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# SYMPLECTIC-N IN STRONGLY CORRELATED MATERIALS

by

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## **ABSTRACT OF THE DISSERTATION**

# Symplectic-N in strongly correlated materials

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Strong correlations between electrons often generate unexpected new collective behavior that we call *emergent phenomena*. Strong interactions can ramp up the relevant scales, creating massive electrons in heavy fermion materials and high transition temperatures in superconductors, or lead to entirely new states of matter with low energy excitations containing a fraction of the original electron. These phenomena provide unique challenges to theorists as they sit at the intersection of kinetic and potential energy scales, where perturbative many body techniques fail.

One useful method here is the large N approach, which generalizes the number of components of the electron spin from 2 to N, providing an artificial perturbation expansion about a strongly correlated state which, if chosen properly, captures the essential physics. To do so, we must ensure that the large N limit maintains the important symmetries. While SU(N) is the traditional large-N limit, not all SU(N) spins invert under time-reversal for N > 2. To treat phenomena like frustrated magnetism and superconductivity that contain particle-particle singlets, we must restrict ourselves to the subgroup of time-reversing spins, SP(N), a large N limit we call symplectic-N.

The correspondance of time-reversal and symplectic symmetry, and its consequences for spin and Hubbard operator representations are discussed in Chapter 2, which provides the mathematical backbone of this dissertation. Chapter 3 develops a symplectic-N treatment of frustrated magnetism, treating ferromagnetic and antiferromagnetic correlations on equal footing, before we move on to unconventional superconductivity. First we show how composite pairs, bound states between local moments and conduction electrons in two orthogonal symmetry channels, emerge from the large N limit of the two channel Kondo model in Chapter 4, and then discuss how composite pairing interacts cooperatively with magnetic pairing in Chapter 5. In Chapter 6, we examine the interplay of composite pairing and valence fluctuations in the two-channel Anderson model. Finally, Chapter 7 studies the effect of Coulomb repulsion on  $s_{\pm}$  pairing in a t - J model of the iron-based superconductors.

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# **Table of Contents**

Abstract				ii
Ac	know	ledgem	ents	iv
Li	st of H	igures		viii
1.	Intro	oductio	<b>n</b>	1
	1.1.	Magne	tism	7
		1.1.1.	Frustration and spin liquids	8
	1.2.	Heavy	Fermion Physics	12
		1.2.1.	The Kondo model	13
		1.2.2.	RKKY coupling, competition and criticality	16
		1.2.3.	Heavy Fermion Superconductivity	18
		1.2.4.	Two channel Kondo impurities	19
		1.2.5.	Valence fluctuations and the Anderson model	21
		1.2.6.	The infinite- $U$ Anderson model and Hubbard operators	24
	1.3.	Adding	g charge fluctuations to a Heisenberg magnet	25
		1.3.1.	Strongly correlated insulators	26
		1.3.2.	Doping a Mott insulator	28
2.	Spin	s, time	reversal and symplectic symmetry	31
	2.1.	What i	s a spin?	31
	2.2.	Time r	eversal in $SU(2)$	33
	2.3.	Time r	eversal in large $N$	34
	2.4.	Decou	pling Spin Hamiltonians	37
	2.5.	Staying	g in the physical subspace: constraints	41
		2.5.1.	Fermionic constraints and SU(2) symmetry	41

		2.5.2.	Bosonic constraints	44
	2.6.	Hubba	rd Operators	46
	2.7.	Symple	ectic Hubbard operators	49
3.	Frus	strated	magnetism	52
		3.0.1.	Previous large $N$ treatments of the Heisenberg model	53
	3.1.	Time r	eversal and symplectic symmetry	56
		3.1.1.	Ground States	59
		3.1.2.	Spin dynamics	61
	3.2.	Solvin	g the symplectic- $N$ Heisenberg model	63
		3.2.1.	Simple Example	68
		3.2.2.	Examining the Ground State	69
	3.3.	Illustra	tion: $J_1 - J_2$ model	71
		3.3.1.	Valence bond structure	73
		3.3.2.	T=0 phase diagram	73
		3.3.3.	Finite Temperatures: the Ising transition	75
			Analytical form of $T_{RVB}$	77
	3.4.	Discus	sion and Conclusions	80
4.	The	two cha	annel Kondo model	86
	4.1.	. Introduction		86
		4.1.1.	The two channel Kondo model	87
		4.1.2.	Spins and large $N$	91
			Large N solution of the $SU(N)$ Kondo model $\ldots \ldots \ldots \ldots \ldots$	92
			Symplectic- <i>N</i>	93
	4.2.	The sy	mplectic- $N$ two channel Kondo lattice $\ldots$	95
		4.2.1.	Composite pairing	99
		4.2.2.	Resonant Andreev scattering	100

		4.2.3. Solving the mean field theory	103	
		4.2.4. Landau theory of composite pairing	107	
	4.3.	Experimental consequences	109	
5.	Tano	lem Pairing and the Cerium 115s	119	
	5.1.	Introduction	119	
	5.2.	Internal structure of a heavy fermion pair	122	
	5.3.	The two channel Kondo-Heisenberg model	124	
	5.4.	Experimental consequences	127	
6.	Sym	plectic Anderson models	134	
	6.1.	Introduction	134	
		6.1.1. The infinite- $U$ Anderson model and Hubbard operators	138	
	6.2.	Symplectic Hubbard operators	141	
	6.3.	The two channel Anderson model	145	
	6.4.	The large $N$ two channel Anderson model $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	148	
		6.4.1. The mean field solution	150	
	6.5.	Charge Redistribution	154	
	6.6.	Conclusions	159	
7.	The	symplectic t-J model	163	
	7.1.	Introduction	163	
		7.1.1. Brief overview of the iron-based superconductors	164	
		7.1.2. $t - J$ model and the Coulomb pseudopotential	166	
	7.2.	The symplectic $t - J$ model $\ldots$ $\ldots$ $\ldots$ $\ldots$ $\ldots$ $\ldots$ $\ldots$ $\ldots$	169	
	7.3.	Mean field solutions	176	
	7.4.	Conclusions	179	
Re	<b>References</b>			
Cu	<b>Curriculum Vita</b>			

# List of Figures

1.1.	Quasiparticles and collective excitations in electron gases.	2
1.2.	Three examples of strongly correlated materials	3
1.3.	Strongly correlated electrons on a lattice	5
1.4.	The large $N$ limit $\ldots$	6
1.5.	Illustrating frustration	9
1.6.	Valence bonds	10
1.7.	The $J_1$ - $J_2$ model and order from disorder	11
1.8.	The Kondo effect: resistance minima and formation of the Kondo resonance	13
1.9.	Hybridization between composite fermions and conduction electrons	16
1.10.	Fermi surface jump in CeRhIn <sub>5</sub> .	17
1.11.	The RKKY interaction and the Doniach Kondo lattice phase diagram	18
1.12.	Comparing the susceptibilities of $UPt_3$ and $CeCoIn_5$ .	20
1.13.	Atomic energy levels and the relationship between f-electron valence and the chem-	
	ical potential.	22
1.14.	The Anderson model and f-electron density of states.	24
1.15.	Localization versus itineracy	27
1.16.	The Hubbard model and superexchange	28
1.17.	Schematic phase diagrams of cuprate and iron-based high temperature supercon-	
	ductors, and a discussion of superconducting gaps.	29
2.1.	The three different types of spins found in real materials: Ising, XY, and Heisenberg.	32
2.2.	The time reversal operator, $\theta$ and rotation operators U acting on a spin must commute.	34
2.3.	The symplectic plane	47
2.4.	Hubbard operators	48
3.1.	The various large $N$ techniques in magnetism.	54

3.2.	Valence bond picture of antiferromagnetism and ferromagnetism	57
3.3.	Ground states of the $SU(N)$ spins	60
3.4.	Integrating out fluctuations along real and imaginary axes	65
3.5.	Valence bond states of the $J_1 - J_2$ model	72
3.6.	Critical spin of the $J_1 - J_2$ model for symplectic-N, $SP(N)$ and spin waves	74
3.7.	Finite temperature phase diagram for $J_1 - J_2$ model	77
3.8.	Triangular and tetragonal plaquettes	81
3.9.	Calculating the first order phase transition in the $J_1 - J_2$ model	84
4.1.	Evidence for local moment behavior in NpPd $_5Al_2$ down to the superconducting	
	transition.	86
4.2.	Microscopic origins of a two channel Kondo impurity	89
4.3.	Adding a composite pair.	99
4.4.	Scattering processes that lead to Kondo hybridization and composite pairing	101
4.5.	Three possible composite pairing gaps	103
4.6.	Composite pair phase diagram	106
4.7.	Leading Feynman diagrams responsible for composite pairing in the two-channel	
	Kondo lattice.	109
4.8.	Upturn in the NMR relaxation rate.	110
4.9.	NMR relaxation rate diagram.	118
5.1.	Local moments in the Curie-Weiss susceptibilities of $CeCoIn_5$ and $NpPd_5Al_2$	120
5.2.	Two domes in the Ce 115 superconductors.	121
5.3.	A tandem pair contains a superposition of magnetic and composite pairing	122
5.4.	The superconducting transition temperature as the RKKY and second Kondo chan-	
	nel couplings vary.	127
5.5.	A possible experimental path through the phase diagram in Figure 5.4, chosen for	
	its similarity to the Ce 115 phase diagram.	129
5.6.	Predicted NQR frequency shift in $CeMIn_5$ .	130

6.1.	Atomic states of a two channel Anderson impurity	135
6.2.	Hilbert space of the two channel Anderson model	147
6.3.	Example phase diagram for the two channel Anderson model	153
6.4.	Mixed valence increases the superconducting transition temperature	154
6.5.	The f-electron valence changes with temperature, with a sharp shift at $T_c$	156
6.6.	Crystal structure of $CeCoIn_5$	158
7.1.	Structure of the FeAs plane, schematic Fermi surface and phase diagram of the	
	iron-based superconductors.	166
7.2.	d-wave and $s_{\pm}$ superconducting gaps	168
7.3.	Relationship between spin and charge fluctuations in the $t - J$ model $\ldots \ldots$	172
7.4.	Gap symmetries for the $J_1 - J_2$ model	174
7.5.	Superconducting transition temperatures for the $t_1 - J_2$ model	177
7.6.	Superconducting transition temperatures for the $t_1 - t_2 - t_3 - J_2$ model	178

# **Chapter 1**

## Introduction

Why is the collective behavior of macroscopic numbers of electrons such a fundamental and exciting problem? After all, the behavior of individual electrons is incredibly well described by quantum electrodynamics. However, when we put 10 or 1000 or  $10^{23}$  electrons together, we can get wildly different behavior that could not have been predicted from quantum electrodynamics, and yet can be described in surprisingly simple and beautiful terms. This idea, that "more is different" [1] is the driving force behind the study of these *emergent phenomena*.

The physics of macroscopic numbers of weakly interacting electrons is fairly well understood, although the field still has some surprises [2]. Free electrons have an energy dispersion,  $\epsilon_k = k^2/2m$ , and at zero temperature, electrons occupy all possible states from zero up to the Fermi energy,  $\epsilon_F$ , set by the total number of electrons. The low energy excitations of the free electron gas are still electrons, excited out of the Fermi sea, or holes, which are missing electrons below the Fermi energy. Amazingly, introducing weak to moderate electron-electron interactions changes relatively little: the low energy excitations are still electron-like *quasi-particles*, which have all the quantum numbers (spin, charge, and momentum) of the original free electrons. Increasing interactions renormalize the mass of the electron - a moving electron increases its inertial mass by scattering off other electrons [3]. While the excitations at low energies are electron-like, there are collective modes at high energies called plasmons, which are quantized oscillations in the charge density [4], shown in Figure 1.1.

In systems with strong interactions, the energy scales of the electron-like and collective excitations can swap, and the low energy excitations are collective modes that look nothing like electrons. Just such a swap happens in the Luttinger liquid - the one dimensional version of an interacting electron gas. Here, the low dimensionality makes any interaction a strong interaction, and the low energy excitations of the Luttinger liquid are charge and spin density waves [5, 6]. The electron has



Figure 1.1: (a) Plasmons are quantized collective charge oscillations where the electrons slide as a whole while the positive ions providing a restoring force; the plasma frequency,  $\omega_p$  is the minimum energy required to excite a plasmon. (b) The low energy excitations of the 2D electron gas are particle-hole pairs that occur when an electron is excited out of the filled Fermi sea, leaving behind a hole. There is a continuum of these excitations, shown in green. In two dimensions, low energy excitations are possible for any momentum because the difference in momentum between particle and hole can span the Fermi surface. (c) In one dimension, the Fermi surface consists of two Fermi points, and there are only low energy particle-hole pairs for  $k = 0, 2k_F$ . (d) Instead, the low energy excitations of one dimensional metals, or *Luttinger liquids* are fractionalized spinons and holons. Holons are the absence of an electron on a site - a charge moving alone, while spinons are domain walls between two antiferromagnetic domains that move by flipping a single spin, leaving the charge distribution unchanged.

been *fractionalized*, and now its charge and spin are separate excitations. This situation, where the low energy excitations are not adiabatically connected to the free constituent particles is the norm in strongly correlated matter.

In fact, this fractionalization can be even more extreme: in very pure, two-dimensional interacting electron gases at extremely high magnetic fields and extremely low temperatures, the fractional quantum hall effect occurs. Fractional quantum hall states, indexed by rational numbers  $\nu$ , contain low energy excitations with both fractional charge and statistics [see Figure 1.2 (a)]. When one particle is moved around another in two dimensions, the wavefunction acquires a phase  $e^{i\theta}$ , where  $\theta = 0$  or  $\pi$  for bosons and fermions, respectively. The excitations of the  $\nu = 1/3$  fractional quantum Hall state have charge e/3 and  $\theta = \pi/3$  [7]. Other fractional quantum hall states are believed to have *non-Abelian* statistics, where the phase becomes a matrix and the final phase of a three particle wavefunction depends how they are moved around one another - a topological property potentially useful for quantum computing [8].



Figure 1.2: Three strongly correlated materials. (a) Some low energy excitations found in strongly correlated systems are found nowhere else. Fractional quantum Hall states contain excitations with a fraction of the electron charge: the  $\nu = 1/3$  state has  $e^* = e/3$ ; these particles also have fractional statistics, where taking one particle around another changes the phase of the wavefunction by  $\pi/3$ . The transverse conductivity,  $\sigma_{xy} = \nu e^2/h$  is quantized, where  $\nu$  is a rational number. (Reproduced from Stormer [7]). (b) Schematic phase diagram of the heavy fermion superconductors, CeMIn<sub>5</sub> (M =Co,Rh,Ir). At high temperatures, these materials contain localized spins in a sea of free electrons, but interactions between these components generates a rich phase diagram at low temperatures, easily tuned between antiferromagnetism and heavy fermion superconductivity. (Adapted from Pagliuso *et al.* [9]). (c) The resistance of normal metals is quadratic at very low temperatures before crossing over to a different power law. Optimally doped La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> is an unconventional superconductor whose resistance is linear over *nearly three decades* above  $T_c$ , from 35K to 800K. The origin of this linear resistance is still a mystery. (Reproduced from Takagi *et al.* [10].)

But most strongly correlated materials are not quite this bizarre. The most common effect of strong interactions is to strip the electron of its charge degrees of freedom. Let us examine a simple model, where we have a "half-filled" lattice of  $\mathcal{N}$  sites on which  $\mathcal{N}$  electrons can sit. Electrons hop between sites, gaining kinetic energy, but when two electrons sit on the same site, the Coulomb repulsion costs potential energy. A site generically has four possible states: empty, one electron, with its spin up or down, and doubly occupied, where the two electrons must have opposite spin. As the strength of the Coulomb repulsion increases, the number of doubly occupied sites is eventually suppressed to zero. Since there are an equal number of electrons and sites, each site has only two possible states: where the spin of the electron is up or down. We call this localized electron a spin, as it has lost all of its charge degrees of freedom, and such a strongly correlated insulator is called a Mott insulator [11, 12]. Spins are neither fermions nor bosons, instead obeying the commutation relations of the Pauli matrices,  $[S_a, S_b] \propto S_c$ , and they are the building blocks of many strongly correlated materials:

- Magnetism: Interacting spins in a Mott insulator will usually order antiferromagnetically, ↑↓↑↓ …. In these materials spins behave like bosons, as they condense into an ordered ground state. If these interactions are frustrated enough, the spins can evade long range ordering down to zero temperature, instead forming a highly correlated quantum state with no broken symmetries known as a spin liquid, whose excitations are further fractionalized into bosonic or fermionic spinons, shown in Figure 1.3(c).
- Heavy fermion physics: Adding a small concentration of spins to a weakly interacting metal can drastically alter its properties. While copper is a boring metal, adding 14% spins makes CeCu<sub>6</sub>, a heavy fermion metal with an effective electron mass over one thousand times that of copper [13]. These spins lost their charge degrees of freedom at very high temperatures, yet at low energies they again form electron-like quasiparticles with the aid of the weakly interacting electrons [Figure 1.3(a)]. They are very sensitive to their environment; changing the material structure slightly can turn a heavy Fermi liquid into an antiferromagnet or a superconductor [see Figure 1.2 (c)].

• Unconventional superconductivity: Conventional superconductivity is an instability of weakly correlated metals, where the electrons attract one another by exchanging phonons [14]. Doping a Mott insulator, as shown in Figure 1.3(b) leads to unconventional superconducting states whose basic interaction is the repulsive Coulomb interaction, and yet have far higher transition temperatures [15]. The phases surrounding the superconducting dome can be even stranger, indicating metals whose constituent particles are not electrons [see Figure 1.2(b)].



Figure 1.3: (a) At high temperatures, heavy fermion materials consist of free spins immersed in a sea of non-interacting conduction electrons. At low temperatures, the spins hybridize with the conduction electrons to form mobile, heavy electrons with masses 100 to 1000 times that of the bare electrons. (b) A doped Mott insulator contains holes hopping in an antiferromagnetic background. For high enough doping, these materials become superconducting. (c) Instead of ordering magnetically, Mott insulators on frustrated lattices may become *spin liquids*, which consist of spin singlet valence bonds (blue) between sites. Excitations are created by breaking valence bonds to form two spin 1/2 spinons.

Strongly correlated problems are especially challenging to theorists, as they tend to sit at the intersection of the kinetic and potential energy scales, where neither real space nor momentum space capture the entire picture. Put simply, these problems lack a natural small parameter to expand about

an exactly solvable non-interacting state, and new theoretical methods must be devised to treat them. The search for simple, controlled approximations which capture the collective behavior of strongly correlated electrons is a key goal of condensed matter theorists. This thesis introduces one such approximation scheme, the *symplectic large N limit* and explores its consequences in several areas of strongly correlated electrons.

The idea behind the large N approach is to take the strongly correlated model of interest and generalize it to a family of models, where the number of internal degrees of freedom is indexed by an integer N. As N goes to infinity, central limit effects allow the underlying collective behavior of the model to be solved exactly (shown in Figure 1.4. Corrections to this strongly correlated mean field theory may then be obtained from a power series expansion in 1/N, where 1/N now acts as an artificial small parameter.



Figure 1.4: The partition function, Z is given by a sum over the possible paths of the fields  $\Psi(\vec{x}, \tau)$ , where each path is weighted by an exponential of the action,  $\exp(-S[\Psi])$  of that path. In the large N limit, the action becomes extensive in N, and is dominated by the path with the smallest action, known as the saddle point path. Fluctuations around the saddle point path are controlled by 1/N.

Witten originally introduced the idea of large N to treat quantum chromodynamics [16], where quarks have an SU(3) symmetry, which Witten replaced with a theory of SU(N) symmetric quarks.

The symmetry of spins can also be generalized, from SU(2) to some larger group - SU(N) is one possibility, but so is the symplectic group, SP(N). SU(N) expansions are extremely useful to particle physicists because there are two types of color singlets: mesons, which are particleantiparticle pairs, or in condensed matter, particle-hole pairs, and baryons, which are products of N particles, forming three quark baryons for SU(3). There is no condensed matter analog for N > 2, and the condensed matter version of SU(N) has only particle-hole pairs. However, the group SP(N) has both particle-hole and particle-particle singlets, which pair a particle with its time reversed twin - e.g. valence bonds [17] or Cooper pairs [18]. The existence of these welldefined singlets is guaranteed by maintaining the inversion of spins under time reversal as the group is generalized from SU(2) to SP(N). The large N limit describing Hamiltonians built exclusively out of these time-reversing, symplectic spins is what we call symplectic-N.

The rest of this introduction reviews the three areas of physics where we apply symplectic-*N*: quantum magnetism, heavy fermion physics, and the unconventional superconductivity originating from doped Mott insulators.

#### 1.1 Magnetism

First, we will discuss insulating magnetic materials derived from Mott insulators, where the spins are arranged in a lattice. Spins at sites i and j interact with each other though an exchange coupling,  $J_{ij}$ . Such systems are described by the Heisenberg model,

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j, \tag{1.1}$$

where  $\vec{S}_j$  is a Heisenberg spin,  $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$  at site *j*. The exchange couplings,  $J_{ij}$  arise from virtual charge fluctuations, known as *superexchange*, where the electron making up a spin at site *i* hops to a nearby site *j*, either directly or through other atoms, and then back again [19].  $J_{ij}$  can be positive or negative, depending on the superexchange path. The simplest lattices are either ferromagnets (all J's < 0) or bipartite antiferromagnets, which can be partitioned into two sublattices, where the only

antiferromagnetic (J > 0) couplings are between sublattices [see Figure 1.5 (a)].

At high temperatures, the spins are free, with a Curie-Weiss-like magnetic susceptibility,

$$\chi(T) = \frac{\mu_{eff}^2}{3k_B \left(T - \theta_{CW}\right)},$$
(1.2)

where  $\mu_{eff}$  is the effective moment,  $\mu_{eff}^2 = g^2 S(S + 1)$ , and  $\theta_{CW} \approx -J$ . Simple lattices develop long range magnetic order at  $T_c \sim \theta_{CW}$  (for ferromagnets) or  $T_N \sim |\theta_{CW}|$  (for antiferromagnets). Dimensionality and geometric frustration can suppress these ordering temperatures far below  $|\theta_{CW}|$ , and the region between  $T_N$  and  $|\theta_{CW}|$  is characterized by strong spin correlations, but no broken symmetries [20]. This region is known as a *spin liquid*, in analogy with liquids like water, which also do not break translational or orientational symmetries, and yet are more strongly correlated than a gas. The free spins above  $|\theta_{CW}|$  could analogously be called a spin gas. While a great deal of experimental and theoretical effort has been made to find materials with a spin liquid *ground state*, the jury is still out [21, 22]. Despite the lack of concrete examples, spin liquids have long attracted great interest because of the high temperature superconductivity found in Heisenberg magnets doped with charged holes, which have a similar frustrating effect. Spin liquids also have intrinsic interest as a state of matter not described in terms of the usual symmetry breaking paradigm, which may require topological order parameters.

#### **1.1.1** Frustration and spin liquids

Spin liquid states were first introduced by Anderson [17], who posited that instead of forming a long range antiferromagnetic state, pairs of neighboring spins,  $\langle ij \rangle$  will form local singlets known as *valence bonds*:  $\Delta_{ij} = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)$ . These valence bonds can be arranged in a lattice, forming a *valence bond solid*, which breaks the lattice symmetry (and is thus not a spin liquid), but not time reversal or spin rotation symmetries [Figure 1.6 (a)]. Or the ground state can be a superposition of all possible configurations, forming a *resonating valence bond* (RVB) state [Figure 1.6 (b)], which breaks no symmetries, and is the spin liquid thought to underlie the cuprate superconductors



Figure 1.5: (a) The two simple ground states: a ferromagnet and a bipartite antiferromagnet, which can be partitioned into two sublattices (red and blue). (b) A frustrated triangle: J is antiferromagnetic each link, yet once the first two spins are anti-aligned, the third spin can rotate freely without any energy cost (left). The compromise ground state of the triangular lattice involves spins rotated by  $120^{\circ}$  (right). (c) Three examples of frustrated lattices: the  $J_1 - J_2$  square lattice, where both nearest ( $J_1$ ) and next-nearest ( $J_2$ ) neighbor bonds are antiferromagnetic, and two geometrically frustrated lattices, the triangular and Kagomé, where all bonds are antiferromagnetic. The less connected the lattice, the greater the frustration.

[23, 24].

Geometric frustration is essential to stabilize spin liquid states in more than one dimension [20, 21, 22]. Any non-bipartite lattices will be *frustrated*, as no spin arrangement simultaneously satisfies all exchange couplings, as can be shown simply in a triangular plaquette: when any two spins are anti-parallel, the exchange couplings with the third spin cancel one another, and it is completely free [Figure 1.5 (b)]. However, the triangular lattice does order at zero temperature, forming three sublattices with 120° order. When discussing one and two dimensional systems, we generally mean *quasi*- one and two dimensional systems. As shown by Mermin and Wagner [25], no continuous symmetry [like the SU(2) spin symmetry] may be broken at any finite temperature in less than three dimensions. Real materials will always have some weak coupling in the third dimension, giving rise to a finite ordering temperature, and this temperature is the one strongly suppressed by frustration. Additional exchange couplings also lead to frustration, as in the  $J_1 - J_2$  square lattice.  $J_1$  connects nearest-neighbor sites in different sublattices, while  $J_2$  couples spins within the same sublattice. For



Figure 1.6: If a system does not develop long range magnetic order, the spins may form valence bonds,  $\Delta_{ij} = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)$ , indicated by the blue bonds. These valence bonds can either form a valence bond solid (a), where 2S bonds emanate from each site, or exist in a superposition of all possible configurations, forming a resonating valence bond state (b).

antiferromagnetic  $J_2 \gg J_1$ , the  $J_1$  couplings cancel, and the classical ground state consists of two decoupled *antiferromagnetic* sublattices [Figure 1.7]. Thermal and quantum fluctuations select out the collinear states from the degenerate ground state manifold [26], a phenomena known as *order by disorder* [27, 28, 29].

The Heisenberg model has one energy scale, J, and the J = 0 state is that of extensively degenerate free spins. There are therefore no natural small parameters with which to conduct perturbation theory, and the Heisenberg model is a prime candidate for large N expansions. Since spins do not satisfy canonical commutation relations, like bosons and fermions, they cannot be treated directly in quantum field theory, and must instead by represented by bilinears of fermions and bosons chosen to satisfy the commutation relations of the spin group.

Large N theories were first introduced in quantum magnetism by Berlin and Kac, who solved the spherical model of ferromagnetism exactly in a large N limit [30]. Simultaneously, Anderson, Dyson and Maleev introduced spin wave theory, which takes the spin S to be large and expands in 1/S [31, 32, 33]. The large S limit is a classical limit, where the spins behave like classical vectors, rotating under the group O(3). The long wavelength fluctuations of quantum spins were studied semi-classically in the nonlinear sigma model [34, 35], where quantum renormalizations to the classical parameters were calculated in the large N limit by extending the order parameter



Figure 1.7: (a) When  $J_2$  is large, the spins anti-align in two antiferromagnetic sublattices. Classically, the exchange coupling between these two sublattices,  $J_1 \vec{S}_i \cdot \vec{S}_j$  cancels, and the two sublattices are decoupled at zero temperature. (b) Thermal and quantum fluctuations are softest around the collinear states, and the system will spend the most time fluctuating about these states. Collinear order is thus selected by these *disordering* fluctuations.

manifold of SU(2) spins,  $CP^1$  to that of SU(N) spins,  $CP^{N-1}$  [36].

The large N quantum limit of magnetism was first treated by Affleck and Marston [37, 38]. They used a fermionic spin representation to treat the S = 1/2 Hubbard and Heisenberg models by extending SU(2) to SU(N), preserving the rotational invariance of the Hamiltonian under SU(N). Since then, other extensions of SU(2) have been used, including SP(2N) by Ran and Wen [39]. Fermionic large N theories capture the physics in the extreme quantum limit,  $S/N \ll 1$ , where the ground state is always disordered. These are useful for studying the possible spin liquid ground states [40], but not for determining if a particular model is a spin liquid in the first place. For that, one needs a bosonic spin representation, where magnetic long range order corresponds to the condensation of the bosons. Arovas and Auerbach introduced the bosonic SU(N) theory [41], which can treat arbitrary ratios of S/N, and both magnetically ordered and disordered states. This theory was quite successful at describing ferromagnets and bipartite antiferromagnets, but is unable to treat frustrated magnets. To resolve this, Sachdev and Read extended the theory to arbitrary antiferromagnetic bonds by limiting the rotational invariance to the group SP(N) [42]. However, neither of these theories preserve the time inversion properties of spins, because for N > 2, not all SU(N) spins invert under time reversal. Although Sachdev and Read's Hamiltonian is invariant under SP(N) rotations, it still contains SU(N) spins with the wrong parity under time reversal. Symplectic-N identifies time reversing spins with the generators of SP(N), and then builds interactions exclusively from these symplectic spins. This condition is more stringent than Sachdev and Read's, and leads to a unique large N limit. In Chapter 3, we develop the bosonic symplectic-N approach for the Heisenberg model, which enables us to treat ferromagnetism and antiferromagnetism on equal footing.

