ k<l}}^{N_i}\sum_{l=1}^{N_j} W_{i,j}(q_k^{(i)}, q_l^{(j)}) \quad (2.2.85)$$

(in self-explanatory notation for the Laplacians) is defined on a suitable subset of the space of admissible wavefunctions, which are those twice-differentiable L^2 functions of $\mathbb{R}^{3(1+N)}$ that are (anti-)symmetric with respect to exchange of any two variables $q_k^{(i)}$ and $q_l^{(i)}$ of the same group.

The change-of-coordinates maps that we seek are in the form $T = \tilde{T}\otimes I_{3\times 3}$, for $\tilde{T} : \mathbb{R}^{1+N} \to \mathbb{R}^{1+N}$ a linear map whose matrix has zeroth row given by

$$(T_{0j}) = \left(\frac{m_0}{M_{\text{Tot}}}, \left[\frac{m_1}{M_{\text{Tot}}}\right]_{N_1}, \dots, \left[\frac{m_n}{M_{\text{Tot}}}\right]_{N_n}\right) \quad (2.2.86)$$

where $M_{\text{Tot}} = m_0 + \sum_i N_i m_i$. Here the notation $[x]_k$ represents a vector $(x, \dots, x)$ with k components. But it's best to label the rows and columns of $\tilde{T}$ with the symbols

$$0, 1^{(1)}, \dots, N_1^{(1)}, 1^{(2)}, \dots, N_2^{(2)}, \dots, 1^{(n)}, \dots, N_n^{(n)} \quad (2.2.87)$$

in this order. For example, the entry in the row corresponding to the third particle of group 5 and the column corresponding to the second-to-last particle of group 1 would then be $T_{3^{(5)},(N_1-1)^{(1)}}$.

Due to permutation symmetry of states, a property analogous to (2.2.39) must hold, which can be stated as follows: for fixed $i = 1, \dots, n$, to each permutation σ of $\{1, \dots, N_i\}$ there must correspond a permutation π comprised of permutations within each group $1, \dots, N$ (not necessarily only group i), such that $\tilde{T}$ remains unchanged under swapping of its rows according to σ followed by swapping of its columns according to π. We shall not attempt to classify all possible ways to construct a π for each σ if π is allowed to permute variables of many groups; instead let us consider that π must only act on group i. In the same way, to each permutation π of columns within a group corresponds a permutation σ of rows of that group such that performing π followed by σ on $\tilde{T}$ leaves it unchanged. Then this implies:

- that the zeroth column must be of the form

$$(T_{k0})_k = \left(\frac{m_0}{M_{\text{Tot}}}, [C_1]_{N_1}, \ldots, [C_n]_{N_n} \right)^t \tag{2.2.88}$$

  for some numbers $C_1, \ldots, C_n$ (consider what happens when swapping any two rows of group i);

- that each of the n square blocks on the main diagonal must be of the form

$$(T_{kl})_{k,l=1^{(i)},\ldots,N_i^{(i)}} = \begin{bmatrix} A_i & B_i & B_i & \cdots & B_i \\ B_i & A_i & B_i & \cdots & B_i \\ B_i & B_i & A_i & \cdots & B_i \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_i & B_i & B_i & \cdots & A_i \end{bmatrix} \tag{2.2.89}$$

  for some numbers A_i, B_i (that is, after a permutation of indices $1^{(i)}, \ldots, N_i^{(i)}$; this is just like the proof in Section 3);

- that, given any $i \neq j$, the rectangular off-diagonal block whose rows are in group i and columns are in group j must have all elements equal to the same number X_{ij} (consider first what happens when swapping rows of group i, then also what happens when swapping columns of group j).

Finally, to prevent cross-terms in the kinetic energy and preserve its symmetries, we require the same condition as in (2.2.28):

$$\tilde{T} R^{-1} \tilde{T}^t = S^{-1} \tag{2.2.90}$$

where now

$$R = \operatorname{diag}\left(m_0, [m_1]_{N_1}, \ldots, [m_n]_{N_m}\right) \quad , \quad S = \operatorname{diag}\left(M_{\text{Tot}}, [\mu_1]_{N_1}, \ldots, [\mu_n]_{N_m}\right) \tag{2.2.91}$$

for some reduced masses $\mu_1, \ldots, \mu_n > 0$. The condition $|\det \tilde{T}| = 1$, present in the quantum context but not the classical one, implies that we must impose

$$m_0 m_1 \cdots m_n = M_{\text{Tot}} \mu_1 \cdots \mu_n \ . \tag{2.2.92}$$

Now it becomes more convenient to normalize the elements of $\tilde{T}$ by considering the matrix

$$U = S^{1/2}\tilde{T}R^{-1/2} \ , \tag{2.2.93}$$

which, according to (2.2.90), must be orthogonal. It is obtained from $\tilde{T}$ by multiplying row 0 by $\sqrt{M_{\mathrm{Tot}}}$ and rows $k^{(i)}$ by $\sqrt{\mu_i}$ and dividing column 0 by $\sqrt{m_0}$ and columns $k^{(i)}$ by $\sqrt{m_i}$. Its zeroth row is then determined:

$$(U_{0j}) = \left(\sqrt{\frac{m_0}{M_{\mathrm{Tot}}}}, \left[\sqrt{\frac{m_1}{M_{\mathrm{Tot}}}}\,\right]_{N_1}, \ldots, \left[\sqrt{\frac{m_n}{M_{\mathrm{Tot}}}}\,\right]_{N_n}\right) \ , \tag{2.2.94}$$

and is already normalized to 1 in Euclidean norm. Let us abbreviate it by using the symbols

$$(U_{0j}) = (\nu_0, [\nu_1]_{N_1}, \ldots, [\nu_n]_{N_n}) \ , \tag{2.2.95}$$

(all of them are determined by the data of the problem) and denote the other elements of U with lowercase letters a_i, b_i, c_i, x_{ij} in the locations corresponding to A_i, B_i, C_i, X_{ij} in $\tilde{T}$. We have thus reduced the question to the following: given real constants $\nu_0, \nu_1, \ldots, \nu_n$ satisfying

$$\nu_0^2 + N_1\nu_1^2 + \cdots + N_n\nu_n^2 = 1 \ , \tag{2.2.96}$$

can one find an orthogonal matrix U in the following format?

$$U = \left[\begin{array}{c|c|c|c|c|c}
\nu_0 & \nu_1\ \nu_1\ \cdots\ \nu_1 & \nu_2\ \nu_2\ \cdots\ \nu_2 & \nu_3\ \nu_3\ \cdots\ \nu_3 & \cdots & \nu_n\ \nu_n\ \cdots\ \nu_n \\ \hline
\begin{matrix} c_1 \\ \vdots \\ c_1 \end{matrix} & \mathcal{U}_{11} & \mathcal{U}_{12} & \mathcal{U}_{13} & \cdots & \mathcal{U}_{1n} \\ \hline
\begin{matrix} c_2 \\ \vdots \\ c_2 \end{matrix} & \mathcal{U}_{21} & \mathcal{U}_{22} & \mathcal{U}_{23} & \cdots & \mathcal{U}_{2n} \\ \hline
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \hline
\begin{matrix} c_n \\ \vdots \\ c_n \end{matrix} & \mathcal{U}_{n1} & \mathcal{U}_{n2} & \mathcal{U}_{n3} & \cdots & \mathcal{U}_{nn}
\end{array}\right] \ , \tag{2.2.97}$$

where the blocks $(\mathcal{U}_{ij})_{N_i \times N_j}$ are of the following form:

$$\mathcal{U}_{ii} = \begin{bmatrix} a_i & b_i & b_i & \cdots & b_i \\ b_i & a_i & b_i & \cdots & b_i \\ b_i & b_i & a_i & \cdots & b_i \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_i & b_i & b_i & \cdots & a_i \end{bmatrix} \quad , \quad \mathcal{U}_{ij} = \begin{bmatrix} x_{ij} & x_{ij} & x_{ij} & \cdots & x_{ij} \\ x_{ij} & x_{ij} & x_{ij} & \cdots & x_{ij} \\ x_{ij} & x_{ij} & x_{ij} & \cdots & x_{ij} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{ij} & x_{ij} & x_{ij} & \cdots & x_{ij} \end{bmatrix} \; (i \neq j) \; . \tag{2.2.98}$$

Now there are n equations imposing norm 1 for each row and n equations imposing orthogonality of each row with the zeroth (within each group these are all the same), plus n equations imposing orthogonality of different rows within the same group, plus $n(n-1)/2$ equations imposing orthogonality of rows in different groups, for a total of $n(n+5)/2$ equations. Meanwhile, there are n variables in the zeroth column of U, 2 in each of its n diagonal blocks, 1 for each one of the $n(n-1)/2$ rectangular blocks above the diagonal, and the same for the blocks below, for a total of $n^2 + 2n$ variables. The number of degrees of freedom is then computed to be $n(n-1)/2$, exactly the same as the number of blocks above or below the diagonal. Hence there won't be a unique solution, but the numbers suggest we might still be able to solve all these equations by also imposing $n(n-1)/2$ conditions; let us impose $x_{ij} = x_{ji}$ for all $i \neq j$. Then the big square block of U consisting of all rows and columns except the zeroth is symmetric. Now consider the equations that impose norm one for the nonzeroth rows and columns:

$$\begin{aligned} c_i^2 + a_i^2 + (N_i - 1)b_i^2 + \sum_{j \neq i} x_{ij}^2 = 1 \quad &, \quad i = 1, \ldots, n \; , \\ \nu_i^2 + a_i^2 + (N_i - 1)b_i^2 + \sum_{j \neq i} x_{ji}^2 = 1 \quad &, \quad i = 1, \ldots, n \; . \end{aligned} \tag{2.2.99}$$

With our choice $x_{ij} = x_{ji}$, we see that $c_i = \pm \nu_i$. We choose

$$c_i = \nu_i \quad , \quad i = 1, \ldots, n \tag{2.2.100}$$

to make U a symmetric matrix. Then it is diagonalizable and admits a basis of orthogonal eigenvectors: there exists an orthogonal matrix $\mathcal{O}$ and a diagonal matrix D such that

$$U = \mathcal{O} D \mathcal{O}^t \; . \tag{2.2.101}$$

Therefore U is going to be orthogonal if and only if

$$I = UU^t = U^2 = \mathcal{O} D^2 \mathcal{O}^t \iff D^2 = I \; , \tag{2.2.102}$$

if and only if its eigenvalues are all ± 1. Of course at least one eigenvalue 1 and one -1 need to be present, otherwise U would be diagonal according to (2.2.101).

Just like what happened in the one-species problem, each a_i depends in a simple way on b_i: subtracting from the first equation in (2.2.99) the equation that says that any two different rows in group i are orthogonal, we have

$$c_i^2 + 2a_ib_i + (N_i-2)b_i^2 + \sum_{j\neq i} x_{ji}^2 = 0\ , \tag{2.2.103}$$

so that

$$a_i^2 - 2a_ib_i + b_i^2 = 1 \iff a_i = b_i \pm 1\ . \tag{2.2.104}$$

We will choose

$$a_i = b_j - 1 \quad \text{for all } i\ . \tag{2.2.105}$$

With this, it is possible to choose values for each b_i and x_{ij} that force U to have eigenvalue -1 with very high multiplicity: choose

$$b_i = \rho\nu_i^2 \quad , \quad x_{ij} = \rho\nu_i\nu_j \tag{2.2.106}$$

for some $\rho > 0$ to be determined shortly. Then $U+I$ has column $k^{(i)}$ equal to

$$(U_{l^{(j)},k^{(i)}})_{l^{(j)}=0,\ldots,N} = (\nu_i, [\rho\nu_1\nu_i]_{N_1}, \ldots, [\rho\nu_n\nu_i]_{N_n})^t\,. \tag{2.2.107}$$

This is a multiple of the vector $(1, [\rho\nu_1]_{N_1}, \ldots, [\rho\nu_n]_{N_n})^t$, which is independent of i or k. So all nonzeroth columns of $U+I$ are multiples of each other, giving this matrix a rank of at most 2, and giving -1 a multiplicity of at most $N-1$. With the further choice

$$\rho = \frac{1}{1+\nu_0}\ , \tag{2.2.108}$$

the zeroth column is also a multiple of that same vector, and -1 will have multiplicity N (we remark that algebraic and geometric multiplicity are the same in this case since U is diagonalizable).

Hence U has just one other eigenvalue, λ, which we must check is equal to 1. For that purpose, note that a basis for the -1 eigenspace is given by vectors $\{w_k^{(i)}\ ;\ i=1,\ldots,n\ ,\ k=1,\ldots,N_i\}$, each having only two nonzero components: the zeroth entry equal to 1 and the $k^{(i)\text{th}}$ entry equal to $-1/\rho\nu_i$. Indeed, these are clearly N independent vectors and

$$(U+I)w_k^{(i)} = \left((1+\nu_0) - \frac{\nu_i}{\rho\nu_i}, \left[\nu_1 - \frac{\rho\nu_1\nu_i}{\rho\nu_i}\right]_{N^1}, \ldots, \left[\nu_n - \frac{\rho\nu_n\nu_i}{\rho\nu_i}\right]_{N^n}\right)^t = 0\ . \tag{2.2.109}$$

A vector orthogonal to all the $w_k^{(i)}$ is easily constructed:

$$w_0 = (1, [\rho\nu_1]_{N_1}, \ldots, [\rho\nu_n]_{N_n})^t \ . \tag{2.2.110}$$

Because U is symmetric, eigenvectors corresponding to different eigenvalues are orthogonal, so the eigenspace corresponding to λ must be spanned by w_0. Now simply note that the zeroth coordinate of Uw_0 is

$$\nu_0 + \sum_{i=1}^{n}\sum_{k=1}^{N_i} \nu_i \rho \nu_i = \nu_0 + \rho \sum_{i=1}^{n} N_i \nu_i^2 \ , \tag{2.2.111}$$

which due to (2.2.96) becomes just

$$\nu_0 + \rho(1-\nu_0^2) = \nu_0 + \frac{1-\nu_0^2}{1+\nu_0} = \nu_0 + (1-\nu_0) = 1 \ , \tag{2.2.112}$$

the same as the zeroth coordinate of w_0 itself. Hence $\lambda = 1$, and U is orthogonal as needed.

Going back through (2.2.108), (2.2.106), (2.2.105), (2.2.100), (2.2.98), (2.2.97), (2.2.95), (2.2.94) and (2.2.93), we can finally write our change of coordinates. Letting $\boldsymbol{\xi} = T\boldsymbol{q}$, we already know that ξ_0 is the center-of-mass of the system, and for the rest we can compute:

$$\begin{aligned}
\xi_k^{(i)} &= \sqrt{\frac{m_0}{\mu_i}}\nu_i q_0 - \sqrt{\frac{m_i}{\mu_i}} q_k^{(i)} + \frac{1}{1+\nu_0}\sum_{j=1}^{n}\nu_i\nu_j \sum_{l=1}^{N_j}\sqrt{\frac{m_j}{\mu_i}} q_l^{(j)} \\
&= \frac{1}{\sqrt{\mu_i}}\left(\sqrt{\frac{m_0 m_i}{M_{\text{Tot}}}} q_0 - \sqrt{m_i} q_k^{(i)} + \frac{1}{1+\sqrt{\frac{m_0}{M_{\text{Tot}}}}}\sum_{j=1}^{n}\frac{m_j\sqrt{m_i}}{M_{\text{Tot}}}\sum_{l=1}^{N_j} q_l^{(j)}\right) \\
&= \sqrt{\frac{m_i}{\mu_i}}\left(\sqrt{\frac{m_0}{M_{\text{Tot}}}} q_0 - q_k^{(i)} + \frac{1}{M_{\text{Tot}} + \sqrt{M_{\text{Tot}} m_0}}\sum_{j=1}^{n} m_j \sum_{l=1}^{N_j} q_l^{(j)}\right) \\
&= \sqrt{\frac{m_i}{\mu_i}}\left(\sqrt{\frac{m_0}{M_{\text{Tot}}}} q_0 - q_k^{(i)} + \left(1 - \sqrt{\frac{m_0}{M_{\text{Tot}}}}\right)\frac{1}{M_{\text{Tot}} - m_0}\sum_{j=1}^{n} m_j \sum_{l=1}^{N_j} q_l^{(j)}\right)
\end{aligned} \tag{2.2.113}$$

where we deliberately arranged for the center-of-mass of all but the zeroth particle to appear. Wrapping it all up in a theorem:

Theorem 2.2.8. *Given positive integers $n \geq 1$, $N_1, \ldots, N_n \geq 2$ and positive real numbers $m_0, \ldots, m_n$, $\mu_1, \ldots, \mu_n$, let $M_{\text{Tot}} = m_0 + N_1 m_1 + \ldots + N_n m_m$. Then a possible linear transformation*

$$\begin{aligned}
T = \tilde{T} \otimes I_{3\times 3} : \mathbb{R}^{3(1+N_1+\ldots+N_n)} &\to \mathbb{R}^{3(1+N_1+\ldots+N_n)} \\
(q_0, (q_k^{(1)})_{k=1,\ldots,N_1}, \ldots, (q_k^{(n)})_{k=1,\ldots,N_n})^t &\mapsto (\xi_0, (\xi_k^{(1)})_{k=1,\ldots,N_1}, \ldots, (\xi_k^{(n)})_{k=1,\ldots,N_n})^t
\end{aligned} \tag{2.2.114}$$

that preserves the permutation symmetries and structure of the many-species Hamiltonian (2.2.85), as well as the symmetry of the admissible states of the $(1+N_1+\cdots+N_n)$*-body problem associated with it, is the following:*

$$\begin{cases} \xi_0 &= \dfrac{1}{M_{\mathrm{Tot}}}\left(m_0 q_0 + \displaystyle\sum_{i=1}^{n} m_i \sum_{k=1}^{N_i} q_k^{(i)}\right) \\ \xi_k^{(i)} &= \sqrt{\frac{m_i}{\mu_i}}\left(\sqrt{\frac{m_0}{M_{\mathrm{Tot}}}}(q_0-\overline{\boldsymbol{q}})+\overline{\boldsymbol{q}}-q_k^{(i)}\right) \end{cases} \tag{2.2.115}$$

where we used this abbreviation:

$$\overline{\boldsymbol{q}} = \frac{1}{M_{\mathrm{Tot}}-m_0}\sum_{j=1}^{n} m_j \sum_{l=1}^{N_j} q_l^{(j)}. \tag{2.2.116}$$

The inverse transformation is obtained from (2.2.93):

$$\tilde{T}^{-1} = (S^{-1/2}UR^{1/2})^{-1} = R^{-1/2}US^{1/2}\ . \tag{2.2.117}$$

We compute:

$$q_0 = \sqrt{\frac{M_{\mathrm{Tot}}}{m_0}}\nu_0\xi_0 + \sum_{j=1}^{n}\sum_{l=1}^{N_j}\sqrt{\frac{\mu_j}{m_0}}\nu_j\xi_l^{(j)} = \xi_0 + \sum_{j=1}^{n}\sqrt{\frac{\mu_j m_j}{M_{\mathrm{Tot}}m_0}}\sum_{l=1}^{N_j}\xi_l^{(j)} \tag{2.2.118}$$

and

$$\begin{aligned} q_k^{(i)} &= \sqrt{\frac{M_{\mathrm{Tot}}}{m_i}}\nu_i\xi_0 - \sqrt{\frac{\mu_i}{m_i}}\xi_k^{(i)} + \frac{1}{1+\nu_0}\sum_{j=1}^{n}\nu_i\nu_j\sum_{l=1}^{N_j}\sqrt{\frac{\mu_j}{m_i}}\xi_l^{(j)} \\ &= \frac{1}{\sqrt{m_i}}\left(\sqrt{m_i}\xi_0 - \sqrt{\mu_i}\xi_k^{(i)} + \frac{1}{1+\sqrt{\frac{m_0}{M_{\mathrm{Tot}}}}}\sum_{j=1}^{n}\frac{\sqrt{m_i m_j \mu_j}}{M_{\mathrm{Tot}}}\sum_{k=1}^{N_j}\xi_l^{(j)}\right) \\ &= \xi_0 - \sqrt{\frac{\mu_i}{m_i}}\xi_k^{(i)} + \frac{1}{M_{\mathrm{Tot}}+\sqrt{M_{\mathrm{Tot}}m_0}}\sum_{j=1}^{n}\sqrt{m_j\mu_j}\sum_{k=1}^{N_j}\xi_l^{(j)}\ . \end{aligned} \tag{2.2.119}$$

Interestingly, unlike what happened in the one-species problem, the analogous quantity to $\overline{\boldsymbol{q}}$, which would be

$$\overline{\boldsymbol{\xi}} = \frac{1}{N_1\mu_1+\cdots+N_n\mu_n}\sum_{j=1}^{n}\mu_j\sum_{l=1}^{N_j}\xi_l^{(j)}\ , \tag{2.2.120}$$

does not appear in these formulas, unless we specifically choose $\mu_i = m_i$ for all i.