#### **1.2 Heavy Fermion Physics**

At high temperatures, local magnetic moments immersed in a metallic host will scatter the conduction electrons in two ways: ordinary potential scattering events leaving the spins of both the local moment and the conduction electron unchanged, and spin-flip scattering events swapping the two spins. As the temperature decreases, these spin-flip events favor the development of a cloud of conduction electrons anti-parallel to the spin, which in turn intensifies the spin flip scattering. This *anti-screening* effect makes the antiferromagnetic interaction between local moments and conduction electrons scale to strong coupling. At high temperatures, the moment is *asymptotically free*: decoupled from the conduction sea, while at low temperatures it is completely compensated by the cloud of conduction electrons, forming a *Kondo singlet* [43, 44]. The Kondo crossover temperature,  $T_K$  separates these two behaviors.

When the local moment is mostly screened, scattering electrons see only a large singlet state acting as a potential scattering center with a very large cross section. As the local moment must bind the equivalent of one conduction electron to form a singlet, the Friedel sum rule, which relates the charge bound by a potential scatterer, Q = 1 to its phase shift at the Fermi energy,  $\delta(\epsilon_F)$ :  $\sum_{\sigma} \frac{\delta_{\sigma}(\epsilon_F)}{\pi} = 1$  indicates that the Kondo singlet is a *resonant* bound state ( $\delta_{\sigma}(\epsilon_F) = \pi/2$ ) [45, 46] pinned to the Fermi energy [47], illustrated in Figure 4.27(a).

The formation of the Kondo resonance has a well-known set of physical consequences. Most



Figure 1.8: (a) At high temperatures, the spin and conduction electrons are decoupled, but at low temperatures the Kondo resonance results as the local moment binds a single conduction electron to form a local singlet bound state (Reproduced from [48]). (b)Here we show the resistivity,  $\rho(T)$  of  $Ce_xLa_{1-x}Cu_6$ . La is a non-magnetic analog of Ce, so x is the concentration of Kondo impurities. For low concentrations, the resistivity reaches a maximum at low temperatures as the spin-flip scattering off the impurity saturates. For larger concentrations the impurities form a Kondo lattice and the scattering off different impurities becomes coherent, and begins to decrease as a heavy Fermi liquid is formed [49].

notably, while the resistivity at high temperatures decreases with temperature as the phonon and impurity potential scattering contributions decrease, the spin-flip scattering begins to increase around  $T_K$ , leading to the characteristic Kondo resistance minimum [43, 44]. The resistance reaches a maximum when the local moment is completely quenched, shown in Figure 4.27(b). The impurity contributions to the zero temperature specific heat coefficient,  $\gamma = \lim_{T\to 0} C/T$  and susceptibility,  $\chi(T = 0)$  resemble those of a very heavy conduction electron [50], where the bandwidth, D has been replaced by the exponentially smaller  $T_K$ .

#### **1.2.1** The Kondo model

The formation of local moments from strongly interacting electrons was first introduced in the Anderson model [51]. However, most of the interesting low energy physics comes from spin fluctuations, contained in the Kondo model: the low energy limit of the Anderson model [52, 53] neglecting charge fluctuations. So we shall discuss this simpler model first, and come back to the Anderson model in section 1.2.5. The Kondo Hamiltonian [43, 44] describes a band of free conduction electrons interacting antiferromagnetically with a local moment,  $\vec{S}$ 

$$H = \sum_{k} \epsilon_k c_k^{\dagger} c_k + J_K \vec{\sigma}(0) \cdot \vec{S}, \qquad (1.3)$$

where  $\vec{\sigma}(0) = c_{0\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{0\beta}$  is the conduction electron spin density at the local moment site. As with superexchange, the antiferromagnetic Kondo interaction,  $J_K$  is generated by virtual charge fluctuations [52], where the localized electron hops off into the conduction sea and a conduction electron hops back on - a process only possible when the spins are anti-aligned. The Kondo temperature is given by  $T_K = D e^{-D/2J_K}$ , where D is the conduction electron bandwidth.

Jun Kondo first elucidated the non-perturbative nature of the Kondo problem in 1962 [43], when he showed that the appearance of a logarithmic term in the resistivity at third order in  $J_K$  signals the failure of perturbation theory caused by the anti-screening effect. This logarithmic term explains the upturn in the resistivity, but non-perturbative techniques are required to capture the low temperature behavior, where the renormalization group concept developed by Wilson [54] was essential to understanding the scaling properties of the Kondo singlet ground state.

Although the Kondo impurity model is amenable to several exact techniques [55, 56], the nature of the Kondo singlet remained unclear until recently, with two competing physical interpretations. The original picture, based on work by Nozières [57], held that the local moment is screened by low energy conduction electrons within  $T_K$  of the Fermi surface. However, this picture runs into difficulty when there is an appreciable concentration of Kondo impurities, as only  $T_K/E_F \ll 1$ low energy conduction electrons are available within each unit cell to screen the spins. For a reasonable  $T_K \sim 10K$ ,  $E_F \sim 10,000K$ , the supply of conduction electrons available for screening is exhausted for  $n_{imp} \sim .1\%$ , while in practice Kondo physics is regularly seen at much larger concentrations [48]. This contradiction is known as *Nozières exhaustion paradox*, and led to the more modern idea that screening is a local phenomena involving energies up to the bandwidth, similar to the formation of Cooper pairs [58]. However, instead of a bosonic pair of two electrons, the relevant bound state is a *composite fermion*, binding a conduction electron to a bosonic spin flip of the local moment,  $f_{\uparrow}^{\dagger} \sim c_{\downarrow}^{\dagger}S_{+}$ . Composite fermions have the charge, *e* and spin, 1/2 of electrons. This composite fermion is injected into the Fermi sea, where it hybridizes with conduction electrons to form the Kondo singlet,  $\langle c^{\dagger}\vec{\sigma}c\cdot\vec{S}\rangle$ . This physical picture emerges from a large *N* solution of the Kondo model, and is easily extended to the Kondo lattice, where the local moments form a dense lattice [59, 60], each interacting with the same conduction sea:

$$H = \sum_{k} \epsilon_k c^{\dagger}_{k\alpha} c_{k\alpha} + J \sum_{j} c^{\dagger}_{j\alpha} c_{j\beta} S_{\alpha\beta}(j), \qquad (1.4)$$

where repeated spin indices are summed over. The composite fermions form a flat band that hybridizes with the conduction electrons, shown in Figure 1.9. The effective mass of the hybridized bands (given by the inverse of the slope) is much larger than the original conduction electron mass. While in the impurity, spin-flip scattering leads to an increasing resistivity at low temperatures, in the lattice the resistivity first rises, as the individual impurities spin-flip scatter, but then drops as coherence develops across the sample at  $T^*$ , as seen in Figure 4.27 (b). The low temperature state is a *heavy Fermi liquid* [61, 62], with resistivity  $\rho(T) = \rho_0 + AT^2$ , where A is enhanced by  $\left(\frac{m^*}{m}\right)^2$ . Similarly, the low temperature specific heat takes a Fermi liquid form,  $C = \gamma T$ , and the susceptibility crosses over from a Curie-Weiss form at high temperatures to an constant enhanced Pauli susceptibility,  $\chi(T) \sim \chi_0$  as the local moments quench into the heavy Fermi liquid.  $\gamma$  and  $\chi_0$  are both enhanced by  $m^*/m \sim T_F/T^*$ , which ranges from 100 - 1000. Interestingly, in normal metals like copper, Fermi liquid behavior can only be observed up to  $\sim 1K$  before phonon corrections wash it out, while in heavy fermion metals the enhanced electronic contributions are dominant to higher temperatures despite their lower Fermi temperatures. The absorption of the spins into the heavy Fermi liquid can be seen experimentally in CeRhIn<sub>5</sub>, where pressure tunes between a heavy Fermi liquid ground state, with a large Fermi surface (including the spins) to an antiferromagnetic



Figure 1.9: (a) At high temperatures, the conduction electrons (blue band) and local moments are decoupled. The conduction electrons have a small Fermi surface. The local moments form a flat band of composite fermions (red), which (b) at low temperatures hybridizes with the conduction electrons to form a heavy band with strongly enhanced effective mass. The Fermi surface is enlarged to include both the conduction electrons and the spins.

ground state, where the spins order magnetically, leaving behind a small Fermi surface. de Haasvan Alphen experiments see this jump in the size of the Fermi surface with pressure [63], shown in Figure 1.10.

## 1.2.2 RKKY coupling, competition and criticality

When Doniach introduced the Kondo lattice as a model for heavy fermion materials [60], he noted the existence of two energy scales, the Kondo scale,  $T^*$  and the RKKY scale,  $T_{RKKY}$ . As a local moment attempts to form a Kondo singlet, it spin-polarizes the conduction sea immediately surrounding it, leading to an oscillating spin-polarization as the conduction sea recovers (see Figure



Figure 1.10: (a) CeRhIn<sub>5</sub> is an local moment antiferromagnet at ambient pressure, but as applied pressure suppresses the Néel temperature to zero, a dome of heavy fermion superconductivity emerges. (b) At high magnetic fields, there is a direct transition at pressure  $p_c$  between an antiferromagnet with a small Fermi sea of light conduction electrons to a heavy Fermi liquid with a large Fermi surface incorporating the spins. This transition can be seen experimentally in de Haasvan Alphen experiments done in high magnetic fields; these can measure both the size of extremal orbits of the Fermi surface (c) and their effective mass (d). The effective masses are seen to diverge at  $p_c$ , where the size of the Fermi surface jumps.

1.11). A second local moment feels this disturbance as an effective field and orients itself along this field. In the lattice, this interaction is typically antiferromagnetic with  $T_{RKKY} \sim J_K^2 \rho(\epsilon_F)$  [64].

The existence of two energy scales  $T_{RKKY} \sim J_K^2 \rho$  and  $T^* \sim D \exp(-D/2J_K)$  allows for a rich phase diagram ( $\rho = D^{-1}$ ), where by tuning  $J_K \rho$  (through pressure, chemical doping or magnetic field), materials can be tuned between heavy Fermi liquids and antiferromagnets [Figure 1.11 (b)]. How the ground state passes from heavy Fermi liquid to antiferromagnet is still unclear, although it is widely believed that the two phases are separated by a *quantum critical point* (QCP): a second order phase transition at zero temperature, which has profound effects in a broad region of



Figure 1.11: (a)A local moment polarizes the conduction sea around it, setting up Friedel oscillations in the conduction electron spin polarization. Nearby local moments align with this effective field, giving rise to the RKKY interaction. (b) Doniach phase diagram: as  $J\rho$  changes, the relative strength of the Kondo and RKKY temperature scales varies, tuning between antiferromagnetic and heavy Fermi liquid ground states, with an intervening quantum critical point. (After Coleman [48]).

finite temperature above the QCP. While both the antiferromagnet and heavy Fermi liquid are Fermi liquids, albeit with vastly different effective masses, we know from experiment that the intervening finite temperature region can have a variety of power-law resistivities,  $\rho(T) = \rho_0 + AT^n$  (n < 2) and logarithmic specific heat,  $C \sim -T \log T$  [65].

#### **1.2.3 Heavy Fermion Superconductivity**

The discovery of superconductivity in the heavy fermion compound, CeCu<sub>2</sub>Si<sub>2</sub> [50] in 1976 was extremely surprising, as the current conventional wisdom was that magnetic moments were anathema to superconductivity. The conventional picture of heavy fermion superconductivity avoids this problem, as it is a two stage process. The local moments first undergo the Kondo effect to form heavy quasiparticles at the coherence temperature,  $T^*$ , and these heavy quasiparticles then pair at  $T_c \ll T^*$  by exchanging residual spin fluctuation modes, just as electrons exchange phonons in BCS superconductivity [14]. The idea that spin-fluctuation mediated superconductivity might give rise to a d-wave superconducting gap to avoid the high Coulomb repulsion cost of on-site s-wave pairing was first introduced in the context of heavy fermion superconductivity [66, 67, 68]. Such a nodal gap is observed in heavy fermion superconductors in the power law NMR relaxation rates,  $1/T_1 \sim T^3$  [69]. The heavy fermion superconductor, UPt<sub>3</sub> [70] fits nicely into this model, as  $T^* \sim 100K$ , and the local moments are completely quenched by 30K [Figure 1.12 (left)]. Superconductivity does not develop until  $T_c = 0.5K$ , so the scales are very well separated. While UPt<sub>3</sub> actually has a p-wave gap [71], many heavy fermion superconductors are in fact d-wave [72]. Many are antiferromagnetic at ambient pressure, like CePd<sub>2</sub>Si<sub>2</sub> and CeIn<sub>3</sub>, with a superconducting dome concealing the point where the Néel temperature vanishes with increasing pressure; these are thought to be mediated by quantum critical spin fluctuations [73, 74, 75]. However, several heavy fermion compounds do not fit into this weak-coupling picture, most notably the 115 family: CeMIn<sub>5</sub> (M = Co,Rh,Ir) [76, 77, 78], PuMGa<sub>5</sub> (M = Co,Rh) [79, 80] and NpPd<sub>5</sub>Al<sub>2</sub> [81], which includes the highest temperature heavy fermion superconductors. In many of these 115 materials, local moments are present right down to the superconducting transition temperature, where they quench into the superconductor [Figure 1.12 (right)]; the quasiparticles appear to be *forming as they pair*, requiring a theory incorporating the non-trivial internal structure of the Cooper pair, as we discuss in Chapters 4 and 5.

#### **1.2.4** Two channel Kondo impurities

So far, we have focused on spin 1/2 local moments screened by a single *channel* of conduction electrons, where both the local moment and conduction electrons have two degrees of freedom. This equality allows the local moment to be perfectly screened, forming a ground state singlet. However, as Nozières and Blandin realized [62], the spin degeneracy, 2S + 1 and the number of conduction electron channels, n, may differ. For 2S + 1 > n, there are not enough conduction electron channels to fully screen the impurity, leaving behind an *underscreened* moment. For 2S + 1 < n, there are too many conduction electron channels, all of which align anti-parallel to the local moment, *overscreening* it. Both of these phenomena have excess entropy at zero temperature and give rise to non-Fermi liquid behavior. The simplest example is the two channel Kondo problem, where a spin 1/2 impurity has two types of screening conduction electrons. When the Kondo



Figure 1.12: (a) The magnetic susceptibility,  $\chi$  of UPt<sub>3</sub>(from Frings 1983 [82]) has a Curie-Weisslike form at high temperatures, but the local moments are completely quenched by  $T \approx 30K$ , forming a Pauli paramagnet well above  $T_c = 0.5K$ . (b) By contrast, the susceptibility of CeCoIn<sub>5</sub>(from Petrovic *et al.* [83]), has a Curie-Weiss form all the way down to its  $T_c$  of 2.3K. (c) The superconducting condensation entropy (calculated by integrating C/T up to  $T_c$ ) for UPt<sub>3</sub> is  $\approx 0.05R \log 2$  indicating that the spins are almost fully quenched by  $T_c$ , while in (d) CeCoIn<sub>5</sub> the condensation entropy is  $\approx 1/3R \log 2$ , and the spins are far from quenched.

coupling in one channel,  $J_1$  is larger than that in the other,  $J_2$ , the screening in channel one scales to strong coupling, while the second conduction electron channel decouples from the problem. At low enough temperatures, the problem is just the one channel Kondo model. When the two channels are degenerate ( $J_1 = J_2$ ), neither channel decouples and the spin is overscreened, giving rise to a QCP. This QCP can be studied with exact methods, notably the Bethe Ansatz [84, 85] and boundary conformal field theory [86], which characterize the effects of this QCP on the finite temperature region above it, including an extensive zero point entropy  $S = \frac{1}{2}R \log 2$ , logarithmically divergent spin susceptibility and specific heat coefficient,  $\chi \sim C/T \sim -\log T$  and a sub-linear power law resistivity,  $\rho(T) = \rho_0 + A\sqrt{T}$  [87]. The conduction electron pair susceptibility also diverges at the QCP [88]. This divergent susceptibility, along with the zero point entropy suggest that the impurity quantum critical point will be screened by the development of superconductivity in the lattice, where the channel symmetry protecting the QCP, is broken between lattice sites. Studies of the two channel Kondo lattice in the limit of infinite dimension also suggest superconductivity [89, 90]. The symplectic-N limit of the two channel Kondo lattice exhibits this superconductivity, where two conduction electrons in orthogonal channels combine with the local moment to form a composite pair, as discussed in Chapter 4.

The two channel Kondo model has a special relationship to the problem of two antiferromagnetically coupled Kondo impurities [91], which can also be tuned through a QCP if the problem is particle-hole symmetric. For large antiferromagnetic coupling,  $J_H$ , the two local moments form a valence bond singlet, off which the conduction electrons scatter only weakly ( $\delta_{\sigma} = 0, \pi$ ), but when the Kondo coupling,  $J_K$  is large, each local moment independently forms a Kondo singlet with the conduction sea ( $\delta_{\sigma} = \pi/2$ ). When  $J_H = 2.2J_K$ , these two effects are degenerate, and the spins are again overscreened, leading to a QCP equivalent to that of the two channel Kondo impurity, again with  $S = \frac{1}{2}R \log 2$  zero-point entropy. While the two QCPs are identical, the leading irrelevant operators around them differ, leading to different thermodynamic behavior - two Kondo impurities have a logarithmically divergent *staggered* susceptibility, and the specific heat coefficient has power law behavior [92]. How these two QCPs relate in the lattice is an intriguing problem considered in Chapter 5.

#### **1.2.5** Valence fluctuations and the Anderson model

The Anderson model [51], where atoms with a strong on-site Coulomb repulsion,  $U_f$  are immersed in a sea of non-interacting conduction electrons, encompasses both the spin fluctuations of the Kondo model and the higher energy charge fluctuations. It describes how local moments form at high temperatures down to how they quench into the heavy Fermi liquid at low temperatures, and how the valence of these f-electrons changes as heavy Fermi liquids, or more exotic heavy fermion phases form. Well within the Kondo limit, charge fluctuations are frozen out and the valence is fixed to an integer value. As the chemical potential of the conduction electrons is tuned, the valence begins to fluctuate between two fixed values (see Figure 1.13 b) [93], and the Kondo temperature rises monotonically with the strength of the valence fluctuations [94]. This increase is especially important to understanding the the 115 family, where the 4f Ce 115s have a maximum  $T_c$  of 2.3K [76], but the much more mixed valent 5f analogues, like PuCoGa<sub>5</sub> have a maximum  $T_c = 18.5K$  [79]. A large N limit capturing both superconductivity and valence fluctuations is thus highly desirable.



Figure 1.13: (a) Energies of the Anderson atomic Hamiltonian. The zero of the energy (the conduction electron  $\mu$ ) is between  $\epsilon_f$  and  $\epsilon_f + U$ . (b) Relationship between the chemical potential,  $\mu$ , density of the conduction electrons,  $n_c$ , and the valence of the f-electrons,  $n_f$ . In the *mixed valent* regimes (gray), where  $n < n_f < n + 1$ , the chemical potential becomes pinned to  $\epsilon_f$  (or  $\epsilon_f + U_f$ ) as the f-level is filled. In this regime, mixing occurs *only* between  $f^n$  and  $f^{n+1}$  valence states, in contrast to noninteracting electrons, whose valences fluctuate between all possible values. A weak hybridization, V between the c- and f- electrons smears out what would otherwise be a sharp cusp between the linear dependence of  $n_c$  on  $\mu$  and the plateau, meaning that the chemical potential is pinned to within a width  $\Delta = \rho(\epsilon_f)V^2$  of  $\epsilon_f$ . Between these plateaus, the f-valence is *nearly integral*, and this region, where  $\Delta \ll \epsilon_f$  defines the Kondo regime. (Adapted from Fazekas [93]).

The Anderson model contains two coexisting species of electrons: one weakly interacting and mobile (c) and one strongly interacting and localized (f),

$$H = H_c + H_f + H_{mix}.$$
(1.5)

The first term describes free conduction electrons and the second is an atomic Hamiltonian with a

strong on-site Coulomb repulsion (the atomic states are shown in Figure 1.13 a),

$$H_c = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}, \quad H_f = \sum_i \epsilon_f f_{i\sigma}^{\dagger} f_{i\sigma} + U_f \hat{n}_{fi\uparrow} \hat{n}_{fi\downarrow}.$$
(1.6)

These two species mix quantum mechanically through a hybridization term [95],

$$H_{mix} = V \sum_{i} c^{\dagger}_{i\sigma} f_{i\sigma} + \text{h.c.}, \qquad (1.7)$$

where here we assume an isotropic s-wave hybridization. While this approximation is sufficient to capture much of the physics of heavy Fermi liquids, the full k- and spin- dependent hybridization will be required to capture the nodal superconductivity explored in Chapter 4. We are primarily interested in the Anderson lattice model given above, although the Anderson impurity model provides the foundation of many dynamical mean field theories [96, 97], which are themselves exact in the limit of infinite dimension. The Anderson lattice model applies naturally to lanthanide and actinide materials, where the core f-electrons (4f or 5f) are close to the nucleus, interacting strongly with one another, while the weakly interacting outer s- and p- electrons constitute the conduction electrons, along with electrons from any other weakly interacting atoms. The Kondo model is obtained from the Anderson model by a Schrieffer-Wolff transformation integrating out the charge fluctuations [53, 52], where the Kondo coupling,

$$J_K = \frac{V^2}{|\epsilon_f|} + \frac{V^2}{\epsilon_f + U},\tag{1.8}$$

arises from virtual charge fluctuations, as discussed previously.

The charge and spin features of the Anderson model can be seen in f-electron spectral function or density of states,  $A(\omega)$  which has three main features: a central Kondo resonance peak of width  $T_K$  pinned to the Fermi level, and two charge fluctuation side peaks at the energies  $E_0 = -\epsilon_f$  and  $E_2 = \epsilon_f + U$ . These features are well-separated in the Kondo limit, as the charge fluctuation energy scales are much larger than the hybridization scale,  $\Delta = \rho(\epsilon_f)V^2$ . This separation requires strong



Figure 1.14: (a) The Anderson model. (b) The f-electron density of states  $A(\omega)$  contains a Kondo resonance of width  $T_K$  is pinned to the Fermi surface, while charge fluctuation side peaks occur at  $-\epsilon_f$  and  $\epsilon_f + U$ . The energy ranges captured in the Kondo, infinite-U Anderson and Anderson models are shown.

interactions: for U = 0, the conduction and f-electrons hybridize,  $A(\omega)$  is just a Lorentzian of width  $\Delta$ , the f-electron valence fluctuates between all possible values (n = 0, 1, 2), and  $T_K = \Delta$  is just this energy scale. As U increases, the charge fluctuation peaks separate out, and the central Kondo resonance narrows significantly.

#### **1.2.6** The infinite-U Anderson model and Hubbard operators

In the limit of large U, electrons hopping into and out of the f-orbital are strongly restricted by the high energy cost of double occupancy. A proper treatment of this infinite U Anderson model requires the introduction of *Hubbard operators* to project out any doubly occupied f-states [98]. These operators,  $X_{ab} = |a\rangle\langle b|$ , act within the atomic Hilbert space  $|a\rangle = |0, \uparrow, \downarrow\rangle$ , where the diagonal Hubbard operators,  $X_{aa}$  are projection operators, and the off-diagonal Hubbard operators,  $X_{\sigma 0}$ and  $X_{0\sigma}$  are projected creation/annihilation operators. The hybridization and atomic Hamiltonians may be rewritten with these Hubbard operators [99],

$$H_{mix} = V \sum_{i} c_{i\sigma}^{\dagger} X_{0\sigma}(i) + \text{h.c.}, \quad H_{a} = |\epsilon_{f}| \sum_{i} X_{00}(i).$$
(1.9)

Since Hubbard operators, like spins, do not obey canonical commutation relations, they also cannot be treated directly within quantum field theory and must be represented as bilinears of fermions and bosons chosen to maintain the Hubbard algebra. In the *slave boson* approach [100, 101], a boson,  $b^{\dagger}$  is introduced to represent the empty state, while fermions,  $f_{\sigma}^{\dagger}$  represent the singly occupied spin states:

$$\begin{aligned} |0\rangle &= b^{\dagger} |\Omega\rangle \\ |\sigma\rangle &= f^{\dagger}_{\sigma} |\Omega\rangle, \end{aligned}$$
 (1.10)

where  $|\Omega\rangle$  is a vacuum containing no fermions or bosons. In effect, we separate the electron,  $X_{0\sigma} = b^{\dagger} f_{\sigma}$  into charged, but spinless holons and neutral spinons, which now have the potential to move separately - the ultimate in collective behavior. We can also ask which large N limit these slave bosons represent. By examining the commutation relations of these operators, we can identify them with the SU(N) large N limit, which can treat heavy Fermi liquids, but not superconductivity. In Chapter 6, we introduce symplectic Hubbard operators, which correspond to symplectic spins to treat the two channel Anderson model.

#### **1.3** Adding charge fluctuations to a Heisenberg magnet

Doping holes into Mott insulators generates the cuprate family of unconventional superconductors, the highest temperature superconductors found to date. Understanding how charge fluctuations are slowly reintroduced into strongly correlated spin systems is widely believed to be essential to understanding the superconducting mechanism.
#### **1.3.1** Strongly correlated insulators

Uncorrelated electrons (with full charge and spin fluctuations), hopping on a lattice,

$$H_c = -\sum_{ij} t_{ij} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} - \mu \sum_i c_{i\sigma}^{\dagger} c_{i\sigma} \right)$$
(1.11)

with amplitude  $t_{ij}$ , are best described in momentum space,

$$H_c = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}, \qquad (1.12)$$

where they form an energy band,  $\epsilon_{\mathbf{k}}$  (the Fourier transform of  $t_{ij}$ ). Generally, there will be many bands of electrons, each with spin degeneracy two, occupied up to the Fermi energy,  $\mu$ . When the Fermi energy lies between bands, there are an even number of electrons per site, and the material will be insulating, while when  $\mu$  lies within a band, it will be metallic [102]. Band theory is essentially a theory of independent electrons, and it works extremely well for a large class of materials. It was therefore quite surprising when, in 1937, de Boer and Verway [103], and Mott and Peierls [11], realized that band theory fails for certain correlated insulators. These materials have an odd number of electrons per unit cell, and should be band metals; they are instead very good insulators, known as *Mott insulators*. Strong electron-electron interactions localize the electrons, which are clearly strongly correlated, as they must know to avoid one another. Tuning the interactions induces a metal-insulator phase transition, or *Mott transition* as a function of pressure or temperature.

Electrons interact through the repulsive Coulomb potential,  $V(\mathbf{r}_i - \mathbf{r}_j) = e^2/|\mathbf{r}_i - \mathbf{r}_j|$ , which is reduced to a short-ranged interaction by screening. The competition between the kinetic energy, favoring metallic behavior, and the Coulomb repulsion, favoring electron localization is captured most simply in the Hubbard model, introduced by Hubbard in 1963 [105],

$$H = -t \sum_{\langle ij \rangle} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) - \mu \sum_{i} c_{i\sigma}^{\dagger} c_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \qquad (1.13)$$

The Hubbard U approximates the Coulomb potential with a local repulsive term, U > 0. Further



Figure 1.15: The periodic table shows broad trends tuning itinerant electrons towards localization as the atoms become more strongly correlated, based on Smith and Kmetko [104]. There are two trends here: first, the decrease in localization as the strongly correlated electrons occupy orbitals with more radial nodes, moving from the most localized 4f to 5f and 3d, and second, the contraction within a row of the periodic table as the nuclear charge increases. Localized electrons tend to order magnetically, but a lot of fascinating physics happens in the electrons on the edge of localization - several of which we discuss in this dissertation (boxed atoms). In the case of the cuprates, the atomic physics is localized, but itineracy is introduced by doping.

neighbor Coulomb interactions can be included in the extended Hubbard model, but the Hubbard model already captures many correlated phases: metals, Mott insulators, magnets and superconductors. These ground states may be tuned by changing the ratio U/t or the filling n (by tuning  $\mu$ ). For small U/t, the Hubbard model can be solved perturbatively, describing a Fermi liquid, but perturbative techniques fail near the metal insulator transition.

Each site has four possible states:  $|0\rangle$ ,  $|\uparrow\rangle$ ,  $|\downarrow\rangle$  or  $|2\rangle = |\uparrow\downarrow\rangle$ , with energies  $E_0 = \mu$ ,  $E_{\uparrow,\downarrow} = 0$ , and  $E_2 = -\mu + U$ , where the energy is measured from the Fermi level. The filling, n ranges from 0 to 2, and most interesting physics takes place near half-filling, n = 1. For sufficiently large U, there are no doubly occupied sites, and the half-filled state is a Mott insulator, with only spin degrees of freedom. At infinite U, these spins are free, and reintroducing virtual charge fluctuations leads to antiferromagnetic order through superexchange, shown in Figure 1.16(b). This process only takes place when the two spins are anti-parallel, and  $H = -4t^2/U \sum_{\langle ij\rangle} P_{S=0}(ij)$  projects out the singlet configuration, where  $P_{S=0}(ij) = 1/4 - \vec{S}_i \cdot \vec{S}_j$  [19]. The low energy Hamiltonian of the half-filled



Figure 1.16: (a) The Hubbard model consists of electrons hopping on a lattice with amplitude, t. When two electrons sit on the same lattice site, it costs a Coulomb repulsion energy, U. (b) For large U, there are virtual processes whereby an electron hops to a neighboring site, creating an intermediate state of an empty and a doubly occupied site that costs energy U, and then hops back again, gaining an energy  $\propto t^2/U$ . These *superexchange* processes can only take place when the neighboring electrons are anti-parallel, due to the Pauli exclusion principle.