2.3 Bosonic atom under Born-Oppenheimer approximation

Let us now describe in detail the main theorem that Kiessling obtains in [Kie10] related to the study of ground-state properties of a bosonic atom under the BO approximation, which we wish to generalize.

2.3.1 Set-up

The work [Kie10] is the study of a quantum-mechanical model of an atom comprised of one nucleus pinned at the origin of space and N electrons assumed to be bosons. To describe it, we adapt the notation from that paper, but we keep the same symbols for the basic constructs:

- $e > 0$ is the elementary charge;
- the charge of each electron is ze, where $z < 0$ is a constant;
- the mass of each electron is m;
- the charge of the nucleus is $Z|z|e$, where $Z > 0$ is a constant (allowing for the possibility that this atom is an ion);
- the ratio $\lambda = Z/N$ is defined.

The goal is to study asymptotic properties of the ground-state configuration as $N \to \infty$, while λ is kept constant.

We denote by $\psi : \mathbb{R}^{3N} \to \mathbb{C}$ a generic wave-function of the system (so $\|\psi\|_{L^2} = 1$). Its argument, written as $(q_1, \ldots, q_N)$ with each $q_j \in \mathbb{R}^3$, is an enumeration of possible positions of each electron in space. Since the nucleus is assumed fixed at the origin, it does not contribute to ψ. And since the electrons are assumed to be bosons, ψ must be symmetric with respect to permutations of the q_j's.

The particles are assumed to interact only through the Coulomb force, so that the Hamiltonian of the system is the operator

$$H^{(N)} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\Delta_j - \lambda N(ze)^2\sum_{j=1}^{N}\frac{1}{|q_j|} + (ze)^2\sum_{\substack{i=1 \\ i<j}}^{N}\sum_{j=1}^{N}\frac{1}{|q_i - q_j|}, \tag{2.3.1}$$

where Δ_j is the Laplacian with respect only to the 3-vector q_j. The domain

$$\mathcal{D}_0(H^{(N)}) = \mathcal{C}_0^\infty(\mathbb{R}^{3N} \setminus \{(q_j)\ ;\ q_j = q_k \text{ for some } j \neq k\}) \tag{2.3.2}$$

is considered as a core, and the fully extended self-adjoint $H^{(N)}$ is taken to be the associated Friedrichs extension, defined via the quadratic form

$$Q^{(N)}(\psi) = \frac{\hbar^2}{2m}\sum_{j=1}^{N}\int|\nabla_j\psi|^2\mathrm{d}^{3N}q - \lambda N(ze)^2\sum_{j=1}^{N}\int\frac{|\psi|^2}{|q_j|}\mathrm{d}^{3N}q + (ze)^2\sum_{\substack{i=1\\i<j}}^{N}\sum_{j=1}^{N}\int\frac{|\psi|^2}{|q_i-q_j|}\mathrm{d}^{3N}q. \tag{2.3.3}$$

Here the integrals are over $\mathbb{R}^{3N}$, and $\nabla_j\psi$ is the gradient 3-vector of ψ with respect to q_j. The domain of $Q^{(N)}$ can be taken to be $\mathcal{D}(Q^{(N)}) = H^1(\mathbb{R}^3)\otimes\cdots\otimes H^1(\mathbb{R}^3)$, which is an N-fold tensor product of Sobolev spaces.

The ground-state energy of the system is

$$E(N) = \inf\left\{Q^{(N)}(\psi)\ ;\ \psi\in\mathcal{D}(Q^{(N)})\ ,\ \|\psi\|_{L^2} = 1\right\}. \tag{2.3.4}$$

If a minimizing wave-function exists, we call it the **ground-state** and denote it by $\psi_{\mathrm{GS}}^{(N)}$. We say that this ground-state is **proper** when the ground-state energy $E(N)$ belongs to the discrete spectrum of $H^{(N)}$. Due to theorems by Zhislin, Benguria and Lieb (see [BL83] and [LS09]), it is known that:

- there exists N^* such that if $\lambda \geq .826$ then a proper ground-state exists for $N \geq N^*$;
- there exists $.826 \leq \lambda^* < 1$ such that if $\lambda \geq \lambda^*$ then a proper ground state exists for all N.

Because of this, all theorems that can be proved by assuming a proper ground state exists must be stated under the assumption that

$$(\lambda \geq \lambda^*) \quad \text{or} \quad (\lambda \geq .826 \text{ and } N \geq N^*). \tag{2.3.5}$$

Define the **asymptotic Hartree functional** $\mathcal{H}_\infty$ on $H^1(\mathbb{R}^3)$ by

$$\mathcal{H}_\infty(\phi) = \frac{\hbar^2}{2m}\int|\nabla\phi|^2\mathrm{d}^3x - \lambda(ze)^2\int\frac{|\phi|^2}{|x|}\mathrm{d}^3x + \frac{1}{2}(ze)^2\iint\frac{|\phi(x)\phi(y)|^2}{|x-y|}\mathrm{d}^3x\mathrm{d}^3y. \tag{2.3.6}$$

It arises naturally when plugging-in a trial ψ of the form $\Phi(q_1)\cdots\Phi(q_N)$ into $Q^{(N)}$, rescaling the arguments with N and taking $N\to\infty$.

The strategy found in [Kie10] is adapted from previous works, especially [Hog11], with the goal of describing the asymptotic behavior of the ground-state energy and wavefunction by methods from classical Statistical Mechanics. The main idea is that the measure

$$\rho(x) = |\psi(x)|^2 \mathrm{d}^{3N} x \tag{2.3.7}$$

can be considered an absolutely continuous probability density, and the main theorem can be quoted as follows:

Theorem 2.3.1. (Kiessling) *The following hold.*

i) The ratio $E(N)/N^3$ grows monotonically as $N \to \infty$, converging to

$$\inf\{\mathcal{H}_\infty(\phi)\ ;\ \phi \in H^1(\mathbb{R}^3)\ ,\ \|\phi\|_{L^2} = 1\}. \tag{2.3.8}$$

ii) $\mathcal{H}_\infty$ has a unique positive minimizer $\phi_{\min}$ with $\|\phi_{\min}\|_{L^2} = 1$.

iii) Let N be given and assume condition (2.3.5). Let

$$\tilde{\psi}^{(N)}_{\mathrm{GS}}(q_1, \dots, q_N) = N^{-3N/2} \psi^{(N)}_{\mathrm{GS}}(N^{-1}q_1, \dots, N^{-1}q_N) \tag{2.3.9}$$

be a rescaled version of the ground-state. Then, for any $n \in \mathbb{N}$, $n \leq N$, we have

$$\int |\tilde{\psi}^{(N)}_{\mathrm{GS}}|^2(q_1, \dots, q_n, u_{n+1}, \dots u_N) \mathrm{d}^3 u_{n+1} \cdots \mathrm{d}^3 u_N \underset{N\to\infty}{\longrightarrow} |\phi_{\min}(q_1)|^2 \cdots |\phi_{\min}(q_n)|^2 \tag{2.3.10}$$

weakly in $L^1 \cap L^{\frac{3n}{3n-2}}$.

2.4 Bosonic atom without Born-Oppenheimer approximation

2.4.1 Set-up

In order to formulate the same model described by the Hamiltonian (2.3.1) without the Born-Oppenheimer approximation, we need to rewrite it by using the general procedure described in section 2.2 (see remark 2.2.6). It gives rise to the following energy functional (unimportant constants have been set equal to 1, and C is the factor $1 \pm r^{-1/2}$ arising from the coordinate change):

$$Q^{(N)}(\rho^{(N)}) = \sum_{j=1}^{N} \int |\nabla_j \sqrt{\rho^{(N)}}|^2 - \sum_{j=1}^{N} \int \frac{\rho^{(N)}}{|\xi_j - C\bar{\boldsymbol{\xi}}|} + \frac{1}{N} \sum_{i<j}\sum \int \frac{\rho^{(N)}}{|\xi_i - \xi_j|}\ . \tag{2.4.1}$$

Proposition 2.4.1. *$Q^{(N)}$ is bounded below in the space of absolutely continuous, compactly supported, permutation-symmetric probability measures $\rho^{(N)}$ in $\mathbb{R}^{3N}$ such that $\nabla\sqrt{\rho^{(N)}} \in L^1$.*

Proof. It is enough to get rid of the third (positive) term and consider only

$$\begin{aligned}\tilde{Q}^{(N)}(\rho^{(N)}) &= \sum_{j=1}^{N}\int |\nabla_j\sqrt{\rho^{(N)}}|^2 - \sum_{j=1}^{N}\int \frac{\rho^{(N)}}{|\xi_j - C\overline{\boldsymbol{\xi}}|} \\ &= N\left(\int |\nabla_1\sqrt{\rho^{(N)}}|^2 - \int \frac{\rho^{(N)}}{|\xi_1 - C\overline{\boldsymbol{\xi}}|}\right) \\ &= N\left(\int |\nabla_1\sqrt{\rho^{(N)}}|^2 - \int \frac{\rho^{(N)}}{|(1-\frac{C}{N})\xi_1 - C(1-\frac{1}{N})\overline{\overline{\boldsymbol{\xi}}}|}\right)\end{aligned} \tag{2.4.2}$$

where

$$\overline{\overline{\boldsymbol{\xi}}} := \frac{\xi_2 + \cdots + \xi_N}{N-1} \; . \tag{2.4.3}$$

Let $\rho^{(N)}$ as in the theorem statement. For every fixed $\boldsymbol{\xi}^{(N-1)} = (\xi_2, \ldots, \xi_N) \in \mathbb{R}^{3(N-1)}$, consider the function

$$\rho_{\boldsymbol{\xi}^{(N-1)}}(\xi) = \rho^{(N)}(\xi, \boldsymbol{\xi}^{(N-1)}) \quad , \quad \xi \in \mathbb{R}^3 \tag{2.4.4}$$