Hubbard model is therefore the antiferromagnetic Heisenberg Hamiltonian (section 1.1).

## 1.3.2 Doping a Mott insulator

Adding even one hole should turn a half-filled Mott insulator into a strongly correlated metal, however disorder localizes this hole immediately, and the antiferromagnetic Mott insulator is stable over a finite region of doping. Such Mott insulators are the parent compounds of the cuprate family of high temperature superconductors, discovered in 1986 by Bednorz and Müller [106]. Conventional, weak-coupling superconductors are described by BCS theory [14], where the attractive phonon interaction forms pairs of electrons into bosonic Cooper pairs [18], which Bose-condense to form a superconducting state, with a maximum  $T_c$  well below the boiling point of liquid nitrogen. By contrast, the cuprate superconductors are strongly coupled, with a maximum  $T_c$  around 150K [107] and their electronic pairing mechanism, resulting from the *repulsive* Coulomb interaction, falls outside BCS theory. The phase diagram of these doped Mott insulators also contains a "pseudogap" phase reminiscent of uncondensed Cooper pairs above the superconducting dome, and a region of non-Fermi liquid, *strange metallic* behavior suggesting a QCP concealed beneath the superconducting dome [15]. Any complete theory must capture all of these exotic phases. While from 1986 to 2007, the cuprates were the sole family of high temperature superconductors (though some heavy fermion superconductors have similarly large values of  $T_c/T^*$ ), a new family of *iron-based* superconductors was discovered in 2008, with a maximum  $T_c$  of 56K [108]. The phase diagram of these materials shares many similarities with the cuprates (Figure 1.17) [109], however, the parent compounds are just on the metallic side of the Mott transition [110].



Figure 1.17: (Top) Schematic phase diagrams of two high temperature superconducting families: the cuprates (left), and the iron-pnictides (right). Both families possess a rich phase diagram, with magnetism at low doping, Fermi liquid physics at large doping, and intermediate non-Fermi liquid finite temperature phases above the superconducting dome, although the parent compounds are on opposite sides of the Mott transition. (Bottom) The BCS superconducting gap,  $\Delta_k = \langle \tilde{\sigma} c_{k\sigma}^{\dagger} c_{-k-\sigma}^{\dagger} \rangle$ is isotropic around the Fermi surface, or s-wave (left). While the Coulomb repulsion disfavors on-site pairing, it scales to weak coupling in BCS [111], allowing an s-wave gap. The Coulomb repulsion cannot be neglected for strongly correlated superconductors, which instead develop nodal gaps, where the pairing with a positive gap (red) is cancelled by that with a negative gap (blue). The cuprates have a d-wave gap (middle), where this cancellation is exact, while the iron-based superconductors have an  $s_+$  gap (right) that has different signs on the two Fermi surfaces [108, 109].

To understand these phase diagrams, we are interested in the low energy physics of the strongly correlated large U limit. The Heisenberg model describes half-filling, but for n < 1 holes will hop around in an antiferromagnetic background. Doubly occupied states must still be avoided, and the hopping is *not* that of free electrons. Rather, it is *projected hopping*, described by the t - J model,

$$H = -t \sum_{\langle ij \rangle} X_{\sigma 0}(i) X_{0\sigma}(j) + \sum_{ij} J_{ij} X_{\sigma \sigma'}(i) X_{\sigma' \sigma}(j), \qquad (1.14)$$

an effective Hamiltonian obtained from the Hubbard model with a canonical transformation similar to the Schrieffer-Wolff transformation [112], and proposed as the relevant model for the cuprate superconductors by Anderson [23]. The Hubbard operators,  $X_{ab}$  (already discussed for the infinite-U Anderson model) ensure that only empty sites, or holes can hop. While mean field theories have played in important role in understanding the t - J model, to date there have been no consistent, superconducting large N treatments. The introduction of symplectic Hubbard operators fills this void, as we discuss in detail for the iron-based superconductors in Chapter 7.

# **Chapter 2**

## Spins, time reversal and symplectic symmetry

#### 2.1 What is a spin?

As we extend the theory of physical electron spins into a family of related theories, we will lose some of the physics unique to these spins, so how do we guarantee that our resulting theories still capture the defining characteristics of interacting spins? What defines magnetism? What defines a spin?

The spin of an electron is an internal angular momentum quantized to have two states,  $\uparrow$  and  $\downarrow$ , pointing along some quantization axis [113]. Thus, the electron is doubly degenerate. The spin state of the electron wavefunction, described by a spinor,  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ , is acted upon by the spin operators  $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ , where  $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  are the Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.1)$$

which generate SU(2), the special unitary group of all  $2 \times 2$  unitary matrices  $[U^{\dagger}U = 1; \det U = 1]$ . 1]. Any SU(2) matrix can be written  $U = \exp(i\vec{\alpha} \cdot \vec{\sigma})$ , and U acting on a spin rotates it within the SU(2) spin space. Technically, the SU(2) group is generated by the su(2) algebra, defined solely by the commutation relations of the Pauli matrices:

$$[\sigma_a, \sigma_b] = 2i\epsilon_{abc}\sigma_c,\tag{2.2}$$

where  $\epsilon_{abc}$  is the Levi-Civita symbol, guaranteeing antisymmetrization. They also anticommute as  $\{\sigma_a, \sigma_b\} = 2\delta_{ab}\mathbf{1}$ . The Pauli matrices are a *representation* of this algebra, but any set of matrices satisfying (2.2) also forms a representation, with larger representation corresponding to larger spins. In real materials, several electrons may align to create a total spin S > 1/2. The spin quantization

axes is still within three dimensional space, but the spins now take on 2S + 1 values, and are proportional to a larger representation of SU(2). The Pauli matrices are the smallest, or *fundamental* representation of SU(2) [114].



Figure 2.1: The three different types of spins found in real materials: Ising, XY, and Heisenberg.

In strongly correlated insulators, electrons lose their charge degrees of freedom and behave like fixed spins. Instead of four states,  $|0\rangle$ ,  $|\uparrow\rangle$ ,  $|\downarrow\rangle$ ,  $|2\rangle = |\uparrow\downarrow\rangle$  per site, a spin points either  $|\uparrow\rangle$  or  $|\downarrow\rangle$ . In the simplest materials, these are Heisenberg spins, those described by SU(2), however, microscopic details like the coupling of spin and orbital degrees of freedom or the effects of the lattice [93] can reduce these down to XY spins, constrained within an easy plane and described by the continuous group  $U(1) = \{e^{i\phi}\}$  or Ising spins, which are constrained to point along an easy axis and are described by the discrete group  $Z_2 = \{\pm 1\}$ .

To understand the defining characteristics of a spin, the first, best place to look is at the symmetries. An SU(2) spin Hamiltonian has two symmetries - invariance with respect to SU(2) rotations and time reversal invariance. XY and Ising spin Hamiltonians also obey time reversal and rotational invariance, but under U(1) or  $Z_2$  rotations. The spins themselves define a unique direction on a manifold,  $CP^1$  for SU(2), and invert under time reversal,  $\vec{S} \rightarrow -\vec{S}$ . The ground states of magnetic Hamiltonians like the Heisenberg model can break the rotational and time reversal symmetries, traditionally simultaneously, as in a ferromagnet, but more recently hypothesized states can break either rotational symmetry, but not time inversion; e.g. a spin-nematic defines a unique direction, but does not have magnetic long range order [115], or chiral spin states which break time reversal, but not rotational symmetry [116]. Certainly there are non-magnetic states, such as liquid crystal displays, which also break rotational symmetry, so the rotational properties of spin are not enough to define magnetism. We propose that both the rotational and time reversal properties of spins are defining symmetries of magnetism, and that a large N theory with broad applicability must maintain both of these properties in the large N limit.

#### **2.2** Time reversal in SU(2)

We begin by demonstrating the link between time reversal and symplectic symmetry. Time reversal is an anti-unitary operator  $\theta$  defined by its action on an electron wave function  $\psi_{\sigma}(\mathbf{x}, t)$ :

$$\theta\psi_{\sigma}(\mathbf{x},t) = \tilde{\sigma}\psi_{-\sigma}^{*}(\mathbf{x},-t), \qquad (2.3)$$

where  $\psi^*$  is the complex conjugate of the wave function, and  $\tilde{\sigma} = \operatorname{sgn}(\sigma)$ . More generally,  $\theta$  is a matrix operator,  $\theta = \hat{\epsilon}K$  [117], where K is the complex conjugation operator,  $K\psi = \psi^*K$  and  $\hat{\epsilon}$  is the antisymmetric matrix  $i\sigma_2 = \tilde{\alpha}\delta_{\alpha,-\beta}$ . A consistent definition of time reversal requires that  $\theta$  commute with the unitary rotation operators U, the members of the group SU(2),  $[U, \theta] = 0$ , shown in Figure 2.2, or written

$$U\theta U^{\dagger} = \theta. \tag{2.4}$$

Using the definition of  $\theta = \hat{\epsilon} K$ , and noting that K converts  $U^{\dagger}$  to  $U^{T}$ , we find

$$U\hat{\epsilon}U^T = \hat{\epsilon} \tag{2.5}$$

This expression is a symplectic condition on the matrices, U because it requires the invariance of an antisymmetric matrix  $\hat{\epsilon}$  under orthogonal transformations. The unusual appearance of the transpose  $U^T$  rather than the Hermitian conjugate  $U^{\dagger}$  reflects the anti-unitary nature of time-reversal. Replacing U by an infinitesimal rotation,  $U = 1 + \vec{\alpha} \cdot \vec{S}$ , the symplectic condition requires that

$$\vec{S} \to \theta \vec{S} \theta^{-1} = \hat{\epsilon} \vec{S}^T \hat{\epsilon} = -\vec{S}.$$
(2.6)

So the symplectic condition is equivalent to the inversion of all SU(2) spins under time-reversal.



Figure 2.2: The time reversal operator,  $\theta$  and rotation operators U acting on a spin must commute. (a) Depicts  $\vec{S} \xrightarrow{\theta U} -R\vec{S}$ . (b)  $\vec{S} \xrightarrow{U\theta} R(-\vec{S})$ , where R is the rotation performed by U. These two are equivalent for all U in SU(2), and SP(N), but not in SU(N).

#### **2.3** Time reversal in large N

To bring the powerful machinery of quantum field theory to bear on condensed matter problems, the fields of interest must be second quantized, which is simple for fermions and bosons because they obey canonical commutation and anti-commutation relations, e.g. -  $[b_a, b_b^{\dagger}] = \delta_{ab}$ ,  $\{f_a, f_b^{\dagger}\} = \delta_{ab}$ . Spins, on the other hand, obey the commutation relations (2.2), and cannot be second quantized directly (to be precise, Wick's theorem is violated [118]). However, spins may be represented with bilinears of bosons or fermions chosen to satisfy spin commutation relations,

$$\hat{S}^a_j = \psi^{\dagger}_{j,\alpha} \sigma^a_{\alpha\beta} \psi_{j,\beta}, \qquad (2.7)$$

where  $\sigma^a$  are the three Pauli matrices, and  $\psi_j^{\dagger} = (\psi_{j,+1}^{\dagger}, \psi_{j,-1}^{\dagger})$  is a two component spinor defined on each site. These representations are known as Schwinger bosons [41] if  $\psi = b$  is bosonic, and Abrikosov pseudo-fermions [45] if  $\psi = f$  is fermionic. The Pauli matrices here are just matrices, not operators. Many representations satisfy (2.2) and different representations are appropriate for different kinds of physics. Some representations, like the Holstein-Primakoff bosons [119], specify a quantization axis and are appropriate for states with long range magnetic order, but the Schwinger and Abrikosov representations are rotationally invariant, more appropriate for states without long range order. These representations may be easily generalized to arbitrary groups by replacing the Pauli matrices with the appropriate generators.

When this treatment is generalized to large N, the number of spin components increases from 2 to an even number N = 2k. Dropping the site index, we have  $\hat{T}_j^a = \frac{1}{2} \psi_{j,\alpha}^{\dagger} T_{\alpha\beta}^a \psi_{j,\beta}$ , where

$$\psi^{\dagger} = \left(\psi^{\dagger}_{+1}, \psi^{\dagger}_{-1}, \psi^{\dagger}_{+2}, \psi^{\dagger}_{-2}, \cdots, \psi^{\dagger}_{+k}, \psi^{\dagger}_{-k}\right)$$
(2.8)

and  $\mathcal{T}^a$  are the generators some larger group, for example, SU(N). As time reversal is a defining property of spins, we want to maintain this essential discrete symmetry as we extend our spin group. However, the SU(N) generators divide into two classes under time reversal (Figure 2.3),

$$\hat{\epsilon} (\mathcal{T}^{a})^{T} \hat{\epsilon} = \begin{cases} -\mathcal{T}^{a} & a \in \{1, 2, \dots, D_{N}\} \\ +\mathcal{T}^{a} & a \in \{D_{N} + 1, \dots, N^{2} + 1\} \end{cases},$$
(2.9)

where  $D_N = \frac{1}{2}N(N+1)$ . The first class can be identified as the generators of the symplectic subgroup, SP(N), whose elements reverse under time reversal, just like the SU(2) spins.  $D_N$ is the number of N dimensional symplectic generators. To avoid confusion, we will label these symplectic spins by  $S^a$ . The second class does not invert under time reversal, and does not form a closed subalgebra of SU(N). When  $\psi_{\alpha}$  is a fermionic operator, we can also define a charge conjugation operator, C that converts particles into holes  $\psi_{\alpha} \stackrel{C}{\to} \tilde{\alpha} \psi^{\dagger}_{-\alpha}$ . The SU(N) spin operator inverts under the combined operation  $C\theta$ ,  $\mathcal{T}^a \stackrel{C\theta}{\to} -\mathcal{T}^a$ , so that when the time reversal parity is ill-defined, the neutrality of the spin is also ill-defined. These generators then behave like *electric* dipoles, not like magnetic moments, so we label them by  $\mathcal{P}^a$ . For N = 2,  $SU(2) \cong SP(2)$ , and there are no antisymplectic generators. However, for any N > 2, the two groups are no longer isomorphic. For example, SU(4) consists of ten symplectic generators

$$\mathcal{S}^{a} \in \left\{ \begin{pmatrix} i\underline{1} \\ -i\underline{1} \end{pmatrix}, \begin{pmatrix} \vec{\sigma} \\ \vec{\sigma} \end{pmatrix}, \begin{pmatrix} \vec{\sigma} \\ \pm \vec{\sigma} \end{pmatrix} \right\}$$
(2.10)

(corresponding to the four Dirac matrices  $\gamma_{\mu}$  and their six commutators  $\frac{i}{2}[\gamma_{\mu}, \gamma_{\nu}]$ ), and five antisymplectic generators

$$\mathcal{P}^{a} \in \left\{ \begin{pmatrix} \underline{1} \\ & -\underline{1} \end{pmatrix}, \begin{pmatrix} & i\vec{\sigma} \\ -i\vec{\sigma} & \end{pmatrix}, \begin{pmatrix} & \underline{1} \\ \underline{1} & \end{pmatrix} \right\}.$$
(2.11)

(corresponding to the  $\gamma_5$  matrix, and its product with the four Dirac matrices  $i\gamma_5\gamma_u$ .)

We can derive an alternate way of writing the SP(N) generators by writing the SU(N) spin operators as,

$$\mathcal{T}_{\alpha\beta} = \psi^{\dagger}_{\alpha}\psi_{\beta} - \left(\frac{n_{\psi}}{N}\right)\delta_{\alpha\beta},\tag{2.12}$$

where  $n_{\psi} = \sum_{\alpha} \psi_{\alpha}^{\dagger} \psi_{\alpha}$  is the number of particles that make up the spin. Under time reversal,  $\mathcal{T}_{\alpha\beta} \xrightarrow{\theta} \tilde{\alpha} \tilde{\beta} \mathcal{T}_{-\beta,-\alpha}$ , SU(N) spins have no well defined parity. By taking antisymmetric or symmetric combinations of the SU(N) spins with their time-reversed version, we may again divide them into two sets, the symplectic spins,

"magnetic" moments 
$$S_{\alpha\beta} = \psi^{\dagger}_{\alpha}\psi_{\beta} - \tilde{\alpha}\tilde{\beta}\psi^{\dagger}_{-\beta}\psi_{-\alpha}, \qquad (\theta, \mathcal{C}) = (-, +)$$
 (2.13)

which invert under time reversal but are neutral under charge conjugation, and antisymplectic spins

"electric" dipoles 
$$\mathcal{P}_{\alpha\beta} = \psi^{\dagger}_{\alpha}\psi_{\beta} + \tilde{\alpha}\tilde{\beta}\psi^{\dagger}_{-\beta}\psi_{-\alpha}, \qquad (\theta, \mathcal{C}) = (+, -), \qquad (2.14)$$

which are invariant under time reversal, but change sign under charge conjugation [120].

Here, the choice of SP(N) is motivated by the desire to maintain the time reversal symmetry of spin in the large N limit, but Sachdev and Read originally developed SP(N) because, unlike SU(N) it contains well defined particle-particle singlets [42]. SU(N) expansions are extremely useful to particle physicists because there are two well defined color singlets - mesons and baryons. Mesons are particle-antiparticle pairs, or in condensed matter, particle-hole pairs, while baryons are products of N particles, forming the three quark baryons for SU(3), which have no condensed matter analog except for N = 2, where these are particle-particle pairs - e.g. valence bonds [17] or Cooper pairs [18]. In the large N limit, the condensed matter version of SU(N) has only particlehole pairs. However, the group SP(N) does have well defined particle-particle singlets, which are the pairing of a particle and its time reversed twin, and particle-hole pairs, but no baryons. The presence of these well defined singlets is only possible because of the existence of a well defined time reversal symmetry of spin.

#### 2.4 Decoupling Spin Hamiltonians

In order to treat the Heisenberg and Kondo Hamiltonians, we would like to rewrite the spin interactions,  $J\vec{S_1} \cdot \vec{S_2}$  without explicit reference to the spin generators. In SU(N), this is done by using the SU(N) completeness relation:

$$\sum_{a} \mathcal{T}^{a}_{\alpha\beta} \cdot \mathcal{T}^{a}_{\gamma\eta} = 2\delta_{\alpha\eta}\delta_{\beta\gamma} - \frac{2}{N}\delta_{\alpha\beta}\delta_{\gamma\eta}$$
(2.15)

We now derive a similar SP(N) completeness relation. Any even dimensional matrix can be split into a symplectic and antisymplectic part:  $M = M_S + M_A$ , where the symplectic part satisfies  $M_S = -\hat{\epsilon}M_S^T\hat{\epsilon}^T$  and the antisymplectic part  $M_A = \hat{\epsilon}M_A^T\hat{\epsilon}^T$ . The symplectic part can be obtained by projection,  $M_S = PM$ , where P is defined such that  $PM_A = 0$ . We recognize that  $M_A - \hat{\epsilon}M_A^T\hat{\epsilon}^T = 0$ , and take

$$PM = \frac{1}{2} \left( M - \hat{\epsilon} M^T \hat{\epsilon}^T \right)$$
(2.16)

$$P^{\alpha\beta}_{\gamma\eta}M^{\eta\gamma} = \frac{1}{2}[M^{\alpha\beta} - \epsilon^{\alpha}_{\gamma}M^{\eta\gamma}\epsilon^{\beta}_{\eta}] \\ = \frac{1}{2}[\delta^{\alpha}_{\eta}\delta^{\beta}_{\gamma} - \epsilon^{\alpha}_{\gamma}\epsilon^{\beta}_{\eta}]M^{\eta\gamma}, \qquad (2.17)$$

so that

$$P^{\alpha\beta}_{\gamma\eta} = \frac{1}{2} [\delta^{\alpha}_{\eta} \delta^{\beta}_{\gamma} - \epsilon^{\alpha}_{\gamma} \epsilon^{\beta}_{\eta}].$$
(2.18)

Since the symplectic matrices form a group,  $M_S$  can always be expanded in the symplectic generators,  $S^a$ ,  $M_S = \sum_a m_a S^a$ . With the normalization  $\text{Tr} \left[S^a S^b\right] = 2\delta_{ab}$ , consistent with the SU(2) Pauli matrices, the coefficient  $m_a = \frac{1}{2} \text{Tr} \left[S^a M\right]$ , giving  $PM = \frac{1}{2} \sum_a \text{Tr} \left[S^a M\right] S^a$ . Expanding both sides in terms of components and canceling  $M^{\eta\gamma}$ , we find

$$P^{\alpha\beta}_{\gamma\eta} = \frac{1}{2} \sum_{a} S^{a}_{\alpha\beta} S^{a}_{\gamma\eta}.$$
(2.19)

Finally, by inserting (2.18), we obtain the SP(N) completeness relation,

$$\sum_{a} (\mathcal{S}^{a})_{\alpha\beta} (\mathcal{S}^{a})_{\gamma\eta} = [\delta^{\alpha}_{\eta} \delta^{\beta}_{\gamma} - \epsilon^{\alpha}_{\gamma} \epsilon^{\beta}_{\eta}].$$
(2.20)

Inserting the spin representation, the symplectic N spin interaction becomes the sum of two terms

$$\hat{S}_1 \cdot \hat{S}_2 = -B_{21}^{\dagger} B_{21} + \eta_{\psi} A_{21}^{\dagger} A_{21} \quad (\eta_{\psi} = \pm 1),$$
(2.21)

where

$$B_{21}^{\dagger} = \frac{1}{2} \sum_{\sigma} \tilde{\sigma} \psi_{2\sigma}^{\dagger} \psi_{1-\sigma}^{\dagger}$$
(2.22)

creates a spin singlet pair between spins 1 and 2, and

$$A_{21}^{\dagger} = \frac{1}{2} \sum_{\sigma} \psi_{2\sigma}^{\dagger} \psi_{1\sigma}$$
(2.23)

creates a particle-hole singlet between these two spins. The signature,  $\eta_{\psi}$  depends on whether  $\psi$  is fermionic ( $\eta_{\psi} = -1$ ) or bosonic ( $\eta_{\psi} = +1$ ). In the large N limit, these bond variables acquire expectation values. For N = 2, this decoupling is one of many alternative mean field theories [121, 122], however in the symplectic N limit, this decoupling is unique. In the context of frustrated magnetism, the two spins are on different sites, 1 = i, 2 = j, and  $B_{ji}^{\dagger}$  creates a valence bond between the two sites, leading to antiferromagnetic correlations, while  $A_{ji}^{\dagger}$  resonates the end of a valence bond between sites *i* and *j*, causing both sites to be simultaneously antiferromagnetically correlated with a third site, thus ferromagnetically correlated with one another. In the case of Kondo physics, the two spins are on the same site, but of different natures:  $S_1$  is the spin-density of the conduction electrons, and  $B_{12}^{\dagger} = \tilde{\alpha} c_{\alpha}^{\dagger} f_{-\alpha}^{\dagger}$  hybridizes a c-electron with an f-hole; the simultaneous condensation of these two bond variables leads to composite pair superconductivity, as we shall show in Chapter 4.

Now we would like to compare this representation with SU(N) [123] and the previous SP(N)treatment [42]. The SU(N) spin Hamiltonian is a dot product between SU(N) spins,  $\hat{T}$ , which can be rewritten using the SU(N) completeness relation(2.15) to obtain the usual sum of ferromagnetic bonds [123] or Kondo hybridization [124, 125, 126],

$$H_{SU(N)} = \frac{J_{ij}}{N} \hat{T}_i \cdot \hat{T}_j = \frac{2J_{ij}}{N} A_{ji}^{\dagger} A_{ji}$$
(2.24)

$$= \frac{J_{ij}}{N} \left( \hat{\mathcal{P}}_i \cdot \hat{\mathcal{P}}_j + \hat{\mathcal{S}}_i \cdot \hat{\mathcal{S}}_j \right), \qquad (2.25)$$

where  $J_{ij}$  is rescaled by N so that H is extensive in N. For simplicity, we have focused on the magnetic case with the spins at two different sites. As one would expect in SU(N), the symplectic and antisymplectic spins are treated on equal footing, which leads to a completely ferromagnetic theory. Bipartite antiferromagnets can also be studied in SU(N) by performing a special transformation (not time reversal) on one sublattice, but SU(N) cannot treat more complicated, e.g.- frustrated, antiferromagnets. The SP(N) Hamiltonian, as defined by Sachdev and Read [42] was originally written in terms of valence bonds,  $H_{SP(N)} = -J_{ij}B_{ji}^{\dagger}B_{ji}$ , in order to treat frustrated antiferromagnets. When we rewrite it in terms of magnetic and electric dipoles, we find

$$H_{SP(N)} = -\frac{J_{ij}}{N} B_{ji}^{\dagger} B_{ji}$$

$$(2.26)$$

$$= \frac{J_{ij}}{2N} \left( \hat{\mathcal{S}}_i \cdot \hat{\mathcal{S}}_j - \hat{\mathcal{P}}_i \cdot \hat{\mathcal{P}}_j \right).$$
(2.27)

Surprisingly, the SP(N) large N theory weights the physical symplectic and unphysical antisymplectic spins equally, but with opposite signs. SP(N) was so called because the Hamiltonian satisfies symplectic symmetry, not because it describes the interactions of symplectic spins. In fact, any combination of the two terms  $B^{\dagger}B$  and  $A^{\dagger}A$  has symplectic symmetry, including SU(N). The requirement that our interactions include only magnetic, symplectic spins is more stringent, and this method is what we call symplectic-N, while we will continue to refer to Sachdev and Read's formulation as SP(N).

Approach	$\mathrm{H}(\mathcal{S},\mathcal{P})$	$\mathrm{H}(b^{\dagger},b)$
SU(N)	$J\left(\mathcal{S}\cdot\mathcal{S}+\mathcal{P}\cdot\mathcal{P}\right)$	$JA^{\dagger}A$
SP(N)	$J\left(\mathcal{S}\cdot\mathcal{S}-\mathcal{P}\cdot\mathcal{P}\right)$	$-JB^{\dagger}B$
Symplectic-N	$JS \cdot S$	$J\left(-B^{\dagger}B + A^{\dagger}A\right)$

Why is it important to exclude the non-time reversing dipoles? Both the symplectic  $(\hat{S}_i \cdot \hat{S}_j)$ and antisymplectic  $(\hat{P}_i \cdot \hat{P}_j)$  interactions are invariant under time reversal, however, the important difference is not in the Hamiltonian, but in the states and the spin dynamics. These are far more coupled than the Hamiltonian suggests because the SU(N) spin  $\hat{T}$  does not act as a vector, and the antisymplectic and symplectic directions are not independent directions, so that  $\hat{T}$  is unable to point in a purely symplectic direction. And even if the ground state is the one of interest, the presence of antisymplectic interactions affects the dynamics of the symplectic spins, dynamically violating the closure of the symplectic subgroup and disrupting any particle-particle singlets.

#### 2.5 Staying in the physical subspace: constraints

The Fock space of the bosonic and fermionic spin representations contain more states than the physical spin space. In the bosonic case, the total spin on the site,  $n_b = 2S$  is allowed to take on any value. The fermionic case has similar problems, as  $n_f$  can take on any value from 0 to N. In order to faithfully represent the spin, we must fix the spin Casimir,  $\vec{S}^2 = S(S+1)$ , which depends on the spin group and representation chosen. This constraint is then implemented by a Lagrange multiplier on each site.

## 2.5.1 Fermionic constraints and SU(2) symmetry

Before we discuss the fermionic spin Casimir, we first wish to discuss the special SU(2) symmetry appearing in the fermionic representation. The existence of this SU(2) symmetry can be seen by introducing the isospin vector,  $\vec{\Psi} = (\Psi_1, \Psi_2, \Psi_3) = \tilde{f}^{\dagger}_{\alpha} \vec{\tau} \tilde{f}_{\alpha}$ , where

$$\Psi_{1} = \left(\Psi^{\dagger} + \Psi\right), \quad \Psi_{2} = -i\left(\Psi^{\dagger} - \Psi\right)$$
  

$$\Psi_{3} = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{\alpha} - f_{-\alpha} f_{-\alpha}^{\dagger} = n_{f} - N/2, \quad (2.28)$$

where  $n_f = \sum_{\alpha} f_{\alpha}^{\dagger} f_{\alpha}$  is the number of fermions and  $\Psi^{\dagger}$  creates an s-wave pair,  $\Psi^{\dagger} = \frac{1}{2} \sum_{\alpha} \tilde{\alpha} f_{\alpha}^{\dagger} f_{-\alpha}^{\dagger}$ . The isospin vector satisfies an SU(2) algebra,  $[\Psi_a, \Psi_b] = 2i\epsilon_{abc}\Psi_c$ . The inversion of spins under time reversal ensure that these pair creation operators,  $\Psi^{\dagger}$  are really creating spin singlets, or in other words, that  $\Psi^{\dagger}$  commutes with  $\hat{\mathbf{S}}$ . This commutation can be seen by computing the commutation relations directly using the spin representation,  $S_{\alpha\beta} = f_{\alpha}^{\dagger}f_{\beta} + \tilde{\alpha}\tilde{\beta}f_{-\alpha}f_{-\beta}^{\dagger}$ . The commutation of a fermion with the spin is,

$$\left[S_{\alpha\beta}, f_{\gamma}^{\dagger}\right] = 2f_{\delta}^{\dagger}P_{\alpha\beta}^{\gamma\delta}, \qquad (2.29)$$

while the time-reversed fermion gives,

$$\left[S_{\alpha\beta}, \tilde{\gamma} f^{\dagger}_{-\gamma}\right] = -2\tilde{\delta} f^{\dagger}_{-\delta} P^{\gamma\delta}_{\alpha\beta}.$$
(2.30)

And the commutator is,

$$\begin{bmatrix} S_{\alpha\beta}, \tilde{\gamma} f_{\gamma}^{\dagger} f_{-\gamma}^{\dagger} \end{bmatrix} = f_{\gamma}^{\dagger} \begin{bmatrix} S_{\alpha\beta}, \tilde{\gamma} f_{-\gamma}^{\dagger} \end{bmatrix} + \begin{bmatrix} S_{\alpha\beta}, f_{\gamma}^{\dagger} \end{bmatrix} \tilde{\gamma} f_{-\gamma}^{\dagger} \\ = f_{\gamma}^{\dagger} \begin{bmatrix} 2P_{\alpha\beta}^{\gamma\delta} - 2P_{\alpha\beta}^{\gamma\delta} \end{bmatrix} \tilde{\delta} f_{-\delta} = 0.$$
(2.31)

So we see that  $[S_{\alpha\beta}, \Psi^{\dagger}] = 0$ , which means not only that pairs are invariant under SP(N) spin rotations, but also that the SP(N) spin generators are invariant under the particle-hole rotations generated by  $\Psi$ . Together with  $[n_f, S_{\alpha\beta}] = 0$ , this commutation relation shows that the spin is invariant under a continuous SU(2) particle-hole transformation,

$$f_{\alpha} \longrightarrow u f_{\alpha} + v \tilde{\alpha} f_{-\alpha}^{\dagger}, \qquad (2.32)$$

where  $|u|^2 + |v|^2 = 1$ . So, for fermionic symplectic spins, the time reversal symmetry gives rise to an SU(2) gauge symmetry. This symmetry was first discovered by Affleck *et al.* for SU(2) spins, and we have now shown that this SU(2) symmetry survives for all N, in fermionic symplectic-N.

We can compute the fermionic spin Casimir, using the completeness relation(2.20), obtaining

$$\hat{\mathbf{S}}^{2} = \sum_{a \in g} (f^{\dagger}_{\alpha}(\sigma^{a}_{N})_{\alpha\beta}f_{\beta})(f^{\dagger}_{\gamma}(\sigma^{a}_{N})_{\gamma\delta}f_{\delta}) \\
= (f^{\dagger}_{\alpha}f_{\beta})(f^{\dagger}_{\gamma}f_{\delta})[\delta_{\alpha\delta}\delta_{\beta\gamma} + \epsilon_{\alpha\gamma}\epsilon_{\delta\beta}].$$
(2.33)

This expression can also be obtained by directly expanding the unconstrained sum  $\frac{1}{2} \sum_{\alpha,\beta} \hat{S}^{\alpha\beta} \hat{S}^{\beta\alpha}$ . By normal ordering the fermion operators in the second term, we obtain

$$\hat{\mathbf{S}}^{2} = (f_{\alpha}^{\dagger}f_{\beta})(f_{\beta}^{\dagger}f_{\alpha}) + \tilde{\alpha}\tilde{\beta}(f_{\alpha}^{\dagger}f_{-\beta})(f_{-\alpha}^{\dagger}f_{\beta})$$

$$= n_{f}(N+2-n_{f}) - \sum_{\alpha,\beta} (\tilde{\alpha}f_{\alpha}^{\dagger}f_{-\alpha}^{\dagger})(\tilde{\beta}f_{-\beta}f_{\beta}),$$

$$= n_{f}(N+2-n_{f}) - 4\Psi^{\dagger}\Psi.$$
(2.34)

We can use the isospin vector, (6.24) to rewrite the spin Casimir simply as,

$$\hat{\mathbf{S}}^{2} = \frac{N}{2} \left(\frac{N}{2} + 2\right) + 2\Psi_{3} - (\Psi_{3})^{2} - \underbrace{\Psi_{1}^{2} + \Psi_{2}^{2} - i[\Psi_{1}, \Psi_{2}]}_{4\Psi^{\dagger}\Psi}$$
$$= \frac{N}{2} \left(\frac{N}{2} + 2\right) - \vec{\Psi}^{2}, \qquad (2.35)$$

since  $[\Psi_1, \Psi_2] = 2i\Psi_3$ . Alternatively,

$$\frac{1}{4}(\mathbf{S}^2 + \vec{\Psi})^2 = j(j+1),$$
  $(j = N/4),$  (2.36)

where, since N is any even number, j is an integer or half-integer. For N = 2, this identity shows that the sum of spin and charge fluctuations are fixed for conventional spin 1/2 fermions, and symplectic-N generalizes this identity for all N. When the isospin is zero,  $\vec{\Psi} = 0$ , the magnitude of the spin is maximal, and  $\mathbf{S}^2 = N/2(N/2+2)$ . When treating spin Hamiltonians, we will always use this maximal spin constraint, however, when we reintroduce charge fluctuations,  $\vec{\Psi}$  will be nonzero. This constraint imposes three conditions on any physical state  $|\psi\rangle$ :

$$\Psi_{3}|\psi\rangle = (n_{f} - N/2)|\psi\rangle = 0,$$
  

$$\Psi^{\dagger}|\psi\rangle = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{-\alpha}^{\dagger}|\psi\rangle = 0,$$
  

$$\Psi|\psi\rangle = \sum_{\alpha>0} f_{\alpha} f_{-\alpha}|\psi\rangle = 0.$$
(2.37)

The first constraint ensures that the state is half-filled,  $n_f = N/2$ , while the last two terms ensure that there are no singlet pairs in any physical state. These additional constraints are especially important when examining superconductivity, as they enforce the strong Coulomb repulsion, eliminating any s-wave pairing.

In the path integral formulation, we impose the above constraints through the following term in

the action

$$H_C = \lambda_- f_\alpha^{\dagger} f_{-\alpha}^{\dagger} + \lambda_3 (n_f - N/2) + \lambda_+ f_{-\alpha} f_\alpha$$
(2.38)

where  $\lambda = (\lambda_1, \lambda_2, \lambda_3)$  is a vector boson field coupling to the isospin  $\tau$  of the f-spin and  $\lambda_{\pm} = \lambda_1 \pm i\lambda_2$ .

#### 2.5.2 Bosonic constraints

In the Schwinger boson representation, with the generators  $\Gamma^a$ , the Casimir is written,

$$\hat{\mathbf{S}}_{j}^{2} = \sum_{a} (\frac{1}{2} b_{j\alpha}^{\dagger} \Gamma_{\alpha\beta}^{a} b_{j\beta}) (\frac{1}{2} b_{j\gamma}^{\dagger} \Gamma_{\gamma\eta}^{a} b_{j\eta}).$$
(2.39)

For symplectic spins, the completeness relation(2.20) is used to rewrite the Casimir as

$$\hat{S}_{j}^{2} = \frac{1}{4} \left( b_{j\alpha}^{\dagger} b_{j\beta} \right) \left( b_{j\gamma}^{\dagger} b_{j\eta} \right) \left[ \delta_{\alpha\eta} \delta_{\beta\gamma} + \epsilon_{\alpha\gamma} \epsilon_{\eta\beta} \right] \\
= \frac{1}{4} \left( b_{j\alpha}^{\dagger} b_{j\beta} b_{j\beta}^{\dagger} b_{j\alpha} + \tilde{\alpha} \tilde{\beta} b_{j\alpha}^{\dagger} b_{j-\beta} b_{j-\alpha}^{\dagger} b_{j\beta} \right) \\
= \frac{1}{4} \left( \left[ b_{j\alpha}^{\dagger} b_{j\alpha} b_{j\beta} b_{j\beta}^{\dagger} - n_{bj} \right] + \left[ \tilde{\alpha} \tilde{\beta} b_{j\alpha}^{\dagger} b_{j-\alpha}^{\dagger} b_{j-\beta} b_{j\beta} + n_{bj} \right] \right) \\
= \frac{1}{4} b_{j\alpha}^{\dagger} b_{j\alpha} b_{j\beta} b_{j\beta}^{\dagger},$$
(2.40)

where  $n_{bj} = \sum_{\alpha} b_{j\alpha}^{\dagger} b_{j\alpha}$  is the number of bosons on a site *j*. The last equality is due to the vanishing of antisymmetric combinations of bosons,  $\tilde{\alpha} b_{j\alpha}^{\dagger} b_{j-\alpha}^{\dagger}$  on site. Thus, for symplectic *N*, the Casimir is given by

$$\hat{\mathcal{S}}_{j}^{2} = \frac{1}{4} n_{bj} \left( n_{bj} + N \right), \qquad (2.41)$$

and is set by fixing the number of bosons on each site. If we choose the convention  $n_{bj} = NS$ , the constraint becomes

$$\hat{\mathcal{S}}_j^2 = \frac{1}{4}N^2S(S+1)$$

The Casimir for SU(N) can be obtained similarly, using the SU(N) completeness relation(2.15)

instead of (2.20):

$$\hat{T}_j^2 = \frac{1}{2} \left( n_b (n_b + N) - n_b - \frac{1}{N} n_b^2 \right), \qquad (2.42)$$

where we have dropped the j index on  $n_b$  for clarity. Using the consistent convention  $n_b = NS$ , the SU(N) constraint becomes

$$\hat{T}_j^2 = \frac{1}{2}(N^2 - N)S(S+1).$$

For N = 2, this reduces to S(S+1) and the SU(N) and SP(N) Casimirs are identical, as required. For all other N,  $\hat{T}_j^2$  will be larger. This means that the antisymplectic spins,  $\hat{\mathcal{P}}_j^2 = \hat{T}_j^2 - \hat{\mathcal{S}}_j^2$  can never be removed for any N > 2. In the large N limit, they are forced to have equal magnitudes:  $\hat{\mathcal{P}}_j^2 = \hat{\mathcal{S}}_j^2$ .

At first sight, this requirement is quite strange. After all, there are  $N^2 - 1$  independent SU(N) generators, which we have been treating as a vector,  $\mathcal{T}$ , why can the spin not point in  $N^2 - 1$  directions? The answer is that not all directions of the SU(N) vector give rise to different spins. The spin itself is given by  $\frac{1}{2}b_j^{\dagger} \cdot \mathcal{T} \cdot b_j$ , and b has N components. The constraint removes one more degree of freedom. For a general state, b is a bosonic vector, but when the spins order,

$$\langle \hat{\mathcal{S}}_{j} \rangle = \frac{1}{2} \langle b_{j\alpha}^{\dagger} \mathcal{S}_{\alpha\beta} b_{j\beta} \rangle = \frac{1}{2} \langle b^{\dagger} \rangle_{j\alpha} \mathcal{S}_{\alpha\beta} \langle b \rangle_{j\beta}, \qquad (2.43)$$

 $\langle b \rangle$  is an N component complex vector, so the spin can only take on 2N-1 different configurations. The spins are constrained to a 2N-1 dimensional manifold  $\mathcal{M}$ .

To be more mathematically precise, this manifold  $\mathcal{M}$  is a "homogeneous space" of SU(N):  $SU(N)/H_x$ , where  $H_x$  is the "stabilizer" of x, the subgroup which leaves an SU(N) element x invariant:

$$H_x = \{ g \in SU(N) | g \cdot x = x \}.$$
(2.44)

Without loss of generality we can choose x to be the spin defined by  $b^T = (1, 0, ..., 0)$ . Rotating b by any matrix which affects only the lowest N-2 entries clearly leaves x invariant, as does rotating the phase of the upper two entries, so  $H_x = SU(N-2) \ge U(1)$ , and

$$\mathcal{M}_{SU(N)} = SU(N)/SU(N-2)\mathbf{x}U(1) \cong CP^{N-1}.$$
 (2.45)

The full SU(N) spin lives on the manifold  $CP^{N-1}$ , while the symplectic spin  $\frac{1}{2}b_j^{\dagger} \cdot S \cdot b_j$  lives on a 2N-1 dimensional manifold, given by

$$\mathcal{M}_{SP(N)} = SP(N)/SP(N-2)\mathbf{x}U(1). \tag{2.46}$$

Since  $\hat{\mathcal{P}}$  is nonzero,  $\mathcal{M}_{SP(N)}$  is not contained within  $\mathcal{M}_{SU(N)}$ ; in fact, the two manifolds have equal dimension, although they are not isomorphic. Rather, any point on  $\mathcal{M}_{SP(N)}$  will correspond to a point on  $\mathcal{M}_{SU(N)}$ . Strictly speaking, this manifold is the order parameter manifold for a long range ordered state, however, it paints a useful picture of the relationship between SU(N)and SP(N) spins. Furthermore, the order parameter manifold will be essential in describing the magnetically ordered state, where, for a spiral state which completely breaks the symmetry, the number of Goldstone modes will be 2N - 1.

## 2.6 Hubbard Operators

When charge fluctuations are reintroduced into strongly correlated spin problems, they must still be strongly restricted by the large on-site repulsion U. Electrons hopping into and out of a Hubbard orbital are constrained by the high energy cost of double occupancy, and a proper treatment of this *projected hopping* requires the introduction of *Hubbard operators* to project out any doubly occupied states [98]. These operators,  $X_{ab} = |a\rangle\langle b|$ , act within the space  $|a\rangle = |0, \uparrow, \downarrow\rangle$ , where the diagonal Hubbard operators,  $X_{aa}$  are projection operators, satisfying the completeness relation,

$$X_{00} + \sum_{\sigma} X_{\sigma\sigma} = 1, \qquad (2.47)$$



Figure 2.3: SU(N) spins consist of two components: symplectic directions that reverse under time reversal, and antisymplectic directions that are invariant under time reversal, which prevent SU(N) spins from forming two particle singlets. However, if the spins are projected into the symplectic plane, these components *can* form two particle singlets, which are well defined as long as the antisymplectic components are noninteracting.

and obeying bosonic commutation relations. The off-diagonal Hubbard operators,  $X_{\sigma 0}$  and  $X_{0\sigma}$  are projected creation/annihilation operators, which obey the anti-commutation relations,

$$\{X_{\sigma 0}, X_{\sigma' 0}\} = X_{\sigma \sigma'} + X_{00}\delta_{\sigma,\sigma'}.$$
(2.48)

We say that the Hubbard operators together satisfy a *graded Lie algebra*, which is bosonic for some components and fermionic for the others. Physically, this expression encodes the relationship between hopping an electron on and off a site and flipping the spin.

Since Hubbard operators, like spins, do not obey canonical commutation relations, they cannot be treated directly within quantum field theory. Also like spins, Hubbard operators may be represented as bilinears of fermions and bosons. In the *slave boson* approach [100, 101], a boson,  $b^{\dagger}$ 



Figure 2.4: A spin flip,  $S_{-} = X_{\uparrow\downarrow}$  is equivalent to hopping an electron off the site and back on again with the opposite spin.

is introduced to represent the empty state, while fermions,  $f_{\sigma}^{\dagger}$  represent the singly occupied spin states:

$$|0\rangle = b^{\dagger}|\Omega\rangle$$
  
$$|\sigma\rangle = f_{\sigma}^{\dagger}|\Omega\rangle, \qquad (2.49)$$

where  $|\Omega\rangle$  is a vacuum containing no fermions or bosons. It can be checked explicitly that the projected hopping operators,

$$X_{0\sigma} = b^{\dagger} f_{\sigma}, \qquad (2.50)$$

satisfy the commutation relations, (6.15), and  $X_{00} = b^{\dagger}b$  counts the number of bosons. In effect, we separate the electron into charged, but spinless holons and neutral spinons, which now have the potential to move separately - the ultimate in collective behavior. Here, we have chosen the holon to be bosonic and the spinon to be fermionic, but we could just have easily made the opposite choice, called the slave fermion representation. As with spins, the physics does not depend on the particular representation for N = 2, but as we go to the large N limit, the slave boson representation easily captures the physics of heavy Fermi liquids and superconductivity, while slave fermions describe magnetism. In this dissertation we are more interested in superconductivity, so we stick with the slave boson representation.

The constraint of no double occupancy fixes the total number of particles,  $n_b + n_f = 1$ , enforced at each site by a Lagrange multiplier,  $\lambda_i$ . This constraint eliminates all but the three physical atomic states (2.49). Since the constraint generally commutes with the Hamiltonian, the physical and nonphysical states do not mix. As these Hubbard operators are invariant under a local U(1)gauge transformation,  $b_i \rightarrow b_i e^{i\theta_i}$ ,  $f_{i\sigma} \rightarrow f_{i\sigma} e^{i\theta_i}$  [127, 128], they are known as U(1) slave bosons. By examining the anti-commutation relations, we see that  $X_{\sigma\sigma'} = f_{\sigma}^{\dagger} f_{\sigma'}$  is an SU(N) spin flip, and these U(1) slave bosons correspond to SU(N) spins in the large N limit.

## 2.7 Symplectic Hubbard operators

In order to develop a symplectic slave-boson approach, we must find a slave boson representation where the spin-flips associated with removed and then replacing an electron,

$$\{X_{\alpha 0}, X_{\beta 0}\} = X_{\alpha \beta} + X_{00}\delta_{\alpha,\beta}, \qquad (2.51)$$

are symplectic spin-flips,

$$S_{\alpha\beta} = f_{\alpha}^{\dagger} f_{\beta} + \tilde{\alpha} \tilde{\beta} f_{-\alpha} f_{-\beta}^{\dagger}.$$
(2.52)

The spin operators,  $S_{\alpha\beta}$  are the traceless forms of the Hubbard operators,  $X_{\alpha\beta}$ ,

$$S_{\alpha\beta} = X_{\alpha\beta} - \frac{X_{\gamma\gamma}}{N},\tag{2.53}$$

where the repeated  $\gamma$  is summed over. We can also rewrite (2.51) as,

$$\{X_{\alpha 0}, X_{\beta 0}\} = S_{\alpha \beta} + \left(X_{00} + \frac{X_{\gamma \gamma}}{N}\right)\delta_{\alpha,\beta}.$$
(2.54)

The algebra requires the introduction of two slave bosons,

$$X_{0\alpha} = b^{\dagger} f_{\alpha} + a^{\dagger} \tilde{\alpha} f_{-\alpha}^{\dagger}$$
  

$$X_{00} = b^{\dagger} b + a^{\dagger} a.$$
(2.55)

Doubling the number of slave bosons preserves the symplectic character of the spins and we shall

see that this encodes the hard-to-enforce absence of double occupancy as a more mathematically tractable SU(2) gauge symmetry. These Hubbard operators can be written more compactly by using the Nambu notation,

$$X_{0\alpha} = B^{\dagger} \tilde{f}_{\alpha}, \ X_{00} = B^{\dagger} B$$
  
where  $B^{\dagger} = \left(b^{\dagger}, \ a^{\dagger}\right), \ \text{and} \ \tilde{f}_{\alpha} = \left(\begin{array}{c} f_{\alpha} \\ \tilde{\alpha} f_{-\alpha}^{\dagger} \end{array}\right).$  (2.56)

Due to their neutrality, the spins are invariant under a continuous particle-hole symmetry,  $f_{\alpha} \rightarrow u f_{\alpha} + v \tilde{\alpha} f_{-\alpha}^{\dagger}$ , which is reflected in the requirement of two types of bosons. The empty state does not distinguish between zero and two fermions, and thus requires two bosons to keep track of the two ways of representing the empty state,  $b^{\dagger} |\Omega\rangle$  and  $a^{\dagger} f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} |\Omega\rangle = a^{\dagger} \Psi^{\dagger} |\Omega\rangle$ , where  $|\Omega\rangle$  is the vacuum containing no particles of any kind. Of course, there is only one physical empty state, as becomes clear when we restrict these Hubbard operators to the physical subspace. As discussed in section 2.5.1, in order to faithfully represent the symplectic spins, the sum of the spin and charge fluctuations must be fixed,  $\vec{S}^2 + \vec{\Psi}^2 = N/2(N/2 + 2)$ . In the pure spin model, this constraint is enforced by setting  $\vec{\Psi} = 0$ , here we must equate our two types of charge fluctuations, by setting  $\vec{\Psi} = -B^{\dagger}\vec{\tau}B$  (these have opposite signs because  $B^{\dagger}$  creates holes). The constraint is therefore  $\vec{Q} = B^{\dagger}\vec{\tau}B + \tilde{f}_{\alpha}^{\dagger}\vec{\tau}\tilde{f}_{\alpha} = 0$ , which commutes with the Hamiltonian, so that the physical subspace does not mix with any unphysical spaces. Written out explicitly,

$$Q_{3} = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{\alpha} - N/2 + b^{\dagger} b - a^{\dagger} a = 0$$

$$Q_{+} = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{-\alpha}^{\dagger} + b^{\dagger} a = 0$$

$$Q_{-} = \sum_{\alpha>0} f_{-\alpha} f_{\alpha} + a^{\dagger} b = 0.$$
(2.57)

The constraint reflects the neutrality of the spins under charge conjugation:  $Q_3$  conserves total electromagnetic charge, and prevents doubly occupancy, while  $Q_{\pm}$  kills any states with s-wave pairs on-site. It is clear from this constraint that b and a have opposite gauge charges, and the only

gauge invariant states satisfying the constraint (for N = 2) are,

$$|\alpha\rangle = = f_{\alpha}^{\dagger}|\Omega\rangle$$
  
$$|0\rangle = = \left(b^{\dagger} + a^{\dagger}\Psi^{\dagger}\right)|\Omega\rangle.$$
 (2.58)

For N = 2, these Hubbard operators are the SU(2) slave bosons introduced by Wen and Lee in the context of the t-J model [129]. Here, it becomes clear that the SU(2) structure is a consequence of symplectic symmetry, present in both the symplectic-N spin and Hubbard operator representations for all N. We can physically interpret the SU(2) symmetry as the result of charge fluctuations in the presence of a particle-hole symmetric spin.

We apply these Hubbard operators both to the two channel Anderson model, in chapter 6 and the t - J model in chapter 7, where the symplectic symmetry allows us to examine superconducting ground states.

# **Chapter 3**

## **Frustrated magnetism**

The search for simple, controlled approximations which capture the collective behavior of matter is a key goal of condensed matter. In quantum magnetism, this search is hindered by the lack of a small parameter; after more than a decade, theorists and experimentalists are still searching for a physically realizable quantum spin liquid [21], and the ground state behavior of highly frustrated magnets, like the kagomé [22, 130, 131], pyrochlore [132, 22] and hyperkagomé [133, 134, 135] lattices is still unclear. One approximation that has proven successful is the "large N" expansion, which generalizes the model of interest to a family of models where the number of internal degrees of freedom is indexed by an integer N. As N goes to infinity, central limit effects permit the underlying collective behavior of the model to be solved exactly, and finite N properties may be obtained from a power series expansion in 1/N about this solution.

The basic equation of quantum magnetism is the Heisenberg Hamiltonian,

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \tag{3.1}$$

where the spin on each site,  $\vec{S}_i$  lives in the group SU(2). The exchange coupling J can be either positive or negative, for simple lattices these lead to antiferromagnetic or ferromagnetic ground states, respectively. Both ground states break both spin rotational and time reversal symmetries, but the antiferromagnet is invariant under the combination of time reversal and translation by one lattice site. More complicated lattices can lead to spins which are not collinear, so called spiral magnets, or possibly to a state in which the spins are not ordered at all, a spin liquid.

#### **3.0.1** Previous large N treatments of the Heisenberg model

The Heisenberg model has one energy scale, J, and the J = 0 state is extensively degenerate. There are therefore no natural small parameters with which to conduct perturbation theory, and the Heisenberg model is a prime candidate for large N expansions. The first class of such limits is semi-classical: the large S limit, which corresponds to taking arbitrarily large spin representations was originally introduced by Anderson [31] and Dyson [32] to study spin fluctuations in magnetically ordered states. In the classical limit,  $S \to \infty$ , spins become three dimensional vectors with magnitude S, and the ground state energy is  $E_0 = -S^2 J(\vec{Q})$ , where  $J(\vec{Q})$  is the Fourier transform of the  $J_{ij}$  evaluated at the ordering vector,  $\vec{Q}$ ; for example,  $\vec{Q} = \vec{0}$ ,  $\vec{\pi}$  describe ferromagnetic and antiferromagnetic orders, respectively. The classical ground state is always ordered, unless there is a degenerate manifold of  $\vec{Q}$ 's, and the O(S) terms describe spin wave fluctuations, which diverge when frustration, dimensionality, or simply temperature, destabilize the ordered state. However, the large S limit gives little information about magnetically disordered states. Meanwhile, a different semi-classical treatment, mapping the long wavelength behavior of a disordered Heisenberg magnet to a continuum nonlinear sigma model yields a lot of information about disordered one dimensional systems, but it is unclear how it fails for small S [36, 34, 35].

It is therefore desirable to develop a *quantum* large N limit, which can be done by generalizing SU(2) to some larger group. The spins are now proportional to the generators of a representation of this larger group. The most natural idea seems to be to generalize SU(2) to SU(N), the group of  $N \times N$  special unitary matrices. SU(N) has many more representations than SU(2) [136, 137], but there are two simple choices: symmetric bosonic representations, where larger representations again represent larger spins set by  $n_b = 2S$  [123]; and an antisymmetrized fermionic representation, which represents spin 1/2 with  $n_f = 1$  [37]. The Heisenberg Hamiltonian can be rewritten,

$$H = \frac{J}{N} \sum_{ij} \vec{S}_i \cdot \vec{S}_j = \frac{J}{N} \sum_{ij} S_{\alpha\beta}(i) S_{\beta\alpha}(j), \qquad (3.2)$$

where  $S_{\alpha\beta} = \psi^{\dagger}_{\alpha}\psi_{\beta}$  are SU(N) spins,  $\alpha \in \{1, \ldots, N\}$ ,  $\psi$  is either fermionic or bosonic, and J



Figure 3.1: The various large N techniques in magnetism. Either the spin, S can become large, in a semi-classical limit, where the ground state is generally ordered (shaded portion of the diagram), or the spin degeneracy, N can become large, giving rise to a quantum mean field which may be either ordered or disordered (unshaded). The fermionic large N theory captures the extreme quantum limit, far from magnetic order, while the bosonic large N theory can keep 2S/N fixed as  $N \to \infty$  and treat both order and disorder, and the nonlinear sigma model (NLSM) treats the phase transition between these two ground states semi-classically. Modified from [136].

is rescaled by N to make H extensive in N. Arovas and Auerbach introduced the bosonic SU(N) $(S_{\alpha\beta} = b^{\dagger}_{\alpha}b_{\beta})$  [123], where

$$H = J \sum_{ij} \left( b_{i\alpha}^{\dagger} b_{j\alpha} \right) \left( b_{j\beta}^{\dagger} b_{i\beta} \right).$$
(3.3)

 $(b_{i\alpha}^{\dagger}b_{j\alpha})$  coherently hops a Schwinger boson between sites, correlating them ferromagnetically. In the large N limit,  $(b_{i\alpha}^{\dagger}b_{j\alpha})$  is replaced by its expectation value,  $\langle b_{i\alpha}^{\dagger}b_{j\alpha} \rangle$ . By transforming  $S_{\alpha\beta} \rightarrow \tilde{S}_{\alpha\beta} = -b_{\beta}^{\dagger}b_{\alpha}$  on one of the two sublattices, this method can also treat bipartite antiferromagnets, where  $(b_{i\alpha}^{\dagger}b_{j\alpha}^{\dagger})$  creates an antiferromagnetic singlet, or valence bond, as can be seen by reversing the transformation [138]. To get a little more technical, the transformation is equivalent to putting spins in representation A on sublattice A and spins in the conjugate representation,  $\bar{A}$  on sublattice B. For SU(2), all representations are *self-conjugate*, and the same representation can be placed on every site. However, the symmetric representations of SU(N) are not self-conjugate for N > 2, requiring this peculiar transformation. The SU(N) mean field theory agrees well with exact Bethe-Ansatz results on spin chains [139], except for half-integral S, where the mean field theory predicts a gap where the ground state is gapless, and the first order in 1/N corrections are necessary (and sufficient) to restore the gapless nature of the state [136]. With this caveat, the large N limit works well for ferromagnets and bipartite antiferromagnets, but the spin transformation is impossible for frustrated lattices with more than two sublattices.

The fermionic SU(N) approach, introduced by Affleck and Marston [37, 140], always has an antisymmetric self-conjugate representation, and can be used to study frustrated lattices, however, S is fixed to 1/2 while N gets large, making S/N extremely small. The fermionic representation describes the extreme quantum limit, and can never capture long range order, which is easily described by Bose condensation in the bosonic representation [141]. The fermionic large N limit is useful for studying spin liquid states, but not for determining if a particular model will have a spin liquid ground state in the first place.