(defined for almost every $\boldsymbol{\xi}^{(N-1)}$). We remark that $\sqrt{\rho_{\boldsymbol{\xi}^{(N-1)}}} \in \dot{H}^1(\mathbb{R}^3)$ for almost every $\boldsymbol{\xi}^{(N-1)}$. Indeed, since

$$\int_{\mathbb{R}^{3(N-1)}}\int \rho_{\boldsymbol{\xi}^{(N-1)}}(\xi)\mathrm{d}^3\xi\mathrm{d}^{3(N-1)}\boldsymbol{\xi}^{(N-1)} = \|\rho^{(N)}\|_1 < \infty \; , \tag{2.4.5}$$

we have

$$\int \rho_{\boldsymbol{\xi}^{(N-1)}}(\xi)\mathrm{d}^3\xi < \infty \text{ for almost all } \boldsymbol{\xi}^{(N-1)} \; ; \tag{2.4.6}$$

similarly, since

$$\int_{\mathbb{R}^{3(N-1)}}\int \nabla\sqrt{\rho_{\boldsymbol{\xi}^{(N-1)}}(\xi)}\mathrm{d}^3\xi\mathrm{d}^{3(N-1)}\boldsymbol{\xi}^{(N-1)} = \int_{\mathbb{R}^{3N}} \nabla_1\sqrt{\rho^{(N)}} = \frac{1}{N}\|\nabla\sqrt{\rho^{(N)}}\|_2^2 < \infty \; , \tag{2.4.7}$$

we have

$$\int \nabla\sqrt{\rho_{\boldsymbol{\xi}^{(N-1)}}(\xi)}\mathrm{d}^3\xi < \infty \text{ for almost all } \boldsymbol{\xi}^{(N-1)} \; . \tag{2.4.8}$$

Now let $u = \rho_{\boldsymbol{\xi}^{(N-1)}}$ for some fixed $\boldsymbol{\xi}^{(N-1)}$ for which $\sqrt{u} \in \dot{H}^1(\mathbb{R}^3)$, and define

$$v(\xi) = \frac{1}{\left(1-\frac{C}{N}\right)^3}u\left(\frac{\xi}{1-\frac{C}{N}}\right) \; , \tag{2.4.9}$$

which also satisfies $\sqrt{v} \in \dot{H}^1(\mathbb{R}^3)$. By the Sobolev embedding, $\sqrt{v} \in L^3(\mathbb{R}^3)$ and there is $K > 0$ such that

$$\|\sqrt{v}\|_6 \leq K\|\nabla\sqrt{v}\|_2 \; . \tag{2.4.10}$$

We have

$$\int \frac{u(\xi)}{\left|\left(1-\frac{C}{N}\right)\xi - C\left(1-\frac{1}{N}\right)\overline{\overline{\boldsymbol{\xi}}}\right|}\mathrm{d}\xi = \int \frac{v(\xi)}{\left|\xi - C\left(1-\frac{1}{N}\right)\overline{\overline{\boldsymbol{\xi}}}\right|}\mathrm{d}\xi \ . \tag{2.4.11}$$

For given $R>0$, let

$$\mathcal{A}(R) = \{\xi \in \mathbb{R}^3 \ ; \ \left|\xi - C\left(1-\frac{1}{N}\right)\overline{\overline{\boldsymbol{\xi}}}\right| < R\} \ . \tag{2.4.12}$$

By the Hölder inequality,

$$\int_{\mathcal{A}(R)} \frac{v(\xi)}{\left|\xi - C\left(1-\frac{1}{N}\right)\overline{\overline{\boldsymbol{\xi}}}\right|}\mathrm{d}\xi < \|v\|_3 \left\| \frac{\chi_{\mathcal{A}(R)}(\cdot)}{|\cdot - C(1-1/N)\overline{\overline{\boldsymbol{\xi}}}|}\right\|_{3/2} = \|v\|_3 \left(\frac{8\pi}{3}\right)^{2/3} R \ , \tag{2.4.13}$$

implying

$$\begin{aligned}
&\int |\nabla\sqrt{u}|^2 - \int \frac{u(\xi)}{|(1-\frac{C}{N})\xi - C(1-\frac{1}{N})\overline{\overline{\boldsymbol{\xi}}}|}\mathrm{d}^3\xi \\
&\qquad = \left(1-\frac{C}{N}\right)^6 \|\nabla\sqrt{v}\|_2^2 - \int_{\mathcal{A}(R)} \frac{v}{|\xi - C(1-\frac{1}{N})\overline{\overline{\boldsymbol{\xi}}}|}\mathrm{d}^3\xi - \int_{\mathbb{R}^3\setminus\mathcal{A}(R)} \frac{v}{|\xi - C(1-\frac{1}{N})\overline{\overline{\boldsymbol{\xi}}}|}\mathrm{d}^3\xi \\
&\qquad > \left(1-\frac{C}{N}\right)^6 \|\nabla\sqrt{v}\|_2^2 - \left(\frac{8\pi}{3}\right)^{2/3} R\|\sqrt{v}\|_6^2 - \frac{1}{R}\|v\|_1 \\
&\qquad > \left(\left(1-\frac{C}{N}\right)^6 - \left(\frac{8\pi}{3}\right)^{2/3} K^2 R\right) \|\sqrt{v}\|_2^2 - \frac{1}{R}\|v\|_1 \ .
\end{aligned} \tag{2.4.14}$$

If we choose R such that the scalar in parenthesis above vanishes, we conclude that

$$\int |\nabla\sqrt{u}|^2 - \int \frac{u(\xi)}{|(1-\frac{C}{N})\xi - C(1-\frac{1}{N})\overline{\overline{\boldsymbol{\xi}}}|}\mathrm{d}^3\xi \geq -C_2\|v\|_1 = -C_2\|\sqrt{v}\|_2^2 \tag{2.4.15}$$

for some $C_2>0$ independent of N. Going back to (2.4.2), we see then that

$$\tilde{Q}^{(N)}(\rho^{(N)}) \geq -NC_2 \int_{\mathbb{R}^{3(N-1)}} \|\sqrt{\rho^{(N)}}(\xi_1, \boldsymbol{\xi^{(N-1)}})\|^2_{L^2(\mathbb{R}^3(\xi_1))} \mathrm{d}^{3(N-1)}\boldsymbol{\xi} = -NC_2\|\sqrt{\rho^{(N)}}\|_2^2 \ , \tag{2.4.16}$$

which then shows that $\tilde{Q}^{(N)}$, and also $Q^{(N)}$, are bounded below. Note that this proof also shows that $Q^{(N)}/N$ is bounded below uniformly in N. □

In all that follows, we must assume the existence of a minimizer $\mu^{(N)}$ for (2.4.1). We don't have a proof that it exists; but, in case it doesn't, the argument outlined from here onwards can be applied instead to a minimizing sequence. We don't write it in that context to keep the notation readable.

Call E_N the corresponding minimum energy:

$$Q^{(N)}(\mu^{(N)}) = E_N = \inf_{\rho^{(N)} \in \mathcal{P}_{\mathrm{Sym}}(\mathbb{R}^{3N})} Q^{(N)}(\rho^{(N)}) \ . \tag{2.4.17}$$

The **Hartree functional at level $\boldsymbol{N}$** is defined by

$$\begin{aligned} h_N(u) &= \frac{1}{N} Q^{(N)}(u^{\otimes N}) \\ &= \int |\nabla\sqrt{u}|^2 - \frac{1}{N}\sum_{j=1}^{N} \int \frac{u(\xi_1)\cdots u(\xi_N)}{|\xi_j - C\bar{\boldsymbol{\xi}}|} \mathrm{d}\boldsymbol{\xi} + \frac{1}{2}\left(1 - \frac{1}{N}\right) \iint \frac{u(x)u(y)}{|x-y|} \mathrm{d}x\mathrm{d}y \\ &= \int |\nabla\sqrt{u}|^2 - \int \frac{u(\xi_1)\cdots u(\xi_N)}{|\xi_1 - C\bar{\boldsymbol{\xi}}|} \mathrm{d}\boldsymbol{\xi} + \frac{1}{2}\left(1 - \frac{1}{N}\right) \iint \frac{u(x)u(y)}{|x-y|} \mathrm{d}x\mathrm{d}y \quad , \quad u \in \mathcal{P}(\mathbb{R}^3) \ . \end{aligned} \tag{2.4.18}$$

Define also the **asymptotic Hartree functional** by the exact same expression as in (2.3.6):

$$h_\infty(u) = \int |\nabla\sqrt{u}|^2 - \int \frac{u(x)}{|x|} \mathrm{d}x + \frac{1}{2} \iint \frac{u(x)u(y)}{|x-y|} \mathrm{d}x\mathrm{d}y \quad , \quad u \in \mathcal{P}(\mathbb{R}^3) \ . \tag{2.4.19}$$

This definition is based on h_N above and justified by the fact (to be proved soon) that

$$\int \frac{u(\xi_1)\cdots u(\xi_N)}{|\xi_1 - C\bar{\boldsymbol{\xi}}|} \mathrm{d}\boldsymbol{\xi} \underset{N\to\infty}{\longrightarrow} \int \frac{u(x)}{|x|} \mathrm{d}x \tag{2.4.20}$$

for all reasonable measures u.

We are now ready to state the main conjecture about our functional (2.4.1), analogous to theorem 2.3.1:

Conjecture 2.4.2. *The following hold.*

i) The ratio $E(N)/N^3$ converges to

$$\inf\{h_\infty(\phi) \ ; \ \phi \in H^1(\mathbb{R}^3) \ , \ \|\phi\|_{L^2} = 1\}. \tag{2.4.21}$$

ii) Let N be given. Then, for any $n \in \mathbb{N}$, $n \leq N$, we have

$$\int \mu^{(N)}(q_1, \ldots, q_n, u_{n+1}, \ldots u_N) \mathrm{d}^3 u_{n+1} \cdots \mathrm{d}^3 u_N \underset{N\to\infty}{\longrightarrow} |\phi_{\min}(q_1)|^2 \cdots |\phi_{\min}(q_n)|^2 \tag{2.4.22}$$

weakly in $L^1 \cap L^{\frac{3n}{3n-2}}$, where $\phi_{\min}$ is as in theorem 2.3.1.

2.4.2 Limit behavior of the new potential

A proof of the fact (2.4.20) mentioned above will require the Central Limit Theorem, so let's first recall how it goes:

Theorem 2.4.3. *(Trivariate Central Limit Theorem) Suppose $u \in \mathcal{P}(\mathbb{R}^3)$ is such that*

$$\int_{\mathbb{R}^3} \boldsymbol{x} u(\boldsymbol{x}) \mathrm{d}^3\boldsymbol{x} = \mathbf{0} \quad , \quad \Sigma = (\sigma_{ij})_{3\times 3} := \left(\int_{\mathbb{R}^3} x_i x_j u(\boldsymbol{x}) \mathrm{d}^3\boldsymbol{x} \right)_{3\times 3} \text{ is invertible } . \tag{2.4.23}$$

If $\boldsymbol{X^{(i)}} = (X^{(i)}, Y^{(i)}, Z^{(i)})$ is a sequence of independent random variables whose probability density function is u, then the random variable

$$\sqrt{N}\overline{\boldsymbol{X}} := \sqrt{N} \frac{\boldsymbol{X^{(1)}} + \cdots + \boldsymbol{X^{(N)}}}{N} \tag{2.4.24}$$

converges in distribution to a normal of mean $\mathbf{0}$ and covariance matrix Σ. What this means is that

$$\lim_{N\to\infty} \int_{B_N(S)} u(\boldsymbol{x^{(1)}}) \ldots u(\boldsymbol{x^{(N)}}) \mathrm{d}^{3N}\boldsymbol{x} = \frac{1}{\sqrt{(2\pi)^3 \det \Sigma}} \int_S \exp\left(-\frac{1}{2} \boldsymbol{x}^T \Sigma^{-1} \boldsymbol{x} \right) \mathrm{d}^3\boldsymbol{x} \tag{2.4.25}$$

uniformly over all $S \subseteq \mathbb{R}^3$ with $\mu(\partial S) = 0$ (where μ is Lebesgue measure), where

$$B_N(S) = \left\{ (\boldsymbol{x^{(1)}}, \ldots, \boldsymbol{x^{(N)}}) \in \mathbb{R}^{3N} \ , \ \frac{\boldsymbol{x^{(1)}} + \cdots + \boldsymbol{x^{(N)}}}{\sqrt{N}} \in S \right\} . \tag{2.4.26}$$

Equivalently, for every bounded and continuous $f : \mathbb{R}^3 \to \mathbb{R}$,

$$\lim_{N\to\infty} \int_{\mathbb{R}^{3N}} f\left(\frac{\boldsymbol{x^{(1)}} + \cdots + \boldsymbol{x^{(N)}}}{\sqrt{N}} \right) u(\boldsymbol{x^{(1)}}) \ldots u(\boldsymbol{x^{(N)}}) \mathrm{d}^{3N}\boldsymbol{x}$$
$$= \frac{1}{\sqrt{(2\pi)^3 \det \Sigma}} \int_{\mathbb{R}^3} f(\boldsymbol{x}) \exp\left(-\frac{1}{2} \boldsymbol{x}^T \Sigma^{-1} \boldsymbol{x} \right) \mathrm{d}^3\boldsymbol{x} . \tag{2.4.27}$$

Remark 2.4.4. Note that, if $u \in \mathcal{P}(\mathbb{R}^3)$ is rotationally symmetric (as we expect to be able to assume of the minimizers $\mu^{(N)}$ or of a minimizing sequence), the covariance matrix Σ will be a multiple of the identity. Indeed, let

$$u(\boldsymbol{x}) = v(|\boldsymbol{x}|) \tag{2.4.28}$$

with

$$1 = \int u = 4\pi \int_{-\infty}^{\infty} r^2 v(r) \mathrm{d}r . \tag{2.4.29}$$

The off-diagonal elements in Σ are all zero; for example

$$\iiint xyu(x,y,z) \mathrm{d}x\mathrm{d}y\mathrm{d}z = \iiint (-x)yu(-x,y,z) \mathrm{d}x\mathrm{d}y\mathrm{d}z = \iiint (-x)yu(x,y,z) \mathrm{d}x\mathrm{d}y\mathrm{d}z . \tag{2.4.30}$$

The diagonal elements are all equal to each other; for example

$$\iiint x^2 u(x,y,z)\mathrm{d}x\mathrm{d}y\mathrm{d}z = \iiint y^2 u(y,x,z)\mathrm{d}x\mathrm{d}y\mathrm{d}z = \iiint y^2 u(x,y,z)\mathrm{d}x\mathrm{d}y\mathrm{d}z \; . \tag{2.4.31}$$

And the sum of the three diagonal elements is

$$\iiint (x^2+y^2+z^2)u(x,y,z)\mathrm{d}x\mathrm{d}y\mathrm{d}z = 4\pi \int r^4 v(r)\mathrm{d}r \; . \tag{2.4.32}$$

Therefore

$$\Sigma = (\sigma_{ij})_{3\times 3} \; , \; \sigma_{ij} = \frac{\delta_{ij}}{12\pi} \int_{-\infty}^{\infty} r^4 v(r)\mathrm{d}r \; . \tag{2.4.33}$$

Lemma 2.4.5. *Let $u \in L^2(\mathbb{R}^3)$. Also suppose that*

$$I := \int_{\mathbb{R}^3} \frac{u(\boldsymbol{y})}{|\boldsymbol{y}|}\, \mathrm{d}^3\boldsymbol{y} < \infty \; . \tag{2.4.34}$$

Then there exists $K \geq 0$ such that, for every $\boldsymbol{a} \in \mathbb{R}^3 \setminus \{\boldsymbol{0}\}$,

$$\int_{\mathbb{R}^3} \frac{u(\boldsymbol{y})}{|\boldsymbol{y}||\boldsymbol{y}-\boldsymbol{a}|}\mathrm{d}^3\boldsymbol{y} \leq K(|\boldsymbol{a}|^{-\frac{1}{2}} + |\boldsymbol{a}|^{-1}) \; . \tag{2.4.35}$$

Proof. For fixed $a \in \mathbb{R}^3$ consider the two complementary regions

$$R_1 = \left\{ y \in \mathbb{R}^3 \; , \; |y-a| \leq \frac{|a|}{2} \right\} \quad , \quad R_2 = \left\{ y \in \mathbb{R}^3 \; , \; |y-a| \geq \frac{|a|}{2} \right\} \; . \tag{2.4.36}$$

For R_2 we immediately have

$$\int_{R_2} \frac{u(y)}{|y||y-a|}\mathrm{d}^3 y \leq \frac{2}{|a|} \int_{R_2} \frac{u(y)}{|y|}\mathrm{d}^3 y \leq \frac{2I}{|a|} \; . \tag{2.4.37}$$

In R_1, we start by noting that

$$|y| = |a+y-a| \geq ||a|-|y-a|| \geq |a|-|y-a| \geq |a| - \frac{|a|}{2} = \frac{|a|}{2} \; , \tag{2.4.38}$$

so that

$$\int_{R_1} \frac{u(y)}{|y||y-a|}\mathrm{d}^3 y \leq \frac{2}{|a|} \int_{R_1} \frac{u(y)}{|y-a|}\mathrm{d}^3 y \; . \tag{2.4.39}$$

Note

$$\left\| \frac{1}{|y-a|} \right\|_{L^2(R_1)}^2 = \int_{R_1} \frac{1}{|y-a|^2}\mathrm{d}y = 4\pi \int_0^{|a|/2} \mathrm{d}y = 2\pi|a| \; , \tag{2.4.40}$$

and hence, using the Hölder inequality for $p = q = 2$ and the functions $1/|y-a|$ and u:

$$\int_{R_1} \frac{u(y)}{|y||y-a|} \leq \frac{2}{|a|}\|u\|_2 \sqrt{2\pi|a|} = \sqrt{8\pi}|a|^{-\frac{1}{2}}\|u\|_2 \; . \tag{2.4.41}$$

Putting the R_1 and R_2 estimates together,

$$\int \frac{u(y)}{|y||y-a|}\mathrm{d}y \leq K(|a|^{-1} + |a|^{-\frac{1}{2}}) \ , \tag{2.4.42}$$

where $K = \max\left(2I, \sqrt{8\pi}\|u\|_2\right)$. □

The next theorem is the rigorous way to state the fact that our new potential energy term behaves like the one from section 2.3 for *reasonable* probability measures u (that is, satisfying the conditions (2.4.43) just ahead):

Theorem 2.4.6. *Let $C \in \mathbb{R}$. Let $u \in \mathcal{P}(\mathbb{R}^3)$ be absolutely continuous with respect to Lebesgue measure. Suppose that $u \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ and that*

$$\int_{\mathbb{R}^3} \boldsymbol{x} u(\boldsymbol{x})\ \mathrm{d}^3\boldsymbol{x} = 0 \quad , \quad \Sigma = (\sigma_{ij})_{3\times 3} := \left(\int_{\mathbb{R}^3} x_i x_j u(\boldsymbol{x})\mathrm{d}^3\boldsymbol{x}\right)_{3\times 3} \ \textit{is defined and invertible.} \tag{2.4.43}$$

Then

$$\lim_{N\to\infty} \int u(\xi_1)\cdots u(\xi_N) \left(\frac{1}{|\xi_1|} - \frac{1}{|\xi_1 - C\overline{\boldsymbol{\xi}}|}\right) \mathrm{d}^{3N}\boldsymbol{\xi} = 0 \ . \tag{2.4.44}$$

Proof. Assume $N > C$ in the argument. We stop using boldface $\boldsymbol{x}$ in favor of just x. We remark that

$$\int_{\mathbb{R}^3} \frac{u(x)}{|x|}\mathrm{d}^3x < \infty \ , \tag{2.4.45}$$

as a consequence of the Hölder inequality and the fact that $u \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$.

First there are some simple steps that clean up the expression above via rescalings in the integral. For each N, consider the following rescaled version of u:

$$u_N(x) = \left(\frac{N}{N-C}\right)^3 u\left(\frac{Nx}{N-C}\right) \ . \tag{2.4.46}$$

As $N \to \infty$, the fraction $N/(N-C)$ tends to 1, making u_N converge pointwise a.e. to u (it converges at every point where u is continuous). Also observe that boundedness of the integral $\int(u/|x|)\mathrm{d}^3x$ implies that there is a uniform-in-N bound on the integrals $\int(u_N/|x|)\mathrm{d}^3x$. Indeed, by using the fraction $N/(N-C)$ to rescale the integration variable of the latter, the integral reverts to the former with a constant $(N-C)/N$ in front of it, but this constant can be uniformly bounded in N since it converges to 1.