In order to treat frustrated antiferromagnets for finite S/N, Sachdev and Read [42, 142] introduced the SP(N) Hamiltonian,

$$H = -\sum_{ij} \frac{J_{ij}}{N} \left( b_{i\alpha}^{\dagger} \tilde{\alpha} b_{j-\alpha}^{\dagger} \right) \left( b_{j-\beta} \tilde{\beta} b_{i\beta} \right), \qquad (3.4)$$

where N must be even,  $\alpha \in \{-N/2, ..., N/2\}$  and  $\tilde{\alpha} = \operatorname{sgn}(\alpha)$ .  $(b_{i\alpha}^{\dagger} \tilde{\alpha} b_{j-\alpha}^{\dagger})$  explicitly creates a valence bond singlet between sites *i* and *j*, and this Hamiltonian can treat antiferromagnetic correlations on any lattice [130, 132, 134, 135]. It turns out (as we showed in Chapter 2) that this Hamiltonian is not constructed from the generators of the SP(N) group; instead it breaks the SU(N) symmetry of the Hamiltonian down to SP(N). Just as SU(N) naturally treats only ferromagnetism, SP(N) can only naturally treat antiferromagnetism. Here, we develop the bosonic symplectic-N approach for the Heisenberg model, which enables us to treat ferromagnetism and antiferromagnetism on equal footing. The structure of this chapter is as follows. In section 3.1, we review the bosonic representation of symplectic spins and discuss the importance of removing the anti-symplectic spins to obtain the correct ground states and spin dynamics. In section 3.2, we derive the mean field equations for a generic Heisenberg magnet in the symplectic-N limit, while in section 3.3, we apply these ideas to the two dimensional  $J_1 - J_2$  model, finding both the zero temperature and finite temperature phase diagrams. Finally, in section 3.4, we draw conclusions about the application of symplectic-N to other models.

### 3.1 Time reversal and symplectic symmetry

An SU(2) spin Hamiltonian has two symmetries - invariance with respect to SU(2) rotations and time reversal invariance, where we have shown in Chapter 2 that the inversion of spins under time reversal,

$$\vec{S} \to \theta \vec{S} \theta^{-1} = \hat{\epsilon} \vec{S}^T \hat{\epsilon} = -\vec{S}, \tag{3.5}$$

is equivalent to the symplectic condition,

$$U\hat{\epsilon}U^T = \hat{\epsilon}.\tag{3.6}$$

So maintaining the time-reversal symmetries of SU(2) spins in the large N limit requires the use of symplectic spins,

$$S_{\alpha\beta} = b_{\alpha}^{\dagger} b_{\beta} - \tilde{\alpha} \tilde{\beta} b_{-\beta}^{\dagger} b_{-\alpha}, \qquad (3.7)$$

where

$$\alpha \in \{-N/2, .., -1, 1, .., N/2\}, \text{ and } \tilde{\alpha} = \operatorname{sgn}(\alpha).$$
 (3.8)

The Heisenberg Hamiltonian, (3.1) is written,

$$\sum_{ij} \frac{J_{ij}}{N} \hat{\mathcal{S}}_i \cdot \hat{\mathcal{S}}_j = \frac{J_{ij}}{N} \left( -B_{ji}^{\dagger} B_{ji} + A_{ji}^{\dagger} A_{ji} \right)$$
(3.9)

where

$$B_{ji}^{\dagger} = \frac{1}{2} \sum_{\sigma} \tilde{\sigma} b_{j\sigma}^{\dagger} b_{i-\sigma}^{\dagger}$$
(3.10)

creates a valence bond, or spin singlet pair, between sites i and j, and

$$A_{ji}^{\dagger} = \frac{1}{2} \sum_{\sigma} b_{j\sigma}^{\dagger} b_{i\sigma}$$
(3.11)

creates a ferromagnetic bond, which implies the coherent hopping of Schwinger bosons from site to site. In the language of valence bonds, a ferromagnetic bond can be thought of as resonating one end of a valence bond between sites i and j, causing both sites to be simultaneously antiferromagnetically correlated with a third site, thus ferromagnetically correlated with one another. In this sense, it is a frustrating field. Most generally, a ferromagnetic bond on a link with antiferromagnetic J, or vice versa, can be considered frustrating fields, however, we will usually be dealing with entirely antiferromagnetic lattices, where any ferromagnetic bond is a frustrated bond. This decoupling is identical to the SU(2) mean field theory introduced by Ceccatto *et al.* [121], now controlled by the large N limit of properly time reversing spins.



Figure 3.2: The symplectic-N Heisenberg Hamiltonian contains terms,  $B^{\dagger}$  that create valence bonds (blue) that antiferromagnetically correlate two spins, and terms,  $A^{\dagger}$  that hop the ends of valence bonds between two sites, so that these two sites become antiferromagnetically correlated with a third site, and thus ferromagnetically correlated with one another (red).

This Hamiltonian must be supplemented with the constraint, derived in section 2.5.2, that  $n_{bj} =$ 

2S on each site to ensure that  $\hat{S}_j^2 = \frac{1}{4}N^2S(S+1)$ . This constraint fixes the size of the symplectic spins, but we must remember that because of the relationship between the spin Casimirs of the SU(N) and SP(N) groups, the anti-symplectic spins have equal magnitudes in the large N limit:  $\hat{\mathcal{P}}_j^2 = \hat{S}_j^2$ , and in general the anti-symplectic spins will always be present for any N > 2.

We now wish to compare this representation with SU(N) [123] and the previous SP(N) treatment [42].

Approach	$\mathrm{H}(\mathcal{S},\mathcal{P})$	$\mathrm{H}(b^{\dagger},b)$
SU(N)	$J\left(\mathcal{S}\cdot\mathcal{S}+\mathcal{P}\cdot\mathcal{P}\right)$	$JA^{\dagger}A$
SP(N)	$J\left(\mathcal{S}\cdot\mathcal{S}-\mathcal{P}\cdot\mathcal{P}\right)$	$-JB^{\dagger}B$
Symplectic-N	$JS \cdot S$	$J\left(-B^{\dagger}B + A^{\dagger}A\right)$

The SU(N) Hamiltonian contains both symplectic and anti-symplectic spins, in equal measure as expected, but surprisingly, the SP(N) large N theory weights the physical symplectic and unphysical antisymplectic spins equally, but with opposite signs.

Why is it important to exclude the non-time reversing dipoles? Both the symplectic  $(\hat{S}_i \cdot \hat{S}_j)$ and antisymplectic  $(\hat{P}_i \cdot \hat{P}_j)$  interactions are invariant under time reversal, however, the important difference is not in the Hamiltonian, but in the ground states and the dynamics. These are far more coupled than the Hamiltonian suggests because the SU(N) spin  $\hat{T}$  does not act as a vector, and the antisymplectic and symplectic directions are not independent directions, so that  $\hat{T}$  is unable to point in a purely symplectic direction. The antisymplectic interactions encourage the antisymplectic spins to order - competing with the ordering of the physical components. This competition eliminates the antiferromagnetic[ferromagnetic] ground state completely for SU(N)[SP(N)]. And finally, even if the ground state is the one of interest, the presence of antisymplectic interactions affects the dynamics of the symplectic spins, dynamically violating the closure of the symplectic subgroup.

## 3.1.1 Ground States

A generic Heisenberg Hamiltonian with symplectic invariance contains both antisymplectic and symplectic interaction terms,

$$H = \sum_{ij} J_{ij} \hat{S}_{i} \cdot \hat{S}_{j} + K_{ij} \hat{\mathcal{P}}_{i} \cdot \hat{\mathcal{P}}_{j}$$
  
$$= \sum_{ij} (K_{ij} - J_{ij}) B_{ij}^{\dagger} B_{ij} + (K_{ij} + J_{ij}) A_{ij}^{\dagger} A_{ij}$$
(3.12)

in a ratio K/J, which is  $\pm 1$  for SU(N) and SP(N), respectively, and zero for symplectic-N. In general, the physical, symplectic spins and and the antisymplectic spins may have different interaction strengths and signs.

In the  $S \to \infty$  classical limit, the system is long range ordered, and all the bosons are condensed. The ordered state is described by the angle between neighboring spins,  $\phi_{ij} \equiv \phi_i - \phi_j$  which is 0 for a ferromagnet and  $\pi$  for an antiferromagnet. If we fix  $\langle b \rangle_i = \sqrt{NS}(1, 0, ...)^T$ , we can rotate the top two coordinates of  $\langle b \rangle_j$  by

$$R(\phi_{ij}) = \begin{pmatrix} \cos\frac{\phi_{ij}}{2} & \sin\frac{\phi_{ij}}{2} \\ -\sin\frac{\phi_{ij}}{2} & \cos\frac{\phi_{ij}}{2} \end{pmatrix},$$
(3.13)

which makes  $\langle b \rangle_j = \sqrt{NS} \left( \sin \frac{\phi_{ij}}{2}, \cos \frac{\phi_{ij}}{2}, 0, \ldots \right)$ , and the two bond expectation values will be

$$B_{ij} = \langle b \rangle_j^T \langle b \rangle_i = NS \sin \frac{\phi_{ij}}{2}$$
  

$$A_{ij} = \langle b \rangle_i^T \langle b \rangle_j = NS \cos \frac{\phi_{ij}}{2}$$
(3.14)

Thus the ground state energy for (3.12) is

$$E = \sum_{ij} (K - J)_{ij} \sin^2 \frac{\phi_{ij}}{2} + (K + J)_{ij} \cos^2 \frac{\phi_{ij}}{2}$$
(3.15)

The three special cases of interest are

$$E_{symp-N} = \sum_{ij} NS^2 J_{ij} \cos \phi_{ij}$$

$$E_{SP(N)} = \sum_{ij} -NS^2 J_{ij} \sin^2 \frac{\phi_{ij}}{2}$$

$$E_{SU(N)} = \sum_{ij} NS^2 J_{ij} \cos^2 \frac{\phi_{ij}}{2}.$$
(3.16)

We see that for antiferromagnetic bonds in SU(N), the ground state energy is zero, identical to that of the paramagnet with  $\langle S \rangle = 0$ , and similarly for the ferromagnetic bonds in SP(N). Only symplectic-N has well defined ground states for both signs of J.



Figure 3.3: A toy picture of SU(N) spins, where the symplectic, time reversing components are represented in blue along the  $\hat{y}$  axis, and the antisymplectic, non time reversing components are in red, along the  $\hat{x}$  axis. The purple spin shows the full SU(N) spin obtained by adding its symplectic and antisymplectic components. (a) depicts a ferromagnetic state. (b) depicts an antiferromagnetic state, where we obtain the antiferromagnet by time reversing every other spin. While the symplectic components are anti-parallel, the antisymplectic components are still aligned, causing the total spins to be orthogonal at neighboring sites.

If we turn to finite S, we can construct ferromagnetic and antiferromagnetic states explicitly out of the SU(N) spins, see Figure 3.3. The antiferromagnetic state is defined by dividing the spins into two ferromagnetic sublattices, where sublattice B spins are the time reverse of A. This state satisfies the lattice translation plus time reversal symmetry of the SU(2) antiferromagnetic ground state. The  $\hat{\mathcal{P}}$ 's are aligned in both ground states, and in the large N limit, the magnitudes of  $\hat{S}$  and  $\hat{\mathcal{P}}$  are the same. In SU(N), K = J, so both interactions are maximally satisfied in the ferromagnet - leading in fact to overstabilization due to excess  $\hat{\mathcal{P}}$  bonds, while the antiferromagnet consists of orthogonal SU(N) spins, the two terms in the Hamiltonian cancel and the ground state energy is zero, just as found classically. When K = -J, as in SP(N), it is the antiferromagnetic ground state that is overstabilized by ferromagnetic  $\hat{\mathcal{P}}$  bonds, and the ferromagnetic state has zero energy. These conclusions hold not only for the full ground state, but for individual bonds; in frustrated lattices there will be both antiferromagnetic and ferromagnetic correlations, even if all J's are positive, but SP(N) indicates ferromagnetic correlations only by the absence of a bond. The energy cost of ferromagnetic correlations is zero in SP(N), but we know that in real lattices these frustrated bonds carry a price. By eliminating the antisymplectic interactions, symplectic-N removes the extraneous bonds between  $\hat{\mathcal{P}}$ 's and restores the ability of SU(2) to simultaneously treat both ferromagnetism and antiferromagnetism.

#### 3.1.2 Spin dynamics

Even if the ground state is correct, as for the bipartite antiferromagnet in SP(N), we still need to be concerned about the spin dynamics. We chose to use the group SP(N) not only because its spins all invert under time reversal, but because the group contains well defined particle-particle singlets. The presence of antisymplectic interactions, *even if they are only interacting with themselves* dynamically violates the closure of the symplectic subgroup.

The dynamics of a symplectic spin component at a site i are given by

$$\frac{d\hat{\mathcal{S}}_{i}^{a}}{dt} = \frac{i}{\hbar} \sum_{kj} \left( J_{kj} \left[ \hat{\mathcal{S}}_{i}^{a}, \hat{\mathcal{S}}_{k} \cdot \hat{\mathcal{S}}_{j} \right] + K_{kj} \left[ \hat{\mathcal{S}}_{i}^{a}, \hat{\mathcal{P}}_{k} \cdot \hat{\mathcal{P}}_{j} \right] \right).$$
(3.17)

We concentrate on the effect of the second term, which is generally nonzero when K is nonzero. Inserting the Schwinger boson representation, we find

$$\begin{bmatrix} \hat{S}_{i}^{a}, \hat{\mathcal{P}}_{k} \cdot \hat{\mathcal{P}}_{j} \end{bmatrix} = \frac{1}{8} \begin{bmatrix} b_{i}^{\dagger} \cdot S^{a} \cdot b_{i}, \left( b_{k}^{\dagger} \cdot \mathcal{P}^{b} \cdot b_{k} \right) \left( b_{j}^{\dagger} \cdot \mathcal{P}^{b} \cdot b_{j} \right) \end{bmatrix}$$
$$= \frac{1}{8} \{ b_{j}^{\dagger} \cdot \mathcal{P}^{b} \cdot b_{j}, \left[ b_{i}^{\dagger} \cdot S^{a} \cdot b_{i}, b_{k}^{\dagger} \cdot \mathcal{P}^{b} \cdot b_{k} \right] \}$$
(3.18)
$$\begin{bmatrix} b_i^{\dagger} \cdot S^a \cdot b_i, b_k^{\dagger} \cdot \mathcal{P}^b \cdot b_k \end{bmatrix} = S^a_{\alpha\beta} \mathcal{P}^b_{\lambda\eta} \begin{bmatrix} b_{i\alpha}^{\dagger} b_{i\beta}, b_{k\lambda}^{\dagger} b_{k\eta} \end{bmatrix}$$
$$= \delta_{ik} b_{i\alpha}^{\dagger} \begin{bmatrix} S^a, \mathcal{P}^b \end{bmatrix}_{\alpha\beta} b_{i\beta}$$
$$= 2i \delta_{ik} g^{ab}{}_c \hat{T}^c_i.$$
(3.19)

where  $g^{ab}{}_{c}$  is the appropriate SU(N) structure factor. Since the commutator,  $[S, \mathcal{P}]$  is odd under time reversal,  $\mathcal{T}_{i}^{c}$  must be an antisymplectic spin. So the evolution of  $S_{i}$  is affected by the antisymplectic spins,

$$\left(\frac{d\hat{S}_i}{dt}\right)_{\hat{\mathcal{P}}\cdot\hat{\mathcal{P}}} = -\frac{1}{\hbar}\hat{\mathcal{P}}_i \times \sum_j K_{ij}\hat{\mathcal{P}}_j \tag{3.20}$$

where  $\times$  is the cross product defined by  $g^{ab}{}_{c}$ . The full dynamics of the symplectic spins are given by

$$\frac{d\hat{S}_i}{dt} = -\frac{1}{\hbar} \left( \hat{S}_i \times \sum_j J_{ij} \hat{S}_j + \hat{\mathcal{P}}_i \times \sum_j K_{ij} \hat{\mathcal{P}}_j \right).$$
(3.21)

These dynamics are identical in form to classical spin wave theory, where the spins are torqued by an effective magnetic field coming from neighboring spins. The symplectic and antisymplectic components of  $\hat{T}_i$  are torqued by the effective magnetic fields given by  $\sum_j J_{ij}\hat{S}_j$  and  $\sum_j K_{ij}\hat{P}_j$ , respectively. The effective field coming from the antisymplectic components is not strictly a magnetic field, as it has even time reversal parity, but most importantly, it rotates  $\hat{\mathcal{P}}$  into  $\hat{S}$ , and vice versa. Ordinary SU(2) spin waves will also break spin singlets, but the excitations remain in the SU(2) space, while the excitations for  $K \neq 0$  will take us out of the SP(N) group. It is clear that to have a theory of interacting SP(N) spins, all the antisymplectic interactions must be eliminated; all other Hamiltonians with symplectic invariance describe anisotropic SU(N) spin interactions.

So we have seen that the inclusion of antisymplectic spin interactions have a rather serious effect on the physics of the Heisenberg model. When these interactions are excluded, as in symplectic-N, the unphysical antisymplectic spins can no longer affect the physical spins. In a sense, they come along for the ride, since they are always there, and they are affected by the symplectic spins, but have no effect on the physics. Now we move on to the application of symplectic-N to general lattices.

### **3.2** Solving the symplectic-*N* Heisenberg model

Now we return to the symplectic-N Heisenberg model(3.9) to discuss how to solve the Hamiltonian in the large N limit, for a general lattice specified by  $J_{ij}$ . As a refresher, the Hamiltonian is

$$H[b] = \sum_{ij} \frac{J_{ij}}{N} \hat{\mathcal{S}}_i \cdot \hat{\mathcal{S}}_j = \sum_{ij} \frac{J_{ij}}{N} \left[ -B_{ji}^{\dagger} B_{ji} + A_{ji}^{\dagger} A_{ji} \right], \qquad (3.22)$$

where  $B_{ji}^{\dagger} = \frac{1}{2}\tilde{\sigma}b_{i\sigma}^{\dagger}b_{j-\sigma}^{\dagger}$  and  $A_{ji}^{\dagger} = \frac{1}{2}b_{i\sigma}^{\dagger}b_{j\sigma}$  and the sum over  $\sigma$  is implied.

The usual prescription for solving these problems is to write the partition function as a path integral,

$$\mathcal{Z} = \int \mathcal{D}b \,\mathrm{e}^{-N\mathcal{S}[b]} \prod_{j\tau} \delta\left(\hat{\mathcal{S}}_j^2(\tau) - N^2 S(S+1)\right)$$
(3.23)

where  $N\mathcal{S}[b]$  is the action

$$N\mathcal{S}[b] = \int_0^\beta d\tau \left[ \sum_i \bar{b}_{i\sigma}(\tau) \partial_\tau b_{i\sigma}(\tau) + H[b(\tau)] \right], \qquad (3.24)$$

and the constraint  $\prod_j \delta \left( \hat{S}_j^2(\tau) - N^2 S(S+1) \right)$  restricts the spins to the physical subspace at every site j and time  $\tau$ . This constraint can be rewritten using a Lagrange multiplier  $\lambda_j(\tau)$ ,

$$\prod_{j\tau} \delta\left(\hat{S}_{j}^{2}(\tau) - NS\right) = \int \mathcal{D}\lambda \exp\left[-\int_{0}^{\beta} d\tau \sum_{j} i\lambda_{j}(\tau) \left(\bar{b}_{j\sigma}(\tau)b_{j\sigma}(\tau) - NS\right)\right].$$
(3.25)

From now on we drop the explicit  $\tau$  dependence of  $b_{i\sigma}$  and  $\lambda_i$ .

In order to evaluate the path integral, Z must be in the form of a Gaussian integral, so the quartic

terms in H are decoupled using the Hubbard-Stratonovich identity,

$$\frac{N}{2\pi i J} \int \mathcal{D}\Delta \,\mathrm{e}^{-N\bar{\Delta}\Delta/J} = 1, \qquad (3.26)$$

After inserting this identity,  $\Delta$  can be shifted to  $\Delta - \frac{J}{N}B$ , eliminating the quartic term  $\frac{J}{N}\overline{B}B$ ,

$$e^{\frac{J}{N}\bar{B}B} \propto \int \mathcal{D}\Delta e^{-N\bar{\Delta}\Delta/J + \bar{\Delta}B + \bar{B}\Delta}.$$
 (3.27)

Now we have exchanged a theory of bosons with four particle interactions for a theory of free bosons interacting with a fluctuating field  $\Delta$ . We can integrate out the bosons exactly, but we will need to use the saddle point approximation to perform the path integral over  $\Delta$  (Figure 3.4(a)), an approximation that becomes exact in the large N limit due to the extensive dependence of the action NS on N. First we must treat the other quartic term,  $-\frac{J}{N}\overline{A}A$ . Naively, we would just change the sign in the exponential in (3.27), which gives

$$e^{-\frac{J}{N}\bar{A}A} \propto \int \mathcal{D}h \, e^{+N\bar{h}h/J-\bar{h}A-\bar{A}h}.$$
(3.28)

However, we must be careful, as the quadratic h term now has a positive sign, and the path integral over h appears not to converge. To understand this, we step back to a simpler case, where A is real and we decouple it with the real field a. We begin with  $e^{-Na^2/J}$ , and can rewrite

$$-Na^{2}/J = +N(ia)^{2}/J \to +(ia + \frac{J}{N}A)^{2}/J$$
  
=  $-Na^{2}/J + 2iAa + \frac{J}{N}A^{2},$  (3.29)

so that the quartic term  $-\frac{J}{N}A^2$  becomes  $-Na^2/J + 2iAa$ . We now define the mean field value of  $ia = h_0$  to be real. In fact, let's redefine  $ia = h = h_0 + i\delta a$ , and the identity becomes

$$e^{-\frac{J}{N}A^2} = \int \mathcal{D}h e^{Nh^2/J + 2Ah},$$
(3.30)

which holds as long as h is integrated along the imaginary axis, with the integral maximized at



Figure 3.4: Integrating out the fluctuations. (a.)  $\Delta$  is integrated along real axes x and y, and its saddle point is a minima at some  $\Delta_0$ . (b.) h is integrated along imaginary axes u and v, with a maximum, real saddle point  $h_0$ .

a real  $h_0$  (see Figure 3.4(b)). This can be generalized to a complex a = u + iv, where u, v are imaginary instead of real. As long as we keep in mind that  $\Delta$  is integrated along the real axis and halong the imaginary axis, we can proceed with the above decouplings,

$$H[b] = \sum_{(ij)} (\bar{b}_{i\sigma} \ \tilde{\sigma} b_{i-\sigma}) \begin{pmatrix} -h_{ij} & \Delta_{ij} \\ \bar{\Delta}_{ij} & -\bar{h}_{ij} \end{pmatrix} \begin{pmatrix} b_{j\sigma} \\ \bar{\sigma} \bar{b}_{j-\sigma} \end{pmatrix} + \frac{\bar{h}_{ij} h_{ij} - \bar{\Delta}_{ij} \Delta_{ij}}{J_{ij}}, \qquad (3.31)$$

where  $\sum_{(ij)}$  is performed only over bonds (ij) with nonzero  $J_{ij}$ . The notation can be simplified by defining the Nambu spinor,  $\tilde{b}_j^T = (b_{j\sigma}, \tilde{\sigma}\bar{b}_{j-\sigma})$ . We now have the partition function

$$\mathcal{Z} = \int \mathcal{D}\left[b, \Delta, h, \lambda\right] e^{-N\mathcal{S}\left[b, \Delta, h, \lambda\right]}$$
(3.32)

where the action can be compactly written

$$N\mathcal{S}[b,\Delta,h,\lambda] = \sum_{i\omega_n,(ij)} \left[ \frac{1}{2} \bar{\tilde{b}}_i \left( i\omega_n \tau_3 + \mathbf{G}_{ij}^{-1} \right) \tilde{b}_j + \frac{N}{J_{ij}} (\bar{h}_{ij}h_{ij} - \bar{\Delta}_{ij}\Delta_{ij}) + i\lambda_i N(S + \frac{1}{2}) \delta_{ij} \right]$$

$$\mathbf{G}_{ij}^{-1} = \begin{pmatrix} i\lambda_i\delta_{ij} - 2h_{ij} & 2\Delta_{ij} \\ 2\bar{\Delta}_{ij} & i\lambda_i\delta_{ij} - 2\bar{h}_{ij} \end{pmatrix}.$$
 (3.33)

We have performed a Fourier transform in imaginary time, and  $\tilde{b}_i$ ,  $h_{ij}$ ,  $\Delta_{ij}$  and  $\lambda_i$  are now functions of the Matsubara frequencies  $i\omega_n$ , although in practice we make the Ansatz that  $h_{ij}$ ,  $\Delta_{ij}$  and  $\lambda_i$  are all static quantities. The factors of  $\frac{1}{2}$  come from rewriting  $\lambda_i \bar{b}_{i\sigma} b_{i\sigma}$  in terms of the Nambu spinors,  $\tilde{b}_i$ .

We can calculate the mean field values of  $h_{ij}$ ,  $\Delta_{ij}$  by approximating the path integral  $\mathcal{Z}$  by its saddle point value, which becomes exact in the large N limit. By minimizing the action with respect to  $h_{ij}$ ,  $\Delta_{ij}$  and  $\lambda_i$ , we find

$$h_{ij} = \frac{J_{ij}}{2N} \langle b_{i\sigma}^{\dagger} b_{j\sigma} \rangle$$
  

$$\Delta_{ij} = \frac{J_{ij}}{2N} \langle \tilde{\sigma} b_{i\sigma}^{\dagger} b_{j-\sigma}^{\dagger} \rangle$$
  

$$NS = \langle b_{i\sigma}^{\dagger} b_{i\sigma} \rangle$$
(3.34)

where  $\langle \cdots \rangle$  denotes the thermal expectation value. However, it is simpler to eliminate the bosons altogether by integrating them out.

In order to proceed further, we must make some Ansatz about  $h_{ij}$ ,  $\Delta_{ij}$  and  $\lambda_i$ . In principle,  $h_{ij}$  and  $\Delta_{ij}$  can take different values on every bond, but for spatially uniform states, we choose an Ansatz with the unit cell of the lattice, where h and  $\Delta$  are defined for each different  $J_{ij}$ . If  $J_{ij} = 0$ on any bond, so must  $h_{ij}$  and  $\Delta_{ij}$ . We make the approximation that  $i\lambda_i(\tau) = \lambda$  on every site, taking a local constraint and enforcing it only globally. As usual, this approximation becomes exact in the large N limit.

For a square lattice with only nearest neighbor couplings, this leads to three parameters, which can be further simplified to just  $\lambda$  and  $\Delta$ , as there are no frustrating interactions. Thus we recover the unfrustrated square lattice as previously studied in SP(N) [42]. However, for frustrated lattices we cannot generally exclude either h or  $\Delta$ . Sometimes the uniform state will not be sufficient. The ground state might break lattice rotational symmetries, in which case  $\Delta_{i,i+\hat{x}}$  and  $\Delta_{i,i+\hat{y}}$  will be different, or translational symmetry, requiring  $\Delta_{i,i+\hat{x}} \neq \Delta_{i+\hat{x},i+2\hat{x}}$ . When rotational symmetry is broken,  $\lambda$  will remain the same on every site, but broken translation symmetry requires  $\lambda_i \neq \lambda_{i+\hat{x}}$ . Since the unit cell is enlarged, there will be more than one branch of  $\omega_k$ , which must be summed over. However, as long as the state may be specified by a finite number of parameters, it may be modeled within symplectic-N. Problems with infinite parameter sets, e.g.- spin glasses [143], can also be treated within symplectic-N, but require more complicated theoretical machinery, and will not be treated here. For the rest of this paper, we assume translational symmetry, with  $i\lambda_i = \lambda$ , but this treatment can be easily generalized.

The Fourier transform of the bosonic Hamiltonian,  $\mathbf{G}_{ij}^{-1}$  is

$$\mathbf{G}_{k}^{-1} = \begin{pmatrix} \lambda - 2h_{k} & 2\Delta_{k} \\ \bar{2}\Delta_{k} & \lambda - 2\bar{h}_{k} \end{pmatrix}.$$
(3.35)

We can now perform a Bogoliubov transformation det $(\omega \tau_3 - \mathbf{G}_k^{-1}) = 0$  to obtain

$$\omega_k = \sqrt{(\lambda - 2h_k)^2 - 4\Delta_k^2},\tag{3.36}$$

and integrate out the bosons to obtain the free energy,  $F[h, \Delta, \lambda] = -\beta^{-1} \text{Tr} \log Z[b, h, \Delta, \lambda]$ , where the trace is over sites (i, j), and the Matsubara frequencies  $i\omega_n$ , in addition to the bosonic degrees of freedom.

$$F = N\beta^{-1} \sum_{k} \log\left[2\sinh\frac{\beta\omega_{k}}{2}\right] + \sum_{(ij)} \frac{N}{J_{ij}} \left(\bar{\Delta}_{ij}\Delta_{ij} - \bar{h}_{ij}h_{ij}\right) - \lambda N\mathcal{N}_{s}(S + \frac{1}{2}).$$
(3.37)

Let us say we have a set of  $\{h_1, h_2, \ldots\}$  and  $\{\Delta_1, \Delta_2, \ldots\}$ , which have the Fourier transforms

$$h_k = \sum_a h_a \gamma_{ak}$$

$$\Delta_k = \sum_a \Delta_a \delta_{ak}, \qquad (3.38)$$

where a labels a bond. The symmetry properties of  $h_{ij} = h_{ji}$  and  $\Delta_{ij} = -\Delta_{ji}$  force  $\gamma_{ak}$  and  $\delta_{ak}$  to be symmetric and antisymmetric in k, respectively. The free energy is now

$$\frac{F}{N\mathcal{N}_s} = \frac{\beta^{-1}}{\mathcal{N}_s} \sum_k \log\left[2\sinh\frac{\beta\omega_k}{2}\right] + \sum_a \frac{z_a}{J_a} \left(|\Delta_a|^2 - |h_a|^2\right) - \lambda(S + \frac{1}{2})$$
(3.39)

where  $z_a$  is the number of bonds of type a per unit cell - for a simple square lattice this is just the coordination number z = 4. The free energy is now minimized by solving the mean field equations  $\partial F/\partial \lambda$ ,  $\partial F/\partial h_a$ , and  $\partial F/\partial \Delta_a$ :

$$S + \frac{1}{2} = \frac{1}{\mathcal{N}_s} \sum_k \frac{\lambda - 2h_k}{\omega_k} \left( n_k + \frac{1}{2} \right)$$
(3.40)

$$\frac{2z_ah_a}{J_a} = -\frac{1}{\mathcal{N}_s} \sum_k \frac{(\lambda - 2h_k) 2\gamma_{ak}}{\omega_k} \left(n_k + \frac{1}{2}\right)$$
(3.41)

$$\frac{2z_a\Delta_a}{J_a} = \frac{1}{N_s}\sum_k \frac{2\Delta_k\delta_{ak}}{\omega_k} \left(n_k + \frac{1}{2}\right).$$
(3.42)

 $n_k$  is the Bose function  $\left(\mathrm{e}^{\beta\omega_k}-1\right)^{-1}$ .

### **3.2.1** Simple Example

Now we examine a simple model in detail, the two dimensional bipartite square lattice. We know the mean field value of h must be zero, however, for pedagogical purposes we keep both h and  $\Delta$ .

$$\omega_k = \sqrt{\left[\lambda - 2h(\cos k_x + \cos k_y)\right]^2 - 4\Delta^2(\sin k_x + \sin k_y)^2}$$
(3.43)

We wish to minimize the free energy, however, we must be careful because h and  $\lambda$  are integrated along the imaginary axis. In fact, the free energy should be maximized along h and  $\lambda$  directions and minimized along  $\Delta$ . To examine the nature of the extremum, we look at the Hessian

$$\bar{\chi} = \begin{pmatrix} \frac{\partial^2 F}{\partial \lambda^2} & \frac{\partial^2 F}{\partial \lambda \partial h} & \frac{\partial^2 F}{\partial \lambda \partial \Delta} \\ \frac{\partial^2 F}{\partial \lambda \partial h} & \frac{\partial^2 F}{\partial h^2} & \frac{\partial^2 F}{\partial h \partial \Delta} \\ \frac{\partial^2 F}{\partial \lambda \partial \Delta} & \frac{\partial^2 F}{\partial h \partial \Delta} & \frac{\partial^2 F}{\partial \Delta^2} \end{pmatrix}$$
(3.44)

where  $\Delta$  and h are both zero, which is the global minimum if the temperature is well above where  $\Delta$  acquires an expectation value. All off diagonal terms vanish at this point,

$$\bar{\chi} = \begin{pmatrix} -\frac{1}{4} \operatorname{csch}^2 \frac{\beta\lambda}{2} & 0 & 0\\ 0 & -\frac{8}{J} - \beta \operatorname{csch}^2 \frac{\beta\lambda}{2} & 0\\ 0 & 0 & \frac{8}{J} - \frac{2}{\lambda} \operatorname{coth} \frac{\beta\lambda}{2} \end{pmatrix}.$$
 (3.45)

Looking at  $\lambda$  and h independently, F is always maximized, as expected at the mean field values of h and  $\lambda$ , while F is minimized along  $\hat{\Delta}$  for small J and maximized for large J, indicating a second order transition to nonzero  $\Delta$  at some intermediate J, dependent on temperature and spin.

### 3.2.2 Examining the Ground State

At zero temperature, we are interested in the ground state energy,

$$\frac{E_0}{NN_s} = \frac{1}{2N_s} \sum_k \omega_k + \sum_a \frac{z_a}{J_a} \left( |\Delta_a|^2 - |h_a|^2 \right) - \lambda(S + \frac{1}{2}),$$
(3.46)

which must again be minimized with respect to the parameters  $\lambda$ ,  $h_a$ , and  $\Delta_a$ . The order of limits is important; to obtain the correct mean field equations or  $\bar{\chi}$ , we must take the derivatives of the free energy first and then take the limit  $T \to 0$ . In the mean field equations(3.40 - 3.42), all temperature dependence is in  $n_k$ . If there is no long range order,  $\lim_{T\to 0} n_k = 0$ . The Mermin-Wagner theorem forbids the breaking of a continuous symmetry, like SU(2) or SP(N) at any finite temperature in one and two dimensions [25], however at T = 0, the Heisenberg magnet may develop long range order, which corresponds to the condensation of the Schwinger bosons [141]. The bosons themselves develop an expectation value,

$$b_{i\sigma} = \langle b \rangle_i + \delta b_{i\sigma}, \tag{3.47}$$

where  $\overline{\langle b \rangle_i}$  and  $\langle b \rangle_i$  are no longer independent variables. Instead  $\langle b \rangle_i$  is a complex N component vector, and  $\overline{\langle b \rangle_i} = \langle b \rangle_i^{\dagger}$ .  $n_k$  will no longer vanish for all k. To see the effects of the long range order, we examine the action(3.33) again, inserting (3.47)

$$NS[b, \Delta, h, \lambda] = \int d\omega \sum_{(ij)} \frac{1}{2} \langle b \rangle_i^{\dagger} \left( i \omega \tau_3 + \mathbf{G}_{ij}^{-1} \right) \langle b \rangle_j + NS[\delta b]$$
  
$$= \frac{1}{2} \sum_{\vec{Q}} \langle b \rangle_{\vec{Q}/2}^{\dagger} \mathbf{G}_{k=\vec{Q}/2}^{-1} \langle b \rangle_{\vec{Q}/2} + NS[\delta b], \qquad (3.48)$$

The linear terms proportional to  $\delta b$  must vanish, and so have been neglected.  $\vec{Q}/2$  are the zeroes of the Schwinger boson spectrum. For ferromagnetism,  $\vec{Q}/2 = (0,0)$ , while for antiferromagnetism,  $\vec{Q}/2 = (\pi/2, \pi/2)$ . The long range order is indicated by the ordering of the *spins*, which are the combination of two Schwinger bosons, so the Goldstone modes in classical spin wave theory will be given by  $\vec{Q}/2 \pm \vec{Q}/2 = \vec{0}$  and  $\vec{Q}$ , which gives the traditional  $(\pi, \pi)$  ordering vector for antiferromagnetism. Now, in addition to the mean field equations, we have the condition

$$\partial S/\partial \langle b \rangle_{\vec{Q}/2} = G_{\vec{Q}/2}^{-1} \langle b \rangle_{\vec{Q}/2} = 0$$
  
=  $\omega_{\vec{Q}/2} \langle b \rangle_{\vec{Q}/2} = 0.$  (3.49)

So either  $\langle b \rangle_{\vec{Q}/2} = 0$ , and we proceed as before, or  $\omega_{\vec{Q}/2} = 0$ , which allows us to find the value of  $\langle b \rangle_{\vec{Q}/2}$  in addition to the original parameters. In fact,  $n_{\vec{Q}/2} = \omega_{\vec{Q}/2} \langle b \rangle_{\vec{Q}/2}^2$ , so we can simply define  $n = n_{\vec{Q}/2} / \omega_{\vec{Q}/2}$  and the mean field equations become

$$\omega_{\vec{Q}/2} \langle b \rangle_{\vec{Q}/2} = 0$$

$$S + \frac{1}{2} = \frac{1}{N_s} \sum_k \frac{\lambda - 2h_k}{2\omega_k} + \sum_{\vec{Q}} n(\lambda - 2h_{\vec{Q}/2})$$
(3.50)

$$\frac{2z_a h_a}{J_a} = \frac{1}{N_s} \sum_k \frac{(2h_k - \lambda)\gamma_{ak}}{\omega_k} + 2\sum_{\vec{Q}} n\gamma_{a\vec{Q}/2} (\lambda - 2h_{\vec{Q}/2})$$
(3.51)

$$\frac{2z_a\Delta_a}{J_a} = \frac{1}{\mathcal{N}_s} \sum_k \frac{2\Delta_k\delta_{ak}}{2\omega_k} + 2\sum_{\vec{Q}} n\delta_{a\vec{Q}/2}\Delta_{\vec{Q}/2}.$$
(3.52)

Now we have set up all the machinery for solving the symplectic-N Heisenberg model on a general one or two dimensional lattice(three dimensional lattices cannot currently be treated by Schwinger bosons [144]). Next we treat a simple example which highlights the differences between symplectic-N and previous large N treatments, the  $J_1 - J_2$  model.

# **3.3** Illustration: $J_1 - J_2$ model

The  $J_1 - J_2$  Heisenberg model is one of the simplest two dimensional frustrated magnets,

$$H = J_1 \sum_{\mathbf{x},\mu} \vec{S}_{\mathbf{x}} \cdot \vec{S}_{\mathbf{x}+\mu} + J_2 \sum_{\mathbf{x},\mu'} \quad \vec{S}_{\mathbf{x}} \cdot \vec{S}_{\mathbf{x}+\mu'}, \qquad (3.53)$$

where  $J_1$  and  $J_2$  describe nearest and next nearest neighbor interactions, respectively. We consider only antiferromagnetic  $J_1$  and  $J_2$ .

For  $J_1 \gg J_2$ , the ground state is a Néel antiferromagnet, with  $\vec{Q} = (\pi, \pi)$  long range order, as long as the spin S is greater than a critical spin  $S_c \approx .2$ . The next nearest neighbors are ferromagnetically aligned, so  $J_2$  introduces frustration which begins to suppress long range order by increasing the critical spin.

For  $J_2 \gg J_1$ , the classical ground state consists of two interpenetrating but decoupled Néel sublattices. For any finite  $J_1$ , both quantum and thermal fluctuations couple the sublattices together through the process of "order from disorder," [27, 28, 29] which leads to a long range ordered state with  $\vec{Q} = (0, \pi)$  or  $(\pi, 0)$ . This transition spontaneously breaks the  $Z_4$  lattice symmetry down to  $Z_2$ , which, as a Ising symmetry breaking, can survive to finite temperatures, despite the loss of the underlying long range magnetic order [26]. In real materials, this transition couples to the lattice



Figure 3.5: The  $J_1 - J_2$  model. (a) depicts antiferromagnetic order as described by antiferromagnetic valence bonds(blue) and ferromagnetic bonds(red, dashed), and the spin order  $\vec{Q} = (\pi, \pi)$ . (b) depicts the collinear order,  $\vec{Q} = (0, \pi)$ , where there are two different antiferromagnetic valence bonds(blue and green) and ferromagnetic bonds(red, dashed).

and causes a structural transition from tetragonal to orthorhombic symmetry [145].

The phase boundary between the two classical ground states is at  $J_1 = 2J_2$ . Conventional spin wave theory predicts that the ordered moments of both states are suppressed to zero even for  $S \to \infty$  at this critical point, leaving a quantum spin liquid state that exists for a small, but finite range of  $J_2/J_1$  for the physical spin S = 1/2 [146]. However, at this point, the 1/S expansion fails [147], and much more theoretical work has been done to see if quantum fluctuations stabilize or destabilize the spin liquid region [148, 149, 150]. The current consensus is that the spin liquid ground state is most likely stable between  $.4 \leq J_2/J_1 \leq .6$  for S = 1/2.

The  $J_1 - J_2$  model is an ideal demonstration of the importance of ferromagnetic bonds because they enforce the frustration price in both Néel and collinear phases. This is most obvious on the Néel side, where, without ferromagnetic bonds, the state remains unchanged as  $J_2$  increases, until a first order transition to the collinear state. The ferromagnetic bonds also enable us to obtain the correct temperature dependence of the Ising transition temperature in a large N theory.

#### 3.3.1 Valence bond structure

First we need to describe the relevant states within our valence bond picture. We assign a  $\Delta$  to each antiferromagnetic bond and an h to each ferromagnetic bond. On the Néel side, we have  $\Delta$  on all nearest neighbor bonds and  $h_d$  on the frustrating diagonal bonds, as shown in Figure 3.5(a). This leads to the dispersion relation:

$$\omega_k^n = \sqrt{(\lambda - 4h_d c_x c_y)^2 - 4\Delta^2 (s_x + s_y)^2)}.$$
(3.54)

In the collinear state, we must allow the breaking of lattice symmetry and consider both  $h_x$ ,  $h_y$  and  $\Delta_x$ ,  $\Delta_y$  on the nearest neighbor bonds, and  $h_d$ ,  $\Delta_d$  on diagonal bonds. In fact, there are two distinct diagonal bonds corresponding to what would be the two decoupled sublattices (see Figure 3.5(b)). Their magnitude must be the same, but the phase between them leads to a U(1) gauge symmetry. If we fix the phase to be  $\pi$  it is most natural to break the lattice symmetry explicitly [151] and choose only  $h_x$  and  $\Delta_y$  to be nonzero of the nearest neighbor bonds, and  $h_d = 0$ , which gives the dispersion

$$\omega_k^c = \sqrt{(\lambda - 2h_x c_x)^2 - (4\Delta_d c_x s_y + 2\Delta_y s_y)^2)}.$$
(3.55)

#### **3.3.2** T=0 phase diagram

To examine the frustrating effects of the ferromagnetic bonds, we focus on the border between long and short range orders at T = 0, as a function of spin,  $S \equiv n_b/N$  and frustration,  $J_2/J_1$ . The more stable the phase, the larger the region of long range order. Long range order is lost as the spin decreases below a critical spin  $S_c$ , which is approximately 1/5 for the unfrustrated Néel lattice, e.g. both  $J_2/J_1 = 0$  and  $J_2/J_1 = \infty$ . To compare our results to the original SP(N) [142], we calculate the phase boundaries both with h free and with h set to zero.

Since we are interested in  $S_c$ , the onset of long range order, we know that both n = 0 and  $\omega_{\vec{Q}/2} = 0$ . The Schwinger boson gap is at  $\vec{Q}/2 = (\pi/2, \pi/2)$  for the Néel phase, and  $\vec{Q}/2 = (0, \pi/2)$  for the collinear state. The gap equation,  $\omega_{\vec{Q}/2} = 0$  and the mean field equations for

h(3.51) and  $\Delta(3.52)$  can be used to solve for the mean field parameters, and then equation (3.50) defines  $S_c$ ,

$$S_c + \frac{1}{2} = \int_k \frac{\lambda - 2h_k}{2\omega_k}.$$
(3.56)

Results from these calculations for both symplectic-N and SP(N) are shown in Figure 3.6. For comparison, we have also drawn the phase boundaries given by conventional spin wave theory [146]. First let us discuss the results far from the critical value of frustration  $J_1 \approx 2J_2$ . The results



Figure 3.6: We compare the critical spin  $S_c = \left(\frac{n_b}{N}\right)_c$ , below which there is no long range order in the ground state, calculated within SP(N) (bold red line), symplectic-N (blue and green lines), and spin wave theory [146] (thin black line). For small  $J_2/J_1$ , the spins configurations are staggered, while for large  $J_2/J_1$ , the ground state breaks lattice symmetry to develop collinear order as shown in the figure. SP(N) (bold red line) tends to overstabilize the long range ordered phases, most dramatically on the one sublattice side, where the critical spin is independent of the strength  $J_2$ of the frustrating diagonal bonds [132]. Symplectic-N restores the frustration-induced fluctuations by treating both ferromagnetic and antiferromagnetic bonds, on equal footing, which corrects this overstabilization. The physical spin, S = 1/2 is indicated by a horizontal dashed line.

are most dramatic for the Néel state, where SP(N) is oblivious to the frustrating effects of the diagonal bonds, drastically overestimating the critical spin. For the collinear state, SP(N) neglects the frustrating  $h_x$ , again overestimating the stability of the long range ordered state. On the other hand, symplectic-N tracks conventional spin wave theory for small amounts of frustration, but they differ in a wide range around the critical  $J_2/J_1$ , where conventional spin wave theory is known to fail, and a spin liquid ground state is predicted for S = 1/2. For symplectic-N, we calculated the location of the first order transition between Néel and collinear long range orders by comparing the ground state energies of both states (see Appendix 3A). Symplectic-N indicates a weakly first order transition for S = 1/2, with no intervening quantum spin liquid, however, 1/N corrections, calculated as Gaussian fluctuations from Ceccatto *et al.*'s mean field theory lead to a small region of spin liquid for  $0.53 \le J_2/J_1 \le 0.64$  [148].

### 3.3.3 Finite Temperatures: the Ising transition

Now we turn our focus to the  $J_2 \gg J_1$  side of the phase transition and examine the finite temperature Ising transition between decoupled sublattices and the collinear phase. This phase transition has several possible experimental realizations, most prominently and recently in the iron arsenides [110, 152, 153, 154, 155].

At high temperatures and large  $J_2/J_1$ , the first bonds to develop are the diagonal bonds,  $\Delta_d$ . From the mean field equations(3.40) and (3.42),

$$(S + \frac{1}{2}) = \int_{k} (n_k + \frac{1}{2}) \frac{\lambda}{\omega_k}$$
 (3.57)

$$\frac{1}{J_2} = \int_k (n_k + \frac{1}{2}) \frac{2(2c_x s_y)^2}{\omega_k}, \qquad (3.58)$$

we can solve for  $\lambda$  and  $\Delta_d$  as functions of temperature and spin. They are both independent of  $J_1$ .  $\Delta_d$  turns on at a temperature

$$T_d = \frac{J_2(S+1/2)}{2\log(1+1/S)}.$$
(3.59)

Now that we have a full description of the decoupled phase, we can look for the next bond fields to turn on as we lower the temperature. For simplicity, we assume that the spin is large enough that the ground state is the long range ordered collinear state, so we know that  $h_x$  and  $\Delta_y$  must turn on at some point. However, we can look for all possible bonds at once by examining the unstable

$$\bar{\chi} = \begin{pmatrix} \frac{\partial^2 F}{\partial \lambda^2} & \frac{\partial^2 F}{\partial \lambda \partial h_a} & \frac{\partial^2 F}{\partial \lambda \partial \Delta_a} \\ \frac{\partial^2 F}{\partial \lambda \partial h_a} & \frac{\partial^2 F}{\partial h_a^2} & \frac{\partial^2 F}{\partial h_a \partial \Delta_b} \\ \frac{\partial^2 F}{\partial \lambda \partial \Delta_a} & \frac{\partial^2 F}{\partial h_a \partial \Delta_b} & \frac{\partial^2 F}{\partial \Delta_a^2} \end{pmatrix},$$
(3.60)

where this is a schematic of the seven by seven Hessian with respect to  $\lambda$ ,  $h_x$ ,  $h_y$ ,  $h_d$ ,  $\Delta_x$ ,  $\Delta_y$ ,  $\Delta_d$ . When det  $\bar{\chi}$  changes sign, the decoupled solution is changing from a free energy minimum to a maximum, indicating the presence of a second order phase transition. By examining the unstable eigenvectors, we know which bond fields are turning on, without having to solve the seven mean field equations.

All of the matrix elements have similar forms, for example

$$\frac{\partial^2 F}{\partial h_x^2} = \int \frac{d^2 k}{(2\pi)^2} \left(n_k + \frac{1}{2}\right) \frac{\partial^2 \omega_k}{\partial h_x^2} - \frac{n_k (n_k + 1)}{T} \left(\frac{\partial \omega_k}{\partial h_x}\right)^2 - \frac{1}{J_1}.$$
(3.61)

Since  $\lambda$  and  $\Delta_d$  are independent of  $J_1$ , we can fix  $J_2 = 1$ , S = 1/2 and easily evaluate  $\bar{\chi}$  for all  $J_1$  at a given T, since the integrals are all independent of  $J_1$ . det  $\bar{\chi} = 0$  can then be solved for  $J_{1c}$  and the phase transition,  $T_c$  mapped out parametrically, as shown in Figure 3.7. The unstable eigenvector is

$$\phi = \begin{pmatrix} -h_x \\ \Delta_y \end{pmatrix}, \tag{3.62}$$

showing that the system does develop long range Ising order. This method finds all possible second order phase transitions, however, it is blind to first order phase transitions. As we see in the figure, there is a temperature dependent first order transition between the short range Néel and decoupled orders which cuts off the second order line (see Appendix 3A for derivation).



Figure 3.7: Finite temperature phase diagram for S = 1/2.  $T_d$ (equation 3.59) and  $T_N$ (equation 3.76) are the transitions into short range two sublattice and Néel antiferromagnetic order, respectively. The Ising transition,  $T_c$  is shown for both symplectic-N(blue) and SP(N)(red). The Ising order is long range, even though the underlying antiferromagnetic order is not. The dashed(green) line indicates a first order transition from Ising order to short range antiferromagnetic order. Just as we saw by examining  $S_c$ , SP(N) overstabilizes the Ising order. Insets show the appropriate valence bond order.

### Analytical form of $T_{RVB}$

Now we derive the analytical form for the Ising transition temperature, in the limit of large  $J_2/J_1$ . At temperatures far below the development of decoupled order  $T_d$ , but above the Ising transition,  $T_c$ , the gap in the spectrum at  $(0, \pi/2)$ ,

$$\Delta_{gap} = \sqrt{\lambda^2 - (4\Delta_d)^2} \tag{3.63}$$

is much smaller than T, and, assuming large S, we can apply spin wave theory to this problem, which implies  $\lambda \approx 4\Delta_d \approx c_{sw} = 4J_2S$ .  $\bar{\chi}$  can be restricted to the two relevant parameters  $h_x$  and  $\Delta_y$ , and we define the quantities  $A_1$ ,  $A_2$  and B,

$$\bar{\chi} = \begin{pmatrix} \frac{\partial^2 F}{\partial h_x^2} & \frac{\partial^2 F}{\partial h_x \partial \Delta_y} \\ \frac{\partial^2 F}{\partial \Delta_y \partial h_x} & \frac{\partial^2 F}{\partial \Delta_y^2} \end{pmatrix} \equiv \begin{pmatrix} A_1 - \frac{1}{J_1} & B \\ B & A_2 + \frac{1}{J_1} \end{pmatrix}.$$
(3.64)

In the limit  $\Delta_{gap} \to 0$ , we find that  $A_1 = A_2 \equiv A = B$  to all divergent orders. This is because our singlet bond fields are decoupled from the S = 1 spin waves becoming gapless. To find  $T_c$ , we need to consider the short wavelength behavior which makes A - B nonzero,

$$\det \bar{\chi} = (A+B)(A-B) - 1/J_1^2 = 0, \tag{3.65}$$

where A + B is of the order  $T/\Delta_{gap}^2$ , but the divergences cancel from A - B and we can calculate this integral to zeroth order in  $\Delta_{gap}$ :

$$A-B = \frac{1}{2} \left( \frac{\partial^2 F}{\partial h_x^2} + \frac{\partial^2 F}{\partial \Delta_y^2} \right) - \frac{\partial^2 F}{\partial h_x \partial \Delta_y}$$
  
$$= 2\lambda^2 \int \frac{d^2 k}{(2\pi)^2} \frac{\cos^2 k_x \cos^4 k_y}{\omega_k^2} \left( \frac{n_k (n_k+1)}{T} - \frac{n_k + \frac{1}{2}}{\omega_k} \right)$$
  
$$= -\frac{1}{3T} \int \frac{d^2 k}{(2\pi)^2} \frac{\cos^2 k_x \cos^4 k_y}{1 - \cos^2 k_x \sin^2 k_y} \equiv -\frac{\pi\gamma}{T}, \qquad (3.66)$$

where  $\gamma = .039$ . Altogether (3.65) gives us

$$\frac{8\gamma}{\Delta_{gap}^2} = \frac{1}{J_1^2}.$$
(3.67)

We can expand the constraint equation (4.36) to find the gap,

$$\frac{\Delta_{gap}}{c} = \exp\left(\frac{-8\pi J_2 S^2}{T}\right),\tag{3.68}$$

which, combined with (3.66) leads us to the Ising transition temperature,

$$T_c = \frac{4\pi J_2 S^2}{\log\left[\frac{2J_2 S}{J_1\sqrt{2\gamma}}\right]}.$$
(3.69)

Chandra, Coleman and Larkin found semi-classically [26],

$$T_{i} = \frac{4\pi J_{2}S^{2}}{\log\left[\frac{2J_{2}}{J_{1}\sqrt{2\gamma_{T}}}\right]},$$
(3.70)

with  $\gamma_T = .318$ . Note that the form of the two temperatures is identical, with only numerical differences inside the logarithm, which are negligible for small spin. This temperature dependence has been confirmed by classical Monte Carlo [156], and quantum numerical studies have show that finite S systems also share the temperature dependence [157].

The same calculation is much simpler in SP(N) where  $\bar{\chi}$  is a one dimensional matrix,  $\partial^2 F / \partial \Delta_y^2 \sim -T/\Delta_{gap}^2 + 1/J_1$ , giving the defining condition  $T_c^{SP(N)}/\Delta_{gap}^2 = \gamma_{SP(N)}/J_1$ . Again inserting the gap(3.67), we find an implicit equation for  $T_c^{SP(N)}$ ,

$$T_c^{SP(N)} = \frac{16\pi J_2 S^2}{\log\left[\frac{16J_2^2 S^2}{J_1 T_c^{SP(N)} \gamma_{SP(N)}}\right]}.$$
(3.71)

The extra  $T_c^{SP(N)}$  in the logarithm acts to increase the Ising temperature, as was also seen in our numerical calculation (Figure 3.7).

This phase transition has several possible experimental realizations. First, there is a direct realization of the two dimensional  $J_1 - J_2$  lattice in Li<sub>2</sub>VOSiO<sub>4</sub>, where a transition to long range collinear order is immediately preceded by a lattice distortion from tetragonal to orthorhombic symmetry [158].

In the iron arsenides, a  $\vec{Q} = (0, \pi)$  spin density wave order develops either coincident with a tetragonal to orthorhombic structural transition, or slightly below [155, 110, 154, 153]. First principles calculations suggest that the system can be described by the  $J_1 - J_2$  model with  $J_1/J_2 \approx$ 1/2 [152], although whether the magnetism is itinerant or local moment is still controversial.

Finally, the spin dimer system, BaCuSi<sub>2</sub>O<sub>6</sub> [159] contains elements of  $J_1 - J_2$  physics despite being three dimensional. The alternating layers of dimers are ordered antiferromagnetically, but decoupled, like the  $J_2$  sublattices, while the interlayer couplings are frustrated like  $J_1$ . The compound can be thought of as a multi-layer  $J_1 - J_2$  model, where the transition to three dimensionality is an Ising transition [160].

### 3.4 Discussion and Conclusions

We have identified the time reversal of spin as a symplectic symmetry and examined the consequences of maintaining this symmetry in the large N limit. In order to write a theory of symplectic spins, all interactions of the unphysical antisymplectic spins must be excluded, leading to a unique large N limit which we call symplectic-N. In this paper, we have examined the bosonic symplectic-N Heisenberg model. The practical consequences are to introduce two mean field parameters,

$$h_{ij} = \langle \frac{J_{ij}}{2N} \sum_{\sigma} b_{j\sigma}^{\dagger} b_{i\sigma} \rangle$$
  

$$\Delta_{ij} = \langle \frac{J_{ij}}{2N} \sum_{\sigma} \tilde{\sigma} b_{j\sigma}^{\dagger} b_{i-\sigma}^{\dagger} \rangle$$
(3.72)

where  $h_{ij}$  measures the ferromagnetic correlations along a bond  $\{ij\}$  and  $\Delta_{ij}$  the antiferromagnetic correlations, and to identify the mean field theory introduced by Ceccatto *et al.* [121] for SU(2)as the unique large N limit. Previous large N methods had either ferromagnetism or antiferromagnetism, and the presence of both means that symplectic-N can treat both ferromagnetic and antiferromagnetic states. In frustrated antiferromagnets, this is especially important because the frustration manifests itself through the presence of ferromagnetic correlations on antiferromagnetic bonds; in these cases we call h the frustration field. Correctly accounting for the price of these frustrated bonds is essential in systems with many competing states close in energy.

Frustrated bonds will occur whenever there are triangles containing two or more antiferromagnetic bonds (see Figure 3.8(top)). In this paper, we studied collinear magnets, where the bonds on the triangle are either exclusively ferromagnetic or antiferromagnetic, e.g. - h and  $\Delta$  do not coexist. In other lattices, like the triangular lattice, non-collinear states are expected. Certainly the classical symplectic-N limit will contain coexisting bonds, as we know  $h_{ij} = SJ_{ij} \cos \frac{\phi_{ij}}{2}$ , and  $\Delta_{ij} = SJ_{ij} \sin \frac{\phi_{ij}}{2}$ , where  $\phi_{ij} \neq 0$  or  $\pi$  for non-collinear ground states. Whether this coexistence persists in the quantum limit is still an open question. In a first attempt, we have examined the triangular plaquette and found the ground state to be the uniform, coextant state. However, the lattice case will likely be different; the plaquette version of the  $J_1 - J_2$  model also has a uniform ground



Figure 3.8: a. The antiferromagnetic triangular plaquette has three possible bond orderings: (left) just a single  $\Delta$  connecting two of the spins and leaving the third completely free; (middle)  $\Delta$ 's(blue) and *h*'s(red, dashed) segregated; and (right) the uniform state, which is the ground state of symplectic-*N*.b. The tetrahedral plaquette. When all sites are assumed to be equivalent, there are three different types of bonds - as shown in black, gray and thin black lines.

state, not the broken symmetry state found in the lattice. In the tetrahedral plaquette, as in SP(N), there is a continuously degenerate ground state manifold [132]. In SP(N), the degeneracy is lifted in the lattice, however, the ground state found in the SP(N) semi-classical limit is inconsistent with linear spin wave theory [161]. Given the many competing states, it is an interesting open question whether the frustrating fields will bring the lattice ground state into agreement with spin wave theory. More generally, we would like to know if including the price of frustration substantially changes the ground states or response for other highly frustrated lattices.