Let's estimate the limit (2.4.44) by taking the absolute value of the integrand. First we separate out the ξ_1 from the empirical average term and perform a change of variables in the ξ_1 variable:

$$\begin{aligned}
&\int u(\xi_1)\cdots u(\xi_N)\left|\frac{1}{|\xi_1|}-\frac{1}{|\xi_1-C\bar{\boldsymbol{\xi}}|}\right|\mathrm{d}^{3N}\boldsymbol{\xi}\\
&\quad=\int_{\mathbb{R}^3}\int_{\mathbb{R}^{3(N-1)}}u(\xi_1)\cdots u(\xi_N)\left|\frac{1}{|\xi_1|}-\frac{1}{|(1-\frac{C}{N})\xi_1-\frac{C}{N}(\xi_2+\cdots+\xi_N)|}\right|\mathrm{d}^{3(N-1)}\boldsymbol{\xi}\mathrm{d}^3\xi_1 \qquad (2.4.47)\\
&\quad=\int_{\mathbb{R}^3}\int_{\mathbb{R}^{3(N-1)}}u_N(\xi_1)u(\xi_2)\cdots u(\xi_N)\left|\frac{\frac{N-C}{N}}{|\xi_1|}-\frac{1}{|\xi_1-\frac{C(N-1)}{N}\frac{\xi_2+\cdots+\xi_N}{N-1}|}\right|\mathrm{d}^{3(N-1)}\boldsymbol{\xi}\mathrm{d}^3\xi_1\ .
\end{aligned}$$

We will abbreviate again

$$\bar{\bar{\boldsymbol{\xi}}}=\frac{\xi_2+\ldots+\xi_N}{N-1}\ . \qquad (2.4.48)$$

Now split the absolute value above as follows:

$$\left|\frac{\frac{N-C}{N}}{|\xi_1|}-\frac{1}{|\xi_1-\frac{C(N-1)}{N}\bar{\bar{\boldsymbol{\xi}}}|}\right|\le\frac{C}{N}\frac{1}{|\xi_1|}+\left|\frac{1}{|\xi_1|}-\frac{1}{|\xi_1-\frac{C(N-1)}{N}\bar{\bar{\boldsymbol{\xi}}}|}\right|\ . \qquad (2.4.49)$$

The integral of the first of these two terms against the u functions is

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^{3(N-1)}}u_N(\xi_1)u(\xi_2)\cdots u(\xi_N)\frac{C}{N}\frac{1}{|\xi_1|}\mathrm{d}^{3(N-1)}\boldsymbol{\xi}\mathrm{d}^3\xi_1=\frac{C}{N}\int_{\mathbb{R}^3}\frac{u_N(\xi_1)}{|\xi_1|}\mathrm{d}^3\xi_1\ , \qquad (2.4.50)$$

which converges to zero due to the fact that the integrals $\int(u_N/|x|)\mathrm{d}^3x$ are uniformly bounded.

Then we need to concentrate our efforts on the integral of the second term in (2.4.49) against the u functions:

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^{3(N-1)}}u_N(\xi_1)u(\xi_2)\cdots u(\xi_N)\left|\frac{1}{|\xi_1|}-\frac{1}{|\xi_1-\frac{C(N-1)}{N}\bar{\bar{\boldsymbol{\xi}}}|}\right|\mathrm{d}^{3(N-1)}\boldsymbol{\xi}\mathrm{d}^3\xi_1\ . \qquad (2.4.51)$$

It's possible to get rid of the term $C(N-1)/N$ by using a change of variables (a rescaling by this exact term). The resulting factor that multiplies the entire integral after this change is bounded away from both 0 and ∞ because the fraction $(N-1)/N$ converges to 1, so it doesn't interfere with the desired convergence to 0. Therefore, what is left is to show that

$$\lim_{N\to\infty}\int_{\mathbb{R}^3}\int_{\mathbb{R}^{3(N-1)}}u(\xi_1)u(\xi_2)\cdots u(\xi_N)\left|\frac{1}{|\xi_1|}-\frac{1}{|\xi_1-\bar{\bar{\boldsymbol{\xi}}}|}\right|\mathrm{d}^{3(N-1)}\boldsymbol{\xi}\mathrm{d}^3\xi_1=0\ . \qquad (2.4.52)$$

We bound the absolute value as

$$\left|\frac{1}{|\xi_1|}-\frac{1}{|\xi_1-\bar{\bar{\boldsymbol{\xi}}}|}\right|\le\frac{\big||\xi_1-\bar{\bar{\boldsymbol{\xi}}}|-|\xi_1|\big|}{|\xi_1||\xi_1-\bar{\bar{\boldsymbol{\xi}}}|}\le\frac{|\bar{\bar{\boldsymbol{\xi}}}|}{|\xi_1||\xi_1-\bar{\bar{\boldsymbol{\xi}}}|}\ . \qquad (2.4.53)$$

For cleaner writing, we also rename ξ_1 as y, ξ_{i+1} as ξ_i, N as $N+1$ and $\overline{\overline{\boldsymbol{\xi}}}$ as $\overline{\boldsymbol{\xi}}$. That is,

$$\overline{\boldsymbol{\xi}} = \frac{\xi_1 + \cdots + \xi_N}{N} \tag{2.4.54}$$

and we must prove

$$\lim_{N\to\infty} \int_{\mathbb{R}^{3N}} \int_{\mathbb{R}^3} \frac{u(y)}{|y||y-\overline{\boldsymbol{\xi}}|} \mathrm{d}^3 y \; |\overline{\boldsymbol{\xi}}| u(\xi_1) \cdots u(\xi_N) \mathrm{d}^{3N} \boldsymbol{\xi} = 0 \; . \tag{2.4.55}$$

This is where the crux of this proof is. Fix $\varepsilon > 0$. Let

$$K = \max\left(2 \int \frac{u(y)}{|y|} \mathrm{d}^3 y, \sqrt{8\pi} \|u\|_2 \right) \tag{2.4.56}$$

(note that $u \in L^2$ because $u \in L^1 \cap L^3$). Lemma (2.4.5) says that

$$\int \frac{u(y)}{|y||y-\overline{\boldsymbol{\xi}}|} \mathrm{d}^3 y \le K(|\overline{\boldsymbol{\xi}}|^{-1} + |\overline{\boldsymbol{\xi}}|^{-1/2}) \tag{2.4.57}$$

for all $|\overline{\boldsymbol{\xi}}| \neq 0$. Also let

$$f(x) = \frac{1}{\sqrt{(2\pi)^3 \det \Sigma}} \exp\left(-\frac{1}{2} x^T \Sigma^{-1} x \right) \tag{2.4.58}$$

be the probability density of the trivariate normal with correlation matrix defined by u (assumed to be well-defined in the hypotheses of the theorem). There is a small $\delta > 0$ such that

$$K(1+\sqrt{\delta}) \int_{|x|<\delta} f(x) \mathrm{d}x < \frac{\varepsilon}{4} \; . \tag{2.4.59}$$

Denote

$$J := \int_{\mathbb{R}^3} |x|^{1/2} f(x) \; \mathrm{d}^3 x \; , \tag{2.4.60}$$

which is finite since the density of the normal distribution has exponential decay at infinity.

For each natural N, consider the regions

$$R_1(N) = \left\{ \boldsymbol{\xi} \in \mathbb{R}^{3N} \; ; \; |\sqrt{N} \overline{\boldsymbol{\xi}}| < \delta \right\} \quad , \quad R_2(N) = \left\{ \boldsymbol{\xi} \in \mathbb{R}^{3N} \; ; \; |\sqrt{N} \overline{\boldsymbol{\xi}}| > \delta \right\} \; . \tag{2.4.61}$$

Pick N_0 large enough that the following three conditions are satisfied:

- we have

$$N_0^{-1/4} J K (1 + 1/\sqrt{\delta}) < \frac{\varepsilon}{4} \; ; \tag{2.4.62}$$

- for $N \geq N_0$, we have

$$\begin{aligned}\int_{R_1(N)} u(\xi_1)\cdots u(\xi_N)\mathrm{d}^{3N}\boldsymbol{\xi} &= \int_{\mathbb{R}^{3N}} \chi_{B_\delta}(\sqrt{N}\overline{\boldsymbol{\xi}})u(\xi_1)\cdots u(\xi_N)\mathrm{d}^{3N}\boldsymbol{\xi} \\ &< \int_{|x|<\delta} f(x)\mathrm{d}x + \frac{\varepsilon/4}{K(1+\sqrt{\delta})} \ ,\end{aligned} \tag{2.4.63}$$

which can be done due to the Central Limit Theorem, considering that χ_{B_δ} is a bounded function; and

- for $N \geq N_0$, we have

$$\begin{aligned}\int_{R_2(N)} |\sqrt{N}\overline{\boldsymbol{\xi}}|^{1/2}u(\xi_1)\cdots u(\xi_N)\mathrm{d}^{3N}\boldsymbol{\xi} &< \int_{\mathbb{R}^3\setminus B_\delta} |x|^{1/2}f(x)\mathrm{d}x + \frac{\varepsilon/4}{K(1+1/\sqrt{\delta})} \\ &< J + \frac{\varepsilon/4}{K(1+1/\sqrt{\delta})} \ .\end{aligned} \tag{2.4.64}$$

Now fix any $N \geq N_0$ and any $\boldsymbol{\xi} \in \mathbb{R}^{3N}$. If $\boldsymbol{\xi} \in R_1(N)$ we have $|\overline{\boldsymbol{\xi}}| < \delta$, implying

$$\int_{\mathbb{R}^3} \frac{u(y)}{|y||y-\overline{\boldsymbol{\xi}}|}\mathrm{d}^3y \leq K(|\overline{\boldsymbol{\xi}}|^{-1} + |\overline{\boldsymbol{\xi}}|^{-1/2}|) \leq K(|\overline{\boldsymbol{\xi}}|^{-1} + |\overline{\boldsymbol{\xi}}|^{1/2}|\overline{\boldsymbol{\xi}}|^{-1}) < K(1+\sqrt{\delta})|\overline{\boldsymbol{\xi}}|^{-1} \ , \tag{2.4.65}$$

so that

$$\begin{aligned}\int_{R_1(N)}\int_{\mathbb{R}^3} \frac{u(y)}{|y||y-\overline{\boldsymbol{\xi}}|}\mathrm{d}^3y\ |\overline{\boldsymbol{\xi}}|u(\xi_1)\cdots u(\xi_N)\mathrm{d}^{3N}\boldsymbol{\xi} &< K(1+\sqrt{\delta})\int_{R_1(N)} u(\xi_1)\cdots u(\xi_N)\mathrm{d}\boldsymbol{\xi} \\ &< K(1+\sqrt{\delta})\int_{|x|<\delta} f(x)\mathrm{d}x + (1+\sqrt{\delta})\frac{\varepsilon/4}{K(1+\sqrt{\delta})} \\ &< \frac{\varepsilon}{2} \ .\end{aligned} \tag{2.4.66}$$