Now we turn to corrections beyond mean field theory, the 1/N corrections. These will not affect the phase boundaries, but can change the nature of the short range phases. Sachdev and Read have shown that the 1/N corrections for SU(N) spins manifest as a gauge field coupling to the Schwinger bosons [136]. In SU(N), this is a U(1) gauge field, which in two dimensions contains instantons that generate nontrivial Berry phases which enforce the discrete nature of valence bonds. For each spin S, each site participates in exactly 2S valence bonds. The ground state alternates periodically between spin-Peierls and valence bond solid phases as  $2S(\mod z)$ , where z is the coordination number of the lattice. Sachdev and Read later showed that this treatment can be extended

to collinear states in SP(N), while non-collinear states do not generally have instantons [142]. To examine the effects of h, we consider the U(1) gauge symmetry in symplectic-N.

In the large N limit of the  $J_1 - J_2$  model, the valence bond fields  $\Delta$  develop between "even" and "odd" sites. This breaks the local U(1) symmetry associated with boson conservation at each site down to a global compact U(1) symmetry, under which  $b_i \rightarrow e^{i\theta}b_i$  on the even sublattice and  $b_i \rightarrow e^{-i\theta}b_i$  on the odd sublattice (corresponding to the conservation of  $\sum_{i \in \text{even}} n_i - \sum_{i \in \text{odd}} n_i$ ). The instanton tunneling configurations considered by Read and Sachdev are space-time monopoles in the electric field associated with this U(1) field. In fact, the frustration fields h link sites on the same sublattice, so that h is invariant under the global U(1) symmetry, so it does not pick up any phase factor when the instanton forms, and it does not modify the the phase factors associated with instanton formation. In this way, the frustration fields do not affect the formation of valence bond solids in collinear states. The effect of the frustration fields on non-collinear states is however, still an open question.

Another way to move beyond the large N limit is to examine the variational wavefunctions which are the ground state of the large N limit. The wavefunction of a pure valence bond state has a Jastrow form [162, 163],

$$|\Psi\rangle = P_S \exp\left(-\sum_{ij} b_{ij} B_{ij}^{\dagger}\right)|0\rangle,$$
(3.73)

where  $P_S$  projects out the unphysical subspace where  $n_b \neq NS$ , as given in equation (3.25). When we include the effects of the frustrating fields,

$$|\Psi\rangle = P_S \exp\left(-\sum_{ij} a_{ij} A_{ij}^{\dagger}\right) \exp\left(-\sum_{ij} b_{ij} B_{ij}^{\dagger}\right) |0\rangle.$$
(3.74)

The  $\exp\left(-\sum_{ij} a_{ij} A_{ij}^{\dagger}\right)$  creates effective valence bonds of all lengths across the system, causing the spins to fluctuate coherently - in the case of the Ising transition, these coherent fluctuations break lattice symmetry without long range magnetic order.

This chapter has addressed the bosonic representation of interacting symplectic spins, but the principles of symplectic closure can equally well be applied to fermionic models, either in Heisenberg physics, where Ran and Wen have used an identical decoupling [39], or Kondo physics, as we do in Chapter 4. In the fermionic spin representation, requiring spins that reverse under time reversal also insures that the spins are neutral under particle-hole transformations, which leads to a local SU(2) gauge symmetry. In bosonic models, this gauge symmetry reduces to the U(1) symmetry discussed earlier because  $\tilde{\sigma} b_{\sigma}^{\dagger} b_{-\sigma}^{\dagger} = 0$  on site due to symmetrization. In parallel with our current treatment of both ferromagnetism and antiferromagnetism in the Heisenberg model, we are able to treat both the Kondo effect and superconductivity within the two channel Kondo model.

The next step is to introduce charge fluctuations while maintaining the symplectic spin closure. One possibility is to introduce the symplectic-N Hubbard operators, which can used to construct the t - J and Anderson models. These ensure that a hole hopping onto a site and off again will generate a symplectic spin flip. In turn, the symplectic closure guarantees that the local SU(2)gauge symmetry survives to all orders in N, even at finite doping, justifying the SU(2) slave boson theory of Wen and Lee in a unique large N limit [129]. The application of this approach as a large N framework for the RVB theory of superconductivity [164, 165] is a matter of great interest for future research, and is discussed in Chapter 7.

### Appendix 3A: $J_1 - J_2$ first order transitions

In principle, calculating first order transitions is simple - one calculates the parameters  $\lambda$ ,  $h_a$  and  $\Delta_a$  for each of the phases from the mean field equations, plugs them into the free energy, or ground state energy at zero temperature and compares the energies. In practice, it is difficult to solve the mean field equations in complicated phases. Second order transitions are much easier because something is going to zero. For the zero temperature phase diagram of the  $J_1 - J_2$  model, Figure 3.7, we know that the transition between Néel and collinear long range order is first order because the second order lines(between short and long range order of the same type) indicate that the phases overlap for  $S \gtrsim .4$ . We have calculated the location of the first order line by comparing the energy of the

long range ordered states, shown in Figure 3.9.



Figure 3.9: Thin lines indicate the second order transitions from short range to long range Néel and collinear orders. For points within the region of collinear long range order, the ground state energies of the two possible orders were compared. Where the collinear order is lower, a circular, blue dot is placed on the phase diagram; when Néel order is lower, the dot is green and square. The black dot indicates the classical, second order phase transition, which was calculated analytically. The physical spin, S = 1/2 is indicated by the dashed line.

As the spins become more classical, the mean field parameters become more difficult to calculate, but the  $S \to \infty$  point can be calculated analytically using the energies from the previous section(3.16). For the Néel state,  $\phi_{ij} = \pi$  for nearest neighbor bonds, and 0 for diagonal bonds, while for the collinear state  $\phi_{ij} = \pi$  on  $\hat{y}$  and diagonal bonds and 0 on  $\hat{x}$  bonds.

$$E_N = -4J_1 + 4J_2$$
  
 $E_c = -4J_2$  (3.75)

Thus, the classical transition is second order at  $J_1 = 2J_2$ , just as found for classical SU(2) spins. The same calculation can be repeated with  $E_{SP(N)}$ , with the same result.

At finite temperatures, there is a first order transition between the two short range orders. We

already have one end of the first order line - the zero temperature point, and we can calculate the other end, which is a second order point where both antiferromagnetic and decoupled short range orders give way to a completely disordered high temperature phase. We already know the decoupled temperature as a function of  $J_2(3.59)$ , and the antiferromagnetic temperature can be similarly found from the mean field equations for  $\lambda$  and  $\Delta$  in the limit of  $\Delta \rightarrow 0$ ,

$$T_N = \frac{J_1(S+1/2)}{2\log\left(1+1/S\right)}.$$
(3.76)

The two temperatures have identical form - the only difference being that where  $T_N$  has  $J_1$ ,  $T_d$  has  $J_2$ . Thus the first order line ends in a second order point at  $J_1 = J_2$ , as show in Figure 3.7. The intermediate line has been extrapolated, but not calculated.

# **Chapter 4**

## The two channel Kondo model

### 4.1 Introduction

The recent discovery of two heavy-fermion materials,  $PuCoGa_5$  and  $NpPd_5Al_2$ , which transform directly from Curie paramagnets into heavy fermion superconductors has revealed a new class of strongly coupled superconductors where local moments quench directly into the superconducting condensate, shown in Figure 4.1. Unlike conventional heavy fermion superconductors, where Cooper pairing is thought to be driven by spin fluctuations [66, 67, 68, 73, 166], these higher transition temperature materials do not appear to be close to a magnetic instability. Moreover, the superconducting condensation entropy is between a quarter and a third of the free spin entropy,  $R \ln 2$ of the Curie paramagnet, indicating that the spin-quenching normally associated with the Kondo effect is an integral part of the development of superconductivity. Motivated by these unusual superconductors, we have revisited the problem of developing a large N theory of heavy fermion superconductivity.



Figure 4.1: (a) Local moments can be seen in the Curie-Weiss-like susceptibility of NpPd<sub>5</sub>Al<sub>2</sub>, which shows no sign of quenching into Pauli paramagnetism. (b) The superconducting condensation entropy is  $\approx 1/3R \log 2$ , a significant fraction of the total spin entropy.

Large N expansions involving SU(N) have been invaluable in describing heavy fermion metals,

but thus far cannot treat superconductivity. The difficulty is that the odd time-reversal parity of the electron spin,  $\vec{S} \rightarrow^{\theta} -\vec{S}$  is not preserved by SU(N) spins. The inversion of spins under time reversal protects singlet superconductivity by ensuring that an electron paired with its time-reversed twin is a singlet. However, for N > 2, some SU(N) spins do not invert under time-reversal, and this protection is lost. The symplectic large-N limit preserves the time-reversal properties of SU(2) spins, restoring singlet superconductivity, and allowing us to treat Kondo physics and superconductivity on equal footing.

In this chapter, we focus on the application of symplectic-N to heavy-fermion superconductivity in  $PuCoGa_5$  and  $NpPd_5Al_2$ , where the appearance of an SU(2) gauge symmetry has marked physical consequences. We show that when a lattice of magnetic ions exchange spin with their metallic environment in two distinct symmetry channels, they can simultaneously satisfy both channels by forming a condensate of composite pairs between local moments and electrons, screening these moments as superconductivity develops. In the tetragonal crystalline environment relevant to  $PuCoGa_5$  and  $NpPd_5Al_2$ , the lattice structure selects a natural pair of spin-exchange channels and predicts a unique anisotropic paired state with either d- or g- wave symmetry.

### 4.1.1 The two channel Kondo model

These materials contain a lattice of local moments immersed in a sea of electrons to form a Kondo lattice. We assume that at low temperatures, the Pu and Np ions in these materials behave as Kramer's doublets. Due to the strong spin-orbit coupling, J is the only good quantum number. For Pu<sup>3+</sup>, which is a  $5f^5$  atom, Hund's rules give J = 5/2, a six-fold degenerate state. The situation in  $NpPd_5Al_2$  is less certain; the Curie moment extracted from the magnetic susceptibility is closest to that of a  $5f^3$  ion with n = 3, which will have J = 9/2, a ten-fold degenerate state. The lattice breaks the spherical symmetry down to a crystal point group and the degenerate levels are split by the electric fields resulting from the crystal structure into several crystal field levels . Because J is half-integral, the minimum degeneracy of any level is guaranteed to be two by Kramer's theorem, where the degenerate levels are related by time-reversal. In a tetragonal crystal, J = 5/2 splits into

three Kramer's doublets, denoted  $\Gamma_7^{\pm}$  and  $\Gamma_6$  for group theoretical reasons,

$$f^{\dagger}_{\tilde{\Gamma}\sigma} = \sum_{m \in [-5/2, 5/2]} \langle \tilde{\Gamma}\alpha | \frac{5}{2}m \rangle f^{\dagger}_{m\sigma}, \qquad (\sigma = \pm)$$
(4.1)

where

$$\Gamma_{6}: \qquad f_{\Gamma_{6}\pm}^{\dagger} = |\pm 1/2\rangle$$

$$\Gamma_{7}^{+}: \qquad f_{\Gamma_{7}^{+}\pm}^{\dagger} = \cos\beta|\mp 3/2\rangle + \sin\beta|\pm 5/2\rangle \qquad (4.2)$$

$$\Gamma_{7}^{-}: \qquad f_{\Gamma_{7}^{-}\pm}^{\dagger} = \sin\beta|\mp 3/2\rangle - \cos\beta|\pm 5/2\rangle$$

Here the mixing angle  $\beta$  fine-tunes the spatial anisotropy of the  $\Gamma_7^{\pm}$  states. Notice how the crystal mixes  $\pm 5/2$  with the  $\mp 3/2$  states: this is because the tetragonal crystalline environment transfers  $\pm 4$  units of angular momentum to the electron. Even though the doublets are not spin 1/2 doublets, they have the same  $R \log 2$  entropy. The exchange of spin with its environment involves virtual valence fluctuations into ionic configurations with one more, or one less f-electron:  $f^n \rightleftharpoons f^{n\pm 1} \mp e^-$ , where n = 3 and 5 for  $NpPd_5Al_2$  and  $PuCoGa_5$  respectively. We assume that the dominant spin fluctuations occur via valence fluctuations into singlet states

$$\begin{array}{cccc} |0\rangle &\rightleftharpoons & |\Gamma_1 \sigma\rangle &\rightleftharpoons & |\phi\rangle \\ f^{n+1} & f^n & f^{n-1}. \end{array}$$

$$(4.3)$$

To illustrate the situation, consider  $PuCoGa_5$ , where  $|0\rangle \equiv |f^6\rangle$  is an empty j = 5/2 f-shell. The  $f^5$  Kramers doublet can be written  $|\Gamma_1\sigma\rangle = f^{\dagger}_{\Gamma_1\sigma}|0\rangle$  where  $f^{\dagger}_{\Gamma\sigma}$  creates an f-hole in one of these three crystal field states. To form a low-energy  $f^4$  singlet, the strong Coulomb interaction between f-electrons forces us to add a second f-hole in a *different* crystal field channel  $\Gamma_2$ . We assume that this state has the form

$$|\phi\rangle \equiv |\Gamma_2 \otimes \Gamma_1\rangle_s = \frac{1}{\sqrt{2}} \sum_{\sigma=\pm 1} \operatorname{sgn}(\sigma) f^{\dagger}_{\Gamma_2 \sigma} f^{\dagger}_{\Gamma_1 - \sigma} |0\rangle.$$
(4.4)



Figure 4.2:  $Pu^{3+}$  (a  $5f^5$  ion) has a J = 5/2 ground state split by the tetragonal crystal field symmetry into three Kramer's doublets, whose electron distribution is shown on the right. The ground doublet can fluctuate either to the "empty" half-filled J = 5/2 state ( $5f^6$ ) or "doubly-occupied" ( $5f^4$ ) state, which is two holes in the half-filled states. Both of these excited states will generically be singlets and have orthogonal symmetries.

In practice, there are many other excited states, but these are the most relevant, because they generate antiferromagnetic Kondo interactions. In a conventional Anderson model,  $\Gamma_2$  and  $\Gamma_1$  are the same channel, but here Hund's coupling forces  $\Gamma_1$  and  $\Gamma_2$  to be different, and it is this physics that introduces new symmetry channels into the charge fluctuations.

The simplified "atomic" model that describes this impurity is then

$$H_{at} = E_0 |0\rangle \langle 0| + E_1 |\Gamma_1 \sigma\rangle \langle \Gamma_1 \sigma| + E_2 |\phi\rangle \langle \phi|$$
(4.5)

where  $E_1 < E_0, E_2$ , as shown in Figure 4.2, and we neglect the excited crystal field doublets. When this atom is immersed into the conduction sea, the f-orbitals hybridize with conduction electrons with the same crystal symmetry. The hybridization Hamiltonian is written

$$H_{hybr} = \sum_{\sigma} \left[ V_{\Gamma_1} \psi^{\dagger}_{\Gamma_1 \sigma} f_{\Gamma_1 \sigma} + V_{\Gamma_2} \psi^{\dagger}_{\Gamma_2 \sigma} f_{\Gamma_2 \sigma} + (\text{H.c}) \right]$$
(4.6)

where  $\psi_{\Gamma\sigma}^{\dagger}$  creates a conduction electron in a Wannier state with crystal symmetry  $\Gamma$ . The matrix elements of this Hamiltonian between the Kramer's doublet and the two excited states are

$$\langle 0|H_{hyb}|\Gamma\sigma\rangle = V_{\Gamma_1}\psi^{\dagger}_{\Gamma_1\sigma} \langle \phi|H_{hyb}|\Gamma\sigma\rangle = V_{\Gamma_2}\psi_{\Gamma_2-\sigma}\tilde{\sigma},$$

$$(4.7)$$

where  $\tilde{\sigma} = \operatorname{sgn}(\sigma)$ . Thus the removal of an electron occurs in a *different symmetry channel* to the addition of an electron. The projected hybridization matrix becomes

$$H_{hybr} = \sum_{\sigma=\pm} \left( V_{\Gamma_1} \psi^{\dagger}_{\Gamma_1 \sigma} |0\rangle \langle \Gamma_1 \sigma | + \tilde{\sigma} V_{\Gamma_2} |\phi\rangle \langle \Gamma \sigma | \psi_{\Gamma_2 - \sigma} + \text{H.c} \right)$$
(4.8)

If we now carry out a Schrieffer Wolff transformation that integrates out the virtual charge fluctuations into the high-energy singlet states, where the energy of the absorbed, or emitted conduction electron is neglected, assuming it lies close to the Fermi energy, then we obtain

$$H_{K} = -\sum_{\sigma',\sigma=\pm 1} \left( J_{1} |\Gamma_{1}\sigma'\rangle \psi_{\Gamma_{1}\sigma'} \psi_{\Gamma_{1}\sigma}^{\dagger} \langle \Gamma_{1}\sigma | + J_{2} \,\tilde{\sigma}' \psi_{\Gamma_{2}-\sigma}^{\dagger} |\Gamma_{1}\sigma'\rangle \langle \Gamma_{1}\sigma | \psi_{\Gamma_{2}-\sigma'}\tilde{\sigma} \right), \tag{4.9}$$

where

$$J_1 = \frac{(V_{\Gamma_1})^2}{E_0 - E_1}, \qquad J_2 = \frac{(V_{\Gamma_2})^2}{E_2 - E_1}, \tag{4.10}$$

This Hamiltonian can be re-written in terms of spin operators as follows

$$\hat{H}_K = \frac{1}{2} \left[ J_1 \boldsymbol{\sigma}^{\Gamma_1} + J_2 \boldsymbol{\sigma}^{\Gamma_2} \right] \cdot \mathbf{S}_f, \tag{4.11}$$

where we have dropped potential scattering terms and introduced the notation

$$\mathbf{S}_{f} = \sum_{\alpha\beta} |\Gamma_{1}\alpha\rangle \boldsymbol{\sigma}_{\alpha\beta} \langle \Gamma_{1}\beta|, \quad \boldsymbol{\sigma}^{\Gamma} = \psi^{\dagger}_{\Gamma\alpha} \boldsymbol{\sigma}_{\alpha\beta} \psi_{\Gamma\beta}, \qquad (4.12)$$

for the spin of the Kramer's doublet and the conduction electron spin density at the local moment

site in channel  $\Gamma$ .

If we now generalize this derivation to a lattice, the interaction (4.11) develops at each site,

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{j} \left[ J_{1} \psi_{\Gamma_{1}j\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} \psi_{\Gamma_{1}j\beta} + J_{2} \psi_{\Gamma_{2}j\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} \psi_{\Gamma_{2}j\beta} \right] \cdot \mathbf{S}_{j},$$
(4.13)

where  $\mathbf{S}_j$  is the spin operator at site j and  $c_{\mathbf{k}\sigma}^{\dagger}$  creates a conduction electron of momentum  $\mathbf{k}$ . We can relate the Wannier states at site j as follows

$$\psi_{\Gamma_1 j \alpha} = \sum_{k\sigma} [\Phi_{1\mathbf{k}}]_{\alpha\sigma} c_{\mathbf{k}\sigma} e^{i\mathbf{k} \cdot \mathbf{R}_j}, \qquad \psi_{\Gamma_2 j \alpha} = \sum_{k\sigma} [\Phi_{2\mathbf{k}}]_{\alpha\sigma} c_{\mathbf{k}\sigma} e^{i\mathbf{k} \cdot \mathbf{R}_j}$$
(4.14)

where

$$[\Phi_{\Gamma \mathbf{k}}]_{\alpha\sigma} = \langle k\Gamma\alpha | \mathbf{k}\sigma \rangle = \sum_{m \in [-3,3]} \langle \Gamma\alpha | 3m, \frac{1}{2}\sigma \rangle Y^3_{m-\sigma}(\hat{\mathbf{k}})$$
(4.15)

is the form factor of the crystal field state. The two channel Kondo lattice Hamiltonian then takes the form

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{j,k,k'} \left[ J_1 \psi_{1\mathbf{k}\alpha}^{\dagger} \psi_{\Gamma_1 \mathbf{k}'\beta} + J_2 \psi_{2\mathbf{k}\alpha}^{\dagger} \psi_{2\mathbf{k}'\beta} \right] S_{\beta\alpha}(j) e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_j}.$$
(4.16)

The presence of two distinct scattering channels plays a central role in our model. For a single magnetic Kondo ion, the strongest spin-screening channel always dominates, forming a local Fermi liquid of the corresponding symmetry. Two perfectly balanced channels give rise to a critical state in which the spin screening fluctuates between the channels. Many groups have speculated that in a lattice environment, the spins will attempt to avoid this critical state through the development of superconductivity [89, 90, 87, 122]. Symplectic N enables us to develop the first controlled realization of this conjecture, which we apply to the new superconductors  $PuCoGa_5$  and  $NpPd_5Al_2$ .

### 4.1.2 Spins and large N

Before delving into a solution of the two channel Kondo lattice, we first discuss the large N solution of the single channel Kondo model, and then refresh the relevant aspects of symplectic-N.

### Large N solution of the SU(N) Kondo model

The SU(N) Kondo lattice [59, 60, 53] replicates the Kondo impurity at every site, each interacting with the same conduction sea:

$$H = \sum_{k} \epsilon_{k} c_{k\alpha}^{\dagger} c_{k\alpha} + \frac{J}{N} \sum_{j} c_{j\alpha}^{\dagger} c_{j\beta} S_{\alpha\beta}(j), \qquad (4.17)$$

where repeated spin indices are summed over, and we have taken a rotationally invariant hybridization for simplicity. While the Kondo impurity is exactly solvable, solving the Kondo lattice requires non-perturbative techniques like large N [124, 125, 167, 126], where Anderson has pointed out that the spin degeneracy, N = 2J + 1 is already relatively large for spin-orbit coupled Ce (N = 6) or Yb (N = 8) moments [168]. Here, the spins are treated with the fermionic representation of SU(N):  $S_{\alpha\beta}(j) = f^{\dagger}_{\alpha}f_{\beta}$ , with the constraint,  $n_f = N/2$  [101]. Inserting this representation into (4.17) leads to a quartic interaction term, which can be decoupling using the Hubbard-Stratonovich identity [169, 170],

$$\frac{J}{N}(c_{j\alpha}^{\dagger}f_{j\alpha})(f_{j\beta}^{\dagger}c_{j\beta}) \longrightarrow \bar{V}_{j}(c_{j\alpha}^{\dagger}f_{j\alpha}) + V_{j}(f_{j\alpha}^{\dagger}c_{j\alpha}) + \frac{N\bar{V}_{j}V_{j}}{J}, \qquad (4.18)$$

in terms of a mean field hybridization, V. The mean field Hamiltonian is [126, 171],

$$H = \sum_{k} \left( c_{k\alpha}^{\dagger} f_{k\alpha}^{\dagger} \right) \begin{pmatrix} \epsilon_{k} & V \\ V & \lambda \end{pmatrix} \begin{pmatrix} f_{k\alpha} \\ c_{k\alpha} \end{pmatrix} + N\mathcal{N}_{s} \left( \frac{V^{2}}{J} - \frac{\lambda}{2} \right), \quad (4.19)$$

where  $\lambda$  is a Lagrange multiplier enforcing the constraint  $n_f = N/2$  on average. This Hamiltonian describes two hybridizing bands of electrons, where V is the uniform hybridization, and  $\lambda$  is the f-"electron" Fermi level [recall Figure 1.9 (a)]. The spectrum is shown in Figure 1.9 (b), which corresponds to an enlarged Fermi surface, encompassing both the conduction electrons *and* the local moments [172, 173]

$$N\frac{\mathcal{V}_{FS}}{(2\pi)^3} = n_c + n_f = n_c + \frac{N}{2}.$$
(4.20)

At finite N, this mean field approximation is no longer exact. In the impurity, we know the violation is temperature dependent [174], so that large N describes the finite N ground state well, but is less appropriate at high temperatures, where, for example, it find a false phase transition at the coherence temperature,  $T^*$ , the lattice version of  $T_K$ .

The original f-"electrons" were neutral objects; how have they acquired a charge? It is not the original charge of the f-electron, since those degrees of freedom were frozen out at high energies. By comparing the original Hamiltonian, (4.17) with the mean field Hamiltonian, (4.19),  $\frac{J}{N}S_{\alpha\beta}c^{\dagger}_{\beta}c_{\alpha}$  is identified with  $\bar{V}f^{\dagger}_{\alpha}c_{\alpha} + Vc^{\dagger}_{\alpha}f_{\alpha}$ . Comparing the coefficients of  $c_{\alpha}$ , we find

$$\frac{J}{N}S_{\alpha\beta}c_{\beta}^{\dagger} = \bar{V}f_{\alpha}^{\dagger}.$$
(4.21)

So the combination of a spin flip,  $S_{\alpha\beta}$  and a conduction electron behaves as a composite fermionic entity at low energies and long times - this is what we call a composite fermion,  $\bar{V}f^{\dagger}$ . As it combines a charge 0, spin 1 spin-flip with a charge e, spin 1/2 conduction electron, it has all the quantum numbers of an ordinary electron [175, 48]. This composite fermion then hybridizes with the conduction electrons to form a band of heavy electrons. It must be emphasized that the appearance of a composite fermion is *not* due to the choice of a fermionic spin representation; the fermionic spin representation is rather the most natural representation because it contains such ready-made fermionic excitations. When we move on to the two channel Kondo lattice, we shall see that these composite fermions pair with conduction electrons in an orthogonal channel to form a singlet composite pair.

### Symplectic-N

There is no room in the SU(N) Kondo lattice for superconductivity, a consequence of the absence of time-reversal symmetry for any N > 2 which makes the formation of Cooper pairs impossible. Symplectic-N restores this time-reversal symmetry, and Cooper pairs appear naturally in this theory. When we are interested in Kondo physics and superconductivity, it is most natural to use the fermionic representation of symplectic spins,

$$\hat{S}_{\alpha\beta}(j) = f_{j\alpha}^{\dagger} f_{j\beta} - \tilde{\alpha} \tilde{\beta} f_{j-\beta}^{\dagger} f_{j-\alpha}, \qquad (4.22)$$

where  $\alpha$  is an integer ranging from

$$\alpha \in \{-N/2, ..., -1, 1, ..., N/2\}, \text{ and } \tilde{\alpha} = \operatorname{sgn}(\alpha).$$
 (4.23)

SU(N) spins commute with the number operator  $n_{fj}$  at each site, giving rise to a U(1) gauge invariance that features heavily in many analyses of correlated electron physics. Symplectic spins commute with  $n_{fj}$  as well, but also with the fermion pair operator  $\Psi_j = \sum_{\alpha} \tilde{\alpha} f_{j,-\alpha} f_{j\alpha}$  since this operator is an SP(N) singlet,

$$[S_{\alpha\beta}, \Psi_j] = [S_{\alpha\beta}, \Psi_j^{\dagger}] = [S_{\alpha\beta}, n_{fj}] = 0.$$
(4.24)

In a lattice, these symmetries apply independently at every spin site j, giving rise to a local SU(2)gauge invariance. This symmetry was first identified for spin-1/2 by Affleck et al. [140], who argued for its central role in defining the neutrality of spin. Symplectic spins allow us to extend this gauge symmetry to large N, provided we build our Hamiltonian exclusively out of symplectic spins, the process we call symplectic-N.

When using a fermionic spin representation, we must be careful to restrict the allowed states to the physical spin subspace by fixing the spin-Casimir. For SP(N), the spin Casimir is given by,

$$\vec{S}^2 + \vec{\Psi}^2 = N/2(N/2+2),$$
 (4.25)

where  $\vec{\Psi} = (\Psi^{\dagger} + \Psi, -i[\Psi^{\dagger} - \Psi], n_f - N/2)$  is the isospin vector (see section 2.5.1 for more details). In treating a spin problem like the Kondo lattice,  $\vec{S}^2$  must be maximized, meaning the spin-Casimir is fixed by setting  $\vec{\Psi} = 0$ , which fixes  $n_f = N/2$  and removes any s-wave pairs,  $\Psi$  from the local moment site. We have already shown in (4.24) that this constraint commutes with the Hamiltonian, which ensures that the Hamiltonian does not mix unphysical states into the physical subspace.

The "dot product" of symplectic spins  $\vec{S}_i \cdot \vec{S}_j = \frac{1}{2}S_{\alpha\beta}(1)S_{\beta\alpha}(2)$  has a unique decoupling in terms of both particle-hole and singlet pairs:

$$\vec{S}_1 \cdot \vec{S}_2 = -\left(B_{21}^{\dagger} B_{21} + A_{21}^{\dagger} A_{21}\right), \qquad (4.26)$$

where  $B_{21}^{\dagger} = \sum_{\sigma} \tilde{\sigma} f_{2\sigma}^{\dagger} f_{1-\sigma}^{\dagger}$  creates a valence bond of spins between sites one and two, while  $A_{21} = \sum_{\sigma} f_{2\sigma}^{\dagger} f_{1\sigma}$  "resonates" valence bonds between sites. In the terms of the Kondo model, the two spins are not at different sites, rather they represent different species of fermions: conduction electrons and "f-electrons," which are not really electrons at all, as they have no charge degrees of freedom. Particle-hole terms hybridize conduction electrons with these "f-electrons"  $c_{\sigma}^{\dagger} f_{\sigma}$ , while particle-particle terms appear to *pair* conduction and "f-electrons",  $\tilde{\sigma} c_{\sigma}^{\dagger} f_{-\sigma}^{\dagger}$ . In the large N limit, these will acquire expectation values. We shall see that both these terms are required for superconductivity, and that two channels are required for the two terms to have real, gauge-invariant meanings.