Otherwise, if $\boldsymbol{\xi} \in R_2(N)$, we have

$$\int_{\mathbb{R}^3} \frac{u(y)}{|y||y-\overline{\boldsymbol{\xi}}|}\mathrm{d}^3y \leq K(|\overline{\boldsymbol{\xi}}|^{-1}+|\overline{\boldsymbol{\xi}}|^{-1/2}|) \leq K(|\overline{\boldsymbol{\xi}}|^{-1/2}|\overline{\boldsymbol{\xi}}|^{-1/2}+|\overline{\boldsymbol{\xi}}|^{-1/2}) < K(1+\frac{1}{\sqrt{\delta}})|\overline{\boldsymbol{\xi}}|^{-1/2} \ , \tag{2.4.67}$$

so that

$$\begin{aligned}\int_{R_2(N)}\int_{\mathbb{R}^3} \frac{u(y)}{|y||y-\overline{\boldsymbol{\xi}}|}\mathrm{d}^3y\ |\overline{\boldsymbol{\xi}}|u(\xi_1)\cdots u(\xi_N)\mathrm{d}^{3N}\boldsymbol{\xi} &= K(1+\frac{1}{\sqrt{\delta}})\int_{R_2(N)} |\overline{\boldsymbol{\xi}}|^{1/2}u(\xi_1)\cdots u(\xi_N)\mathrm{d}\boldsymbol{\xi} \\ &= N^{-1/4}K(1+\frac{1}{\sqrt{\delta}})\int_{R_2(N)} |\sqrt{N}\overline{\boldsymbol{\xi}}|^{1/2}u(\xi_1)\cdots u(\xi_N)\mathrm{d}\boldsymbol{\xi} \\ &< N^{-1/4}K(1+\frac{1}{\sqrt{\delta}})\left(J + \frac{\varepsilon/4}{K(1+1/\sqrt{\delta})}\right) \\ &< N^{-1/4}KJ(1+1/\sqrt{\delta}) + \frac{\varepsilon/4}{4} \\ &< \frac{\varepsilon}{2} \ .\end{aligned} \tag{2.4.68}$$

Altogether,

$$\int_{\mathbb{R}^{3N}}\int_{\mathbb{R}^3}\frac{u}{|y||y-\overline{\boldsymbol{\xi}}|}\mathrm{d}^3yu(\xi_1)\cdots u(\xi_N)\mathrm{d}^{3N}\boldsymbol{\xi}<\varepsilon \tag{2.4.69}$$

as we wanted. □

In the remainder of this section, we pave some of the ground for establishing the Hartree limit of a bosonic atom without BO approximation by proving that the minimum of the Hartree functional of a bosonic atom with BO approx also supplies a rigorous upper bound to the $\limsup_{N\to\infty}$ of the rescaled N-body energy per particle of the bosonic atom without BO approximation. This goes half the way towards proving conjecture 2.4.2. We also outline what is needed to complete the proof of that conjecture, but this requires new ideas that have to be supplied in future work.

2.4.3 Proof sketch for theorem 2.3.1

After the appropriate mean-field rescaling, we can reduce the problem to studying the following functional of permutation-symmetric absolutely continuous measures $\rho^{(N)}\in\mathcal{P}_{\mathrm{Sym}}(\mathbb{R}^{3N})$:

$$Q^{(N)}(\rho^{(N)})=\sum_{j=1}^N\int|\nabla_j\sqrt{\rho^{(N)}}|^2-\sum_{j=1}^N\int\frac{\rho^{(N)}}{|q_j|}+\frac{1}{N}\sum\sum_{i<j}\int\frac{\rho^{(N)}}{|q_i-q_j|}\ . \tag{2.4.70}$$

Let $\mu^{(N)}$ denote the minimizer, with corresponding energy E_N:

$$Q^{(N)}(\mu^{(N)})=E_N=\inf_{\rho^{(N)}\in\mathcal{P}_{\mathrm{Sym}}(\mathbb{R}^{3N})}Q^{(N)}(\rho^{(N)})\ . \tag{2.4.71}$$

Given $\rho^{(N)}$, we use the symbol $\rho_n^{(N)}$ to denote its n-th marginal ($n\le N$):

$$\rho_n^{(N)}(q_1,\ldots,q_n)=\int\rho^{(N)}(q_1,\ldots,q_N)\mathrm{d}q_{n+1}\cdots\mathrm{d}q_N \tag{2.4.72}$$

(it doesn't matter which variables are integrated out because of the permutation symmetry in ρ). The **Hartree functional at level $\boldsymbol{N}$** is defined as

$$\begin{aligned}h_N(u)&=\frac{1}{N}Q^{(N)}(u^{\otimes N})\\&=\int|\nabla\sqrt{u}|^2-\int\frac{u(x)}{|x|}\mathrm{d}x+\frac{1}{2}\left(1-\frac{1}{N}\right)\iint\frac{u(x)u(y)}{|x-y|}\mathrm{d}x\mathrm{d}y\quad,\quad u\in\mathcal{P}(\mathbb{R}^3)\ .\end{aligned} \tag{2.4.73}$$

Let e_N denote its infimum:

$$e_N=\inf_{u\in\mathcal{P}(\mathbb{R}^3)}h_N(u)\ . \tag{2.4.74}$$

The **asymptotic Hartree functional** is defined a form of limit of h_N — that is, the $1/N$ term goes away:

$$h_\infty(u) = \int |\nabla\sqrt{u}|^2 - \int \frac{u(x)}{|x|}\mathrm{d}x + \frac{1}{2}\iint \frac{u(x)u(y)}{|x-y|}\mathrm{d}x\mathrm{d}y \quad , \quad u \in \mathcal{P}(\mathbb{R}^3) \ . \tag{2.4.75}$$

Let u_∞ denote its unique minimizer, and e_∞ the corresponding value:

$$h_\infty(u_\infty) = e_\infty = \inf_{u\in\mathcal{P}(\mathbb{R}^3)} h_\infty(u) \ . \tag{2.4.76}$$

What the theorem claims is that:

- $\lim_{N\to\infty} \frac{E_N}{N} = e_\infty$;
- for any given n, $\lim_{N\to\infty} \mu_n^{(N)} = u_\infty^{\otimes n}$ weakly in $L^1(\mathbb{R}^{3n}) \cap L^{\frac{3n}{3n-2}}(\mathbb{R}^{3n})$.

First, it's clear by the definitions that

$$\frac{E_N}{N} \le e_N \ . \tag{2.4.77}$$

Also, the only way in which h_N depends on N is through the increasing term $1 - 1/N$, so that $e_N < e_\infty$ for all N, and hence

$$\limsup_{N\to\infty} \frac{E_N}{N} \le e_\infty \ . \tag{2.4.78}$$

The following Lemma will be needed shortly:

Lemma 2.4.7. (Kiessling) *For a fixed n, suppose that a sequence $\rho^{(N_k)} \in \mathcal{P}_{Sym}(\mathbb{R}^{3N_k})$ is such that*

$$\lim_{k\to\infty} \sqrt{\rho_n^{(N_k)}} = \sqrt{\nu^{(n)}} \quad \textit{weakly in } H^1(\mathbb{R}^{3n}) \ . \tag{2.4.79}$$

Then

$$\limsup_{k\to\infty} \frac{1}{N_k} Q^{(N_k)}(\rho^{(N_k)}) \ge \frac{1}{n} Q^{(n)}(\nu^{(n)}) \ . \tag{2.4.80}$$

Proof. We show it is true for each of the three parts in the energy functional. We will actually prove (2.4.80) for lim inf instead of just lim sup, but we will only need to use this inequality later with lim sup in it, and the point is that, in our context of no BO approximation, it may be the case that only an inequality with lim sup can be proven.

For the kinetic energy part, lower semicontinuity of the Fisher functional gives

$$\begin{aligned}\sum_{j=1}^{n}\int|\nabla_j\sqrt{\nu^{(n)}}|^2 &= \int|\boldsymbol{\nabla}\sqrt{\nu^{(n)}}|^2\\ &\le \liminf_{k\to\infty}\int|\boldsymbol{\nabla}\sqrt{\rho_n^{(N_k)}}|^2 \\ &= \liminf_{k\to\infty}\sum_{j=1}^{n}\int|\nabla_j\sqrt{\rho_n^{(N_k)}}|^2\ .\end{aligned} \tag{2.4.81}$$

Given k and n, let $N_k = a(k,n)n + r(k,n)$ with $a(k,n), r(k,n) \in \mathbb{N}$, $0 \le r(k,n) < n$ (Euclidean division). Note that

$$\lim_{k\to\infty}\frac{a(k,n)}{N_k} = \frac{1}{n}\ . \tag{2.4.82}$$

Because of subadditivity of the Fisher functional,

$$\frac{a(k,n)}{N_k}\sum_{j=1}^{n}\int|\nabla_j\sqrt{\rho_n^{(N_k)}}|^2 \le \frac{1}{N_k}\sum_{j=1}^{N_k}\int|\nabla_j\sqrt{\rho^{(N_k)}}|^2\ . \tag{2.4.83}$$

Taking a limit in k,

$$\frac{1}{n}\sum_{j=1}^{n}\int|\nabla_j\sqrt{\nu^{(n)}}|^2 \le \liminf_{k\to\infty}\frac{1}{N_k}\sum_{j=1}^{N_k}\int|\nabla_j\sqrt{\rho^{(N_k)}}|^2\ . \tag{2.4.84}$$

For the Coulomb repulsion between electrons, symmetry and the definition of the marginal give

$$\frac{1}{N_k-1}\frac{1}{N_k}\sum\sum_{1\le i<j\le N_k}\int\frac{\rho^{(N_k)}}{|q_i-q_j|} = \frac{1}{n-1}\frac{1}{n}\sum\sum_{1\le i<j\le n}\int\frac{\rho_n^{(N_k)}}{|q_i-q_j|}\ . \tag{2.4.85}$$

Rearranging slightly and bounding $n-1$ by n:

$$\frac{1}{N_k^2}\sum\sum_{1\le i<j\le N_k}\int\frac{\rho^{(N_k)}}{|q_i-q_j|} \ge \left(1-\frac{1}{N_k}\right)\frac{1}{n^2}\sum\sum_{1\le i<j\le n}\int\frac{\rho_n^{(N_k)}}{|q_i-q_j|}\ . \tag{2.4.86}$$

Then

$$\begin{aligned}\liminf_{k\to\infty}\frac{1}{N_k^2}\sum\sum_{1\le i<j\le N_k}\int\frac{\rho^{(N_k)}}{|q_i-q_j|} &\ge \liminf_{k\to\infty}\frac{1}{n^2}\sum\sum_{1\le i<j\le n}\int\frac{\rho_n^{(N_k)}}{|q_i-q_j|}\\ &\ge \frac{1}{n^2}\sum\sum_{1\le i<j\le n}\int\frac{\nu^{(n)}}{|q_i-q_j|}\end{aligned} \tag{2.4.87}$$

with the last step being justified by weak-lower semicontinuity of the Coulomb potential.