### **4.2** The symplectic-N two channel Kondo lattice

Now we proceed to develop the symplectic-N treatment for the two channel Kondo lattice,

$$\hat{H} = \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} c_{\mathbf{k}\alpha} + \frac{1}{N} \sum_{j} \left[ J_{1} \psi_{1\mathbf{k}\alpha}^{\dagger} \psi_{\Gamma_{1}\mathbf{k}'\beta} + J_{2} \psi_{2\mathbf{k}\alpha}^{\dagger} \psi_{2\mathbf{k}'\beta} \right] S_{\beta\alpha}(j) e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_{j}}, \qquad (4.27)$$

To develop a solvable mean field theory, we examine the family of models where

$$\hat{S}_{\alpha\beta}(j) = f_{j\alpha}^{\dagger} f_{j\beta} - \tilde{\alpha} \tilde{\beta} f_{j-\beta}^{\dagger} f_{j-\alpha}.$$
(4.28)

are the N component symplectic representation of the magnetic moment at each site j. The physical system corresponds to the limit N = 2. We will use a path integral approach to write the partition function,

$$\mathcal{Z} = \int \mathcal{D}[f, \psi] e^{-N\mathcal{S}[f, \psi]} \prod_{j} \delta\left(\vec{\Psi}_{j}\right), \qquad (4.29)$$

where  $N\mathcal{S}[f, \psi]$  is the action,

$$N\mathcal{S}[f,\psi] = \exp\left[-\int_0^\beta d\tau \sum_{j\alpha} \left(\psi_{j\alpha}^\dagger \partial_\tau \psi_{j\alpha} + f_{j\alpha}^\dagger \partial_\tau f_{j\alpha} + H[f,\psi]\right)\right],\tag{4.30}$$

and  $\prod_j \delta\left(\vec{\Psi}_j\right)$  enforces the SU(2) constraint,  $\vec{\Psi}_j = 0$  at every site. When we expand the Kondo interaction in equation (4.27), we obtain  $H_K(j) = \sum_{\Gamma=1,2} H_{\Gamma}(j)$ , where

$$H_{\Gamma}(j) = -\frac{J_{\Gamma}}{N} \left[ (\psi_{j\Gamma}^{\dagger} f_j) (f_j^{\dagger} \psi_{j\Gamma}) + (\psi_{j\Gamma}^{\dagger} \epsilon^{\dagger} f_j^{\dagger}) (f_j \epsilon \psi_{j\Gamma}) \right]$$
(4.31)

describes the spin exchange at site j in channels  $\Gamma = 1, 2$  and  $\psi_{j\Gamma}^{\dagger} = \sum_{\mathbf{k}} \psi_{\mathbf{k}\Gamma}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{R}_{j}}$  creates an electron in a Wannier state of symmetry  $\Gamma$  at site j. This interaction exhibits the local SU(2) gauge symmetry,

$$f_{\alpha} \to \cos \theta f_{\alpha} + \sin \theta \tilde{\alpha} f^{\dagger}_{-\alpha}. \tag{4.32}$$

The important point here, is that this symmetry survives for all even N. Earlier efforts have been made to develop SU(2) gauge theories of heavy electron systems [122], but were not justified in terms of a controlled expansion.

When the Kondo interaction is factorized, it decouples into a Kondo hybridization V and pairing field  $\Delta$  as follows

$$H_{\Gamma}(j) \to \sum_{\alpha} \left[ \left( f_{\alpha}^{\dagger} V_{\Gamma} + \tilde{\alpha} f_{-\alpha} \Delta_{\Gamma} \right) \psi_{\Gamma\alpha} + \text{H.C} \right] + N \left( \frac{|V_{\Gamma}|^2 + |\Delta_{\Gamma}|^2}{J_{\Gamma}} \right)$$
(4.33)

where we have suppressed the site indices j for clarity. The SU(2) gauge transformation becomes,

$$\begin{pmatrix} V_{\Gamma} \\ \Delta_{\Gamma} \end{pmatrix} \to g \begin{pmatrix} V_{\Gamma} \\ \Delta_{\Gamma} \end{pmatrix}, \qquad \begin{pmatrix} f_{\alpha} \\ \tilde{\alpha}f^{\dagger}_{-\alpha} \end{pmatrix} \to g \begin{pmatrix} f_{\alpha} \\ \tilde{\alpha}f^{\dagger}_{-\alpha} \end{pmatrix}$$
(4.34)

where  $g = \begin{pmatrix} u & v^* \\ v & -v^* \end{pmatrix}$  is an SU(2) matrix. The mean-field Hamiltonian defined by this decoupling

becomes exact in the large N limit. Despite the appearance of "pairing terms" in the Kondo interaction, the formation of Kondo singlets in a single channel does not lead to superconductivity; an SU(2) gauge transformation on the f-electron can always absorb the pairing term  $\Delta$  into a redefinition of the f-electron:

$$\bar{V}f_{\alpha}^{\dagger} + \bar{\Delta}\tilde{\alpha}f_{-\alpha} \to \sqrt{|V|^2 + |\Delta|^2}f_{\alpha}^{\dagger}.$$
(4.35)

For the one channel Kondo lattice, the SU(N) and symplectic-N limits are thus identical.

For two channels, this is no longer the case. Here it is convenient to rewrite the decoupled Hamiltonian,

$$H_{\Gamma K} = \sum_{j,\alpha>0} \left[ (\tilde{\psi}_{j\Gamma\alpha}^{\dagger} \mathcal{V}_{\Gamma j}^{\dagger} \tilde{f}_{j\alpha}) + (\tilde{f}_{j\alpha}^{\dagger}) \mathcal{V}_{\Gamma j} \tilde{\psi}_{\Gamma j\alpha} \right] + \frac{N}{2J_{\Gamma}} \operatorname{Tr}[\mathcal{V}_{\Gamma j}^{\dagger} \mathcal{V}_{\Gamma j}]$$
(4.36)

by introducing the Nambu spinors,

$$\tilde{f}_{j\alpha} = \begin{pmatrix} f_{j\alpha} \\ \tilde{\alpha}f_{j-\alpha}^{\dagger} \end{pmatrix}, \qquad \tilde{\psi}_{\Gamma j\alpha} = \begin{pmatrix} \psi_{\Gamma j\alpha} \\ \tilde{\alpha}\psi_{\Gamma j-\alpha}^{\dagger} \end{pmatrix}, \qquad (4.37)$$

and two corresponding matrix SU(2) order parameters,

$$\mathcal{V}_{\Gamma j} = \begin{pmatrix} V_{\Gamma j} & \bar{\Delta}_{\Gamma j} \\ \\ \Delta_{\Gamma j} & -\bar{V}_{\Gamma j} \end{pmatrix}, \qquad (4.38)$$

which transform identically under an SU(2) gauge transformation  $g_j$ ,  $\tilde{f}_j \rightarrow g_j \tilde{f}_j$ ,  $\mathcal{V}_{\Gamma j} \rightarrow g_j \mathcal{V}_{\Gamma j}$ . These represent the hybridization in channel  $\Gamma$  at site j, and generically have both particle-hole and particle-particle contributions.

We seek uniform mean-field solutions, where  $\mathcal{V}_{\Gamma j}$  is constant at each site. In this situation, its convenient to re-write the Wannier states and f-states in a momentum state basis, switching back to the Bloch wave basis for the conduction electrons,  $c_{\mathbf{k}}^{\dagger}$ , and absorbing the form-factors into  $\mathcal{V}_{\mathbf{k}} \longrightarrow \mathcal{V}_1 \Phi_{1\hat{\mathbf{k}}} + \mathcal{V}_2 \Phi_{2\hat{\mathbf{k}}}$ , which is a 2 × 2 matrix in spin-space. For simplicity, we suppress the spin indices here and consider  $\mathcal{V}_{\mathbf{k}}$  to be spin-diagonal We can group these terms into a matrix that
concisely describes the mean-field theory as follows

$$H = \sum_{\mathbf{k},\alpha>0} (c_{\mathbf{k}\alpha}^{\dagger}, \tilde{f}_{\mathbf{k}\alpha}^{\dagger}) \begin{pmatrix} \epsilon_{\mathbf{k}} \tau_3 & \mathcal{V}_{\mathbf{k}}^{\dagger} \\ \mathcal{V}_{\mathbf{k}} & \vec{\lambda} \cdot \vec{\tau} \end{pmatrix} \begin{pmatrix} \tilde{c}_{\mathbf{k}\alpha} \\ \tilde{f}_{\mathbf{k}\alpha} \end{pmatrix} + N\mathcal{N}_s \left( \frac{\operatorname{Tr}[\mathcal{V}_1^{\dagger}\mathcal{V}_1]}{2J_1} + \frac{\operatorname{Tr}[\mathcal{V}_2^{\dagger}\mathcal{V}_2]}{2J_2} \right).$$
(4.39)

The summation over  $\alpha$  is restricted to positive values to avoid overcounting, and we have absorbed the constraint  $\vec{\Psi}_j = \sum_{\alpha>0} \tilde{f}_{j\alpha}^{\dagger} \vec{\tau} \tilde{f}_{j\alpha} = 0$  into the Hamiltonian by using a Lagrange multiplier,  $\vec{\lambda}_j = \vec{\lambda}$  that enforces the constraint on average (an approximation that is exact in the large Nlimit). When the two Kondo channels are orthogonal, it is sufficient to enforce the  $\tau_3$  component of the constraint,  $n_f = N/2$  with a single Lagrange multiplier,  $\lambda$ . This form of the mean-field theory can be elegantly generalized to include the effects of spin-orbit coupled crystal fields by restoring the two-dimensional matrix structure to the form-factors  $\Phi_{\Gamma \mathbf{k}}$ , as we discuss in Appendix 4B. Diagonalizing this mean-field Hamiltonian reveals the heavy-fermion band structure, where we see that hybridization in channels one and two both give rise to hybridization gaps, but the second gap is pinned to the Fermi surface, behaving as a BCS superconducting gap.

Ostensibly, our mean-field theory is that of a two-band BCS superconductor, with hybridization processes that pair the heavy electrons, and Hamiltonian described by

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} \tau_3 & \mathcal{V}_{\mathbf{k}}^{\dagger} \\ \mathcal{V}_{\mathbf{k}} & \lambda \tau_3 \end{pmatrix}$$
(4.40)

However, hidden beneath the hood of the theory is the underlying gauge invariance that maintains the neutrality of the f-spins. To understand the pairing, we must look not to the hybridization pairing terms, which are gauge dependent, but to the gauge-invariant variables in the theory. Indeed, it is not possible to say whether the pairing is in channel one or in channel two. The SU(2) gauge invariant quantity is the product  $\mathcal{V}_{2j}^{\dagger}\mathcal{V}_{1j}$  has an off-diagonal component  $\Psi = (V_{1j}\Delta_{2j} - V_{2j}\Delta_{1j})$ : this quantity preserves the local SU(2) invariance, but it *breaks* the global U(1) gauge invariance associated with physical charge, and plays the role of a superconducting order parameter. If we carry out an SU(2) gauge transformation that removes the  $\Delta_{1j}$ , the composite order parameter  $\Psi_j = V_{1j} \Delta_{2j}.$ 

### 4.2.1 Composite pairing

Physically, we may understand this phenomenon as the consequence of the formation of a condensate of composite pairs: where triplet pairs of conduction electrons (necessarily in orthogonal Kondo channels) form a bound-state singlet in combination with a local moment that collectively condenses (Figure 4.3). Such composite order parameters were originally considered in odd-frequency superconductivity [176], and introduced in heavy fermion superconductivity by Coleman, Andrei, Tsvelik and Kee in 1999 [122]. Our large-*N* analysis provides the first solvable limit in which this mechanism can be rigorously validated, while at the same time incorporating the detailed spin-orbit physics of the crystal field split screening channels.



Figure 4.3: Creating a composite pair involves adding a triplet pair of conduction electrons while flipping the local moment, creating an overall singlet. In order to add a triplet of conduction electrons, they must be in orthogonal channels, A and B.

When an electron scatters off a magnetic impurity, the quantity  $\Psi$  determines the amplitude for emitting an Andreev hole and leaving behind a composite pair. Detailed analysis (see Appendix 4A) confirms this insight and demonstrates the formation of composite order with expectation value

$$\langle \Psi_{N-2} | \psi_{1\downarrow}(j) \psi_{2\downarrow}(j) S_f^+(j) | \Psi_N \rangle \propto (V_{1j} \Delta_{2j} - V_{2j} \Delta_{1j}).$$
(4.41)

The order parameter can be written explicitly as an SP(N) singlet,  $\langle \psi_1^{\dagger}(\boldsymbol{\sigma}_N \cdot \mathbf{S}) \epsilon \psi_2^{\dagger} \rangle$ , where  $\vec{\sigma}_N$  is the SP(N) generalization of the Pauli matrices,  $\vec{\sigma}$ . In a single impurity model, this order parameter is forbidden, because electrons can never change between scattering channels, but in the lattice, electrons travelling between sites no longer conserve the channel index, permitting composite order. Once composite order develops, the Kondo singlets resonate between the two screening channels, and the resonance energy this gives rise to stabilizes the coherent state.

### 4.2.2 Resonant Andreev scattering

Composite pairing manifests itself as the development of an Andreev reflection component to the resonant scattering off magnetic impurities (see Figure 4.4). We can capture this scattering in the mean-field theory by integrating out the f-electrons, which leads to a conduction electron Green's function of the form

$$G(\kappa)^{-1} = \omega - \epsilon_{\mathbf{k}} \tau_3 - \Sigma(\kappa), \qquad \Sigma(\kappa) = \mathcal{V}_{\mathbf{k}}^{\dagger} (\omega - \lambda \tau_3)^{-1} \mathcal{V}_{\mathbf{k}}$$

where  $\kappa \equiv (\mathbf{k}, \omega)$ . The hybridization matrices are written  $\mathcal{V}_{\mathbf{k}} = \mathcal{V}_1 \hat{\Phi}_{1\mathbf{k}} + \mathcal{V}_2 \hat{\Phi}_{2\mathbf{k}}$  where we take  $\mathcal{V}_1 = iv_1$  and  $\mathcal{V}_2 = \Delta_2 \tau_2$ .

It is convenient at this stage to examine the off-diagonal structure of the  $\hat{\Phi}_{\Gamma \mathbf{k}}$ . The matrix  $\hat{\Phi}_{\Gamma \mathbf{k}}$  takes the form  $\phi_{\Gamma \mathbf{k}} \mathcal{U}_{\Gamma \mathbf{k}}$  where  $\phi_{\Gamma_{\mathbf{k}}}$  is a scalar and  $\mathcal{U}_{\Gamma \mathbf{k}}$  is a two-dimensional unitary matrix defining the interconversion between Bloch states and spin-orbit coupled Wannier states. When an electron "enters" the Kondo singlet, its spin quantization axis is rotated according to the matrix  $\mathcal{U}_{\Gamma \mathbf{k}}$ . When it leaves the ion in the same channel, this rotation process is undone, and the net hybridization matrix  $\hat{\Phi}_{\Gamma \mathbf{k}}^{\dagger} \hat{\Phi}_{\Gamma \mathbf{k}} = (\phi_{\Gamma \mathbf{k}})^2 \mathbf{1}$  is spin-diagonal. However, in the presence of composite pairing an incoming electron in channel 1 can Andreev scatter from the ion as a hole in channel 2. This leads to a net rotation of the spin quantization axis through an angle  $\zeta_{\mathbf{k}}$  about an axis  $\mathbf{n}_{\mathbf{k}}$  that both depend on the location on the Fermi surface, as follows

$$\hat{\Phi}_{2\mathbf{k}}^{\dagger} \cdot \hat{\Phi}_{1\mathbf{k}} = \phi_{2\mathbf{k}} \phi_{1\mathbf{k}} [c_{\mathbf{k}} + is_{\mathbf{k}} (\mathbf{n}_{\mathbf{k}} \cdot \boldsymbol{\sigma})]$$



Figure 4.4: The scattering processes which lead to Kondo hybridization are intra-channel, where a conduction electron (solid line) enters and leaves the Kondo singlet in the same channel. The orange insets show the angular dependence of the hybridization functions for the different channels, where  $\Gamma_1 = \Gamma_7^+$  and  $\Gamma_2 = \Gamma_6$ . However, the formation of a composite pair leads to Andreev scattering of conduction electrons between the two channels, leaving behind a composite pair with a superconducting gap symmetry given by the trace of the overlap between the two hybridization functions. For these two channel symmetries, the Andreev scattering process transfers two units of angular momentum, giving rise to a d-wave gap function.

where  $c_{\mathbf{k}} = \cos(\zeta_{\mathbf{k}}/2), s_{\mathbf{k}} = \sin(\zeta_{\mathbf{k}}/2).$ 

When we expand the self energy, we obtain a normal and an Andreev component,  $\Sigma = \Sigma_N + \Sigma_A$ where the normal component is given by

$$\Sigma_{N}(\kappa) = \frac{v_{1\mathbf{k}}^{2}}{\omega - \lambda \tau_{3}} + \frac{v_{2\mathbf{k}}^{2}}{\omega + \lambda \tau_{3}} = \frac{1}{\omega^{2} - \lambda^{2}} \left[ \omega(v_{1\mathbf{k}}^{2} + v_{2\mathbf{k}}^{2}) + \lambda(v_{1\mathbf{k}}^{2} - v_{2\mathbf{k}}^{2})\tau_{3} \right], \qquad (4.42)$$

denoting  $v_{1\mathbf{k}} = v_1 \phi_{1\mathbf{k}}, v_{2\mathbf{k}} = \Delta_2 \phi_{2\mathbf{k}}$ . By contrast, the Andreev terms take the form

$$\Sigma_{A}(\kappa) = V_{1}\Delta_{2} \left( \frac{i\omega\tau_{2} - \lambda\tau_{1}}{(\omega^{2} - \lambda^{2})} \Phi_{2\mathbf{k}}^{\dagger} \Phi_{1\mathbf{k}} + \text{H.c} \right)$$
  
$$= \frac{2v_{1\mathbf{k}}v_{2\mathbf{k}}}{(\omega^{2} - \lambda^{2})} \left[ -\lambda c_{\mathbf{k}}\tau_{1} + \omega s_{\mathbf{k}}(\mathbf{n}_{\mathbf{k}} \cdot \boldsymbol{\sigma})\tau_{2} \right]$$
(4.43)

Notice how the Andreev scattering contains two terms:

• a scalar term  $\frac{2v_{1\mathbf{k}}v_{2\mathbf{k}}}{(\lambda^2-\omega^2)}\lambda c_{\mathbf{k}}\tau_1$  that is finite at the Fermi energy ( $\omega = 0$ ), with gap symmetry of

the form

$$\Delta_{\mathbf{k}} \propto \mathrm{Tr} \Phi_{2\mathbf{k}}^{\dagger} \Phi_{1\mathbf{k}} \sim \phi_{1\mathbf{k}} \phi_{2\mathbf{k}} c_{\mathbf{k}}$$

• a "triplet" term  $-\omega \frac{2v_{1\mathbf{k}}v_{2\mathbf{k}}}{(\lambda^2 - \omega^2)} [s_{\mathbf{k}}(\mathbf{n}_{\mathbf{k}} \cdot \boldsymbol{\sigma})\tau_2]$  which is *odd* in frequency and vanishes on the Fermi surface.

In practice, the nodes of the pair wavefunction are dominated by the symmetry of the function  $c_{\mathbf{k}}$ . When an electron Andreev reflects through one hybridization channel into the other, it acquires orbital angular momentum. For example, the "up" states of the  $\Gamma_7^+ \sim |-3/2\rangle$  and  $\Gamma_7^- \sim |+5/2\rangle$  differ by l = 4 units of angular momentum, so the resulting gap has the symmetry of an l = 4 spherical harmonic, or g- wave symmetry. By contrast, the up states of the  $\Gamma_7^+ \sim |-3/2\rangle$  and  $\Gamma_6 \sim |+1/2\rangle$  differ by l = 2 units of angular momentum, and the resulting gap has the symmetry of an l = 2 spherical harmonic, or d- wave symmetry. In our model, we have chosen  $\Gamma_1 \equiv \Gamma_7^+$ , which maximizes the overlap with the out-of-plane ligand atoms and  $\Gamma_2 \equiv \Gamma_7^-$  corresponding to the in-plane ligand atoms. In this case, we find the gap has the form

$$\phi_{1\mathbf{k}}\phi_{2\mathbf{k}}c_{\mathbf{k}} = \frac{v_1\Delta_2}{4}\operatorname{Tr}[\Phi_{2\mathbf{k}}^{\dagger}\Phi_{1\mathbf{k}} + \text{H.c.}] = \cos(2\beta)\Delta_{g1}(\mathbf{k}) - \sin(2\beta)\Delta_{g2}(\mathbf{k})$$

where  $\Delta_{g1}$  and  $\Delta_{g2}$  are g-wave gap functions of the form

$$\Delta_{g1}(\mathbf{k}) = \frac{\sqrt{5}}{16\pi} \cos(4\phi) \sin^2[\theta]; \qquad \Delta_{g2}(\mathbf{k}) = \frac{3}{16\pi} \sin^2(\theta) (3 + \cos(2\theta)) \tag{4.44}$$

For small  $\beta$ , the gap is dominated by  $\Delta_{g1}(\mathbf{k})$ .



Figure 4.5: Three possible composite pairing gaps for the three Kramer's doublets of a J = 5/2 ion, like Pu or Ce, where  $\beta = .1\pi$  and red (blue) indicate positive (negative) gap regions.  $\Gamma_7^+ \otimes \Gamma_7^-$  (left) is g-wave, while  $\Gamma_7^\pm \otimes \Gamma_6$  is d-wave.

## 4.2.3 Solving the mean field theory

To derive the mean-field theory of the uniform composite pair state, we must diagonalize the meanfield Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} \tau_3 & \mathcal{V}_{\mathbf{k}}^{\dagger} \\ \mathcal{V}_{\mathbf{k}} & \lambda \tau_3 \end{pmatrix}$$
(4.45)

with  $\mathcal{V}_{\mathbf{k}} = \mathcal{V}_1 \Phi_{1\mathbf{k}} + \mathcal{V}_2 \Phi_{2\mathbf{k}}$ . Treating the full spin-orbit form factors is complicated, so we relegate this treatment to Appendix 4B, and here take a simplified model where we assume the  $\Phi_{\Gamma \mathbf{k}} = \phi_{\Gamma \mathbf{k}} \mathbf{1}$  are spin-diagonal. To examine the uniform pairing state we may fix the SU(2) gauge so that hybridization in channel 1 is in the particle-hole channel, with  $V_1 = iv_1$ ,  $\Delta_1 = 0$ , i.e  $\mathcal{V}_1 = iv_1$  while the hybridization in channel 2 is in the Cooper channel,  $V_2 = 0$  and  $\mathcal{V}_2 = \Delta_2 \tau_2$ . The eigenvalues  $\omega_{\mathbf{k}}$  of  $H_{\mathbf{k}}$  are determined by

$$\det(\omega \underline{1} - H_{\mathbf{k}}) = \omega^4 - 2\alpha_{\mathbf{k}}\omega^2 + \gamma_{\mathbf{k}}^2 = 0.$$

where we have introduced the notation:

$$\alpha_{\mathbf{k}} = v_{\mathbf{k}+}^2 + \frac{1}{2} \left( \epsilon_{\mathbf{k}}^2 + \lambda^2 \right), \quad \gamma_{\mathbf{k}}^2 = (\epsilon_{\mathbf{k}} \lambda - v_{\mathbf{k}-}^2)^2 + 4 (v_{1\mathbf{k}} v_{2\mathbf{k}} c_{\mathbf{k}})^2, \tag{4.46}$$

$$v_{1\mathbf{k}} = v_1 \phi_{1\mathbf{k}}, \qquad v_{2\mathbf{k}} = \Delta_2 \phi_{2\mathbf{k}}, \qquad v_{\mathbf{k}\pm}^2 = v_{1\mathbf{k}}^2 \pm v_{2\mathbf{k}}^2.$$
 (4.47)

The quantity  $c_{\mathbf{k}}$  measures the amplitude for singlet Andreev reflection, and is unity for the simplified spin-diagonal model. When the form factors  $\Phi_{\Gamma \mathbf{k}}$  contain off-diagonal components, the above equations still hold, but with the definitions

$$\phi_{\Gamma\mathbf{k}}^{2} = \frac{1}{2} \operatorname{Tr} \left[ \Phi_{\Gamma\mathbf{k}}^{\dagger} \Phi_{\Gamma\mathbf{k}} \right]$$

$$c_{\mathbf{k}} = \frac{\operatorname{Tr} \left[ \Phi_{2\mathbf{k}}^{\dagger} \Phi_{1\mathbf{k}} + \Phi_{1\mathbf{k}}^{\dagger} \Phi_{2\mathbf{k}} \right]}{4\phi_{1\mathbf{k}}\phi_{2\mathbf{k}}} = \frac{\operatorname{Re}\operatorname{Tr} \left[ \Phi_{2\mathbf{k}}^{\dagger} \Phi_{1\mathbf{k}} \right]}{\sqrt{\operatorname{Tr} \left[ \Phi_{1\mathbf{k}}^{\dagger} \Phi_{1\mathbf{k}} \right] \operatorname{Tr} \left[ \Phi_{2\mathbf{k}}^{\dagger} \Phi_{2\mathbf{k}} \right]}}$$

$$(4.48)$$

The eigenvalues of  $H_{\bf k}$  are given by  $\omega=\omega_{{\bf k}\pm}$  and  $\omega=-\omega_{{\bf k}\pm},$  where

$$\omega_{\mathbf{k}\pm} = \sqrt{\alpha_{\mathbf{k}} \pm (\alpha_{\mathbf{k}}^2 - \gamma_{\mathbf{k}}^2)^{1/2}}.$$
(4.49)

The quantity

$$\Delta_{\mathbf{k}} \sim v_{1\mathbf{k}} v_{2\mathbf{k}} c_{\mathbf{k}}$$

plays the role of the gap in the spectrum. Quasiparticle nodes develop on the heavy Fermi surface defined by  $\epsilon_{\mathbf{k}} = v_{\mathbf{k}-}^2/\lambda$  in directions where  $\Delta_{\mathbf{k}} = 0$ .

The mean field equations are obtained by minimizing the free energy

$$\mathcal{F} = -NT \sum_{\mathbf{k},\pm} \log[2\cosh(\beta\omega_{\mathbf{k}\pm}/2)] + N\mathcal{N}_s \sum_{\Gamma=1,2} \frac{v_{\Gamma}^2}{J_{\Gamma}}$$
(4.50)

with respect to  $\lambda$  and  $(v_{\Gamma})^2$  ( $\Gamma = 1, 2$ ), which yields

$$\frac{1}{\mathcal{N}_{s}} \sum_{\mathbf{k}\pm} \frac{\tanh(\omega_{\mathbf{k}\pm}/2T)}{2\omega_{\mathbf{k}\pm}} \left( \lambda \pm \frac{\lambda\alpha_{\mathbf{k}} - \epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}}\lambda - v_{\mathbf{k}-}^{2})}{\sqrt{\alpha_{\mathbf{k}}^{2} - \gamma_{\mathbf{k}}^{2}}} \right) = 0,$$

$$\frac{1}{\mathcal{N}_{s}} \sum_{\mathbf{k}\pm} \phi_{1\mathbf{k}}^{2} \frac{\tanh(\omega_{\mathbf{k}\pm}/2T)}{2\omega_{\mathbf{k}\pm}} \left( 2 \pm \frac{(\epsilon_{\mathbf{k}} + \lambda)^{2} + 4(v_{2\mathbf{k}}s_{\mathbf{k}})^{2}}{\sqrt{\alpha_{\mathbf{k}}^{2} - \gamma_{\mathbf{k}}^{2}}} \right) = \frac{4}{J_{1}},$$

$$\frac{1}{\mathcal{N}_{s}} \sum_{\mathbf{k}\pm} \phi_{2\mathbf{k}}^{2} \frac{\tanh(\omega_{\mathbf{k}\pm}/2T)}{2\omega_{\mathbf{k}\pm}} \left( 2 \pm \frac{(\epsilon_{\mathbf{k}} - \lambda)^{2} + 4(v_{1\mathbf{k}}s_{\mathbf{k}})^{2}}{\sqrt{\alpha_{\mathbf{k}}^{2} - \gamma_{\mathbf{k}}^{2}}} \right) = \frac{4}{J_{2}},$$
(4.51)

where we have put  $s_{\mathbf{k}}^2 = 1 - c_{\mathbf{k}}^2$ . In the normal phase either  $v_1$  or  $v_2$  is nonzero, corresponding to the development of the Kondo effect in the strongest channel. Therefore, there are two types of normal phase with two different Fermi surfaces:

•  $J_1 > J