For the Coulomb attraction to the nucleus, we can actually get equality in (2.4.80). Symmetry and the definition of the marginal give

$$-\frac{1}{N_k}\sum_{j=1}^{N_k}\int\frac{\rho^{(N_k)}}{|q_j|} = -\frac{1}{n}\sum_{j=1}^{n}\int\frac{\rho_n^{(N_k)}}{|q_j|}\ . \tag{2.4.88}$$

So we can take the k limit:

$$-\lim_{k\to\infty}\frac{1}{N_k}\sum_{j=1}^{N_k}\int\frac{\rho^{(N_k)}}{|q_j|}=-\frac{1}{n}\sum_{j=1}^{n}\int\frac{\nu^{(n)}}{|q_j|}\ . \tag{2.4.89}$$

This concludes the proof of the Lemma. □

Now fix an arbitrary subsequence $\mu^{(N_k)}$ of the minimizers of (2.4.70). For any n, due to weak compactness granted by the Sobolev embedding, there exists a sub-subsequence N_{k_l} such that the marginals $\mu_n^{(N_{k_l})}$ converge weakly to some $\nu^{(n)}\in\mathcal{P}_{\mathrm{Sym}}(\mathbb{R}^{3n})$ as $l\to\infty$. (To be precise, all that can be initially justified is that $\nu^{(n)}(\mathbb{R}^{3n})\leq 1$, that is, it may not be a probability measure, but this is a technical point that is dealt with appropriately in [Kie10]).

By a diagonal extraction argument, we may assume that the same N_{k_l} works for any n:

$$\lim_{l\to\infty}\mu_n^{(N_{k_l})}=\nu^{(n)}\quad\text{for all } n\ . \tag{2.4.90}$$

Lemma (2.4.7) then says

$$\limsup_{l\to\infty}\frac{1}{N_{k_l}}Q^{(N_{k_l})}(\mu^{(N_{k_l})})\geq\frac{1}{n}Q^{(n)}(\nu^{(n)})\ . \tag{2.4.91}$$

Due to weak convergence and the Kolmogorov extension theorem, we can find $\nu\in\mathcal{P}_{\mathrm{Sym}}((\mathbb{R}^3)^\infty)$ whose marginals are the $\nu^{(n)}$. And, according to the de Finetti theorem, these marginals are a convex combination of product measures using a measure m on the space $\mathcal{P}(\mathbb{R}^3)$ that only depends on ν:

$$\nu^{(n)}=\int_{\mathcal{P}(\mathbb{R}^3)}u^{\otimes n}\mathrm{d}m(u)\ . \tag{2.4.92}$$

In particular

$$\frac{1}{n}Q^{(n)}(\nu^{(n)})=\int_{\mathcal{P}(\mathbb{R}^3)}\frac{1}{n}Q^{(n)}(u^{\otimes n})\mathrm{d}m(u)=\int_{\mathcal{P}(\mathbb{R}^3)}h_n(u)\mathrm{d}m(u)\ . \tag{2.4.93}$$

Note that moving the functional $Q^{(n)}$ inside the integral is not a trivial step because it's not obvious that the kinetic energy part is affine linear, but it is true. (This part too is a technical point that can be found in [Kie10]. Then

$$e_\infty\geq\limsup_{N\to\infty}\frac{E_N}{N}=\limsup_{l\to\infty}\frac{1}{N_{k_l}}Q^{(N_{k_l})}(\mu^{(N_{k_l})})\geq\frac{1}{n}Q^{(n)}(\nu^{(n)})=\int_{\mathcal{P}(\mathbb{R}^3)}h_n(u)\mathrm{d}m(u)\ . \tag{2.4.94}$$

Taking an n limit:

$$e_\infty\geq\int_{\mathcal{P}(\mathbb{R}^3)}h_\infty(u)\mathrm{d}m(u)\geq e_\infty\ . \tag{2.4.95}$$

This shows that the inequalities in the chain above must all be equalities and in particular

$$\lim_{N\to\infty} \frac{E_N}{N} = e_\infty \ . \tag{2.4.96}$$

Furthermore, the integral $\int_{\mathcal{P}(\mathbb{R}^3)} h_\infty(u)\mathrm{d}m(u)$ can only ever be equal to e_∞ if m is supported on minimizers of h_∞ (and there's only one, which we called u_∞ above). Hence

$$m = \delta_{u_\infty} \tag{2.4.97}$$

and the de Finetti statement about the weak limits $\nu^{(n)}$ becomes

$$\lim_{l\to\infty} \mu_n^{(N_{k_l})}(\boldsymbol{q}) = u_\infty(q_1)\cdots u_\infty(q_n) \quad \text{for all } n \ . \tag{2.4.98}$$

Looking back carefully, what we have proved is that **every** subsequence N_k admits a further subsubsequence N_{k_l} such that the limit above is true for all n. Since the limit object, $u_\infty^{\otimes n}$, is independent of (N_k), this is enough to prove that

$$\lim_{N\to\infty} \mu_n^{(N)} = u_\infty^{\otimes n} \quad \text{for all } n \ . \tag{2.4.99}$$

2.4.4 Adaptation to conjecture 2.4.2

Let us see what happens if the proof strategy outlined above is attempted for our conjecture.

Proposition 2.4.8. *We have*

$$\limsup_{N\to\infty} \frac{E_N}{N} \le e_\infty \ . \tag{2.4.100}$$

Proof. Let $\varepsilon > 0$. Find a $u \in \mathcal{P}(\mathbb{R}^3)$ for which the Theorem (2.4.6) applies and such that

$$h_\infty(u) < e_\infty + \frac{\varepsilon}{2} \ . \tag{2.4.101}$$

The theorem implies that there is N such that

$$\int \frac{u(\xi_1)\cdots u(\xi_N)}{|\xi_1 - C\overline{\boldsymbol{\xi}}|} > \int \frac{u(x)}{|x|} - \frac{\varepsilon}{2} \ . \tag{2.4.102}$$

Plug in the trial function $\rho^{(N)} = u^{\otimes N}$ into $Q^{(N)}$:

$$
\begin{aligned}
\frac{1}{N}Q^{(N)}(u^{\otimes N}) &= \int |\nabla\sqrt{u}|^2 - \left(\frac{1}{N}\sum_{j=1}^{N}\int \frac{u(\xi_1)\cdots u(\xi_N)}{|\xi_j - C\overline{\boldsymbol{\xi}}|}\mathrm{d}\boldsymbol{\xi}\right) + \frac{1}{2}\left(1-\frac{1}{N}\right)\iint \frac{u(x)u(y)}{|x-y|}\mathrm{d}x\mathrm{d}y \\
&\le \int |\nabla\sqrt{u}|^2 - \left(\frac{1}{N}\sum_{j=1}^{N}\int \frac{u(\xi_1)}{|\xi_1|}\mathrm{d}\xi_1 - \varepsilon/2\right) + \frac{1}{2}\iint \frac{u(x)u(y)}{|x-y|}\mathrm{d}x\mathrm{d}y \\
&= h_\infty(u) + \frac{\varepsilon}{2} \\
&\le e_\infty + \varepsilon
\end{aligned}
\tag{2.4.103}
$$

Since ε is arbitrary, the infimum $E(N)/N$ of the expression $(1/N)Q^{(N)}(\rho^{(N)})$ can be at most $\le e_\infty$.

□

A similar lemma to 2.4.7 now needs to be proved. The rest of the argument shown in section 2.3 after it is transferable word-by-word. Hence the sticking point is the statement analogous to that lemma, which is the following:

Conjecture 2.4.9. *For a fixed n, suppose that a sequence $\rho^{(N_k)} \in \mathcal{P}_{Sym}(\mathbb{R}^{3N_k})$ is such that*

$$
\lim_{k\to\infty} \sqrt{\rho_n^{(N_k)}} = \sqrt{\nu^{(n)}} \quad \text{weakly in } H^1(\mathbb{R}^{3n}) \ . \tag{2.4.104}
$$

Then, for the functional $Q^{(N)}$ given in (2.4.1),

$$
\limsup_{k\to\infty} \frac{1}{N_k} Q^{(N_k)}(\rho^{(N_k)}) \ge \frac{1}{n} Q^{(n)}(\nu^{(n)}) \ . \tag{2.4.105}
$$

A proof of this conjecture would imply that conjecture 2.4.2 is true. To try to prove it, fix an n. The kinetic energy and Coulomb repulsion parts of our energy functional are the same as for the one in section 2.3. But, when dealing with the Coulomb attraction part (after replacing the sum $\frac{1}{N_k}\sum_{j=1}^{N_k}\int \frac{\cdots}{|\xi_j - \cdots|}$ with $\int \frac{\cdots}{|\xi_1 - \cdots|}$, which is granted by symmetry), we need to prove that

$$
\limsup_{k} \left(- \int_{\mathbb{R}^{3N}} \frac{\rho^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_{N_k}}|} \right) \ge - \int_{\mathbb{R}^{3n}} \frac{\nu^{(n)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_n}|} \ , \tag{2.4.106}
$$

or, what is the same,

$$
\liminf_{k} \int_{\mathbb{R}^{3N}} \frac{\rho^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_{N_k}}|} \le \int_{\mathbb{R}^{3n}} \frac{\nu^{(n)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_n}|} \ . \tag{2.4.107}
$$

Here the notation of empirical average with a subindex indicates the number of variables involved:

$$\overline{\boldsymbol{\xi}_m} = \frac{\xi_1 + \cdots + \xi_m}{m} \ . \tag{2.4.108}$$

By assumption, we have

$$\lim_{k\to\infty} \int_{\mathbb{R}^{3N}} \frac{\rho^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_n}|} = \lim_{k\to\infty} \int_{\mathbb{R}^{3n}} \frac{\rho_n^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_n}|} = \int_{\mathbb{R}^{3n}} \frac{\nu^{(n)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_n}|} \ . \tag{2.4.109}$$

Hence (2.4.107) is equivalent to

$$\liminf_k \int_{\mathbb{R}^{3N}} \frac{\rho^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_{N_k}}|} \le \lim_k \int_{\mathbb{R}^{3N}} \frac{\mu^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_n}|} \ , \tag{2.4.110}$$

which is now a statement about a general sequence of measures (but not any sequence; we know their n marginals converge, and we may even assume this is true for all n). This is now a problem about understanding what happens with the integral

$$\int_{\mathbb{R}^{3N}} \frac{\rho^{(N_k)}}{|\xi_1 - C\overline{\boldsymbol{\xi}_m}|} \tag{2.4.111}$$

when we let m grow together with N_k versus when we hold m fixed.

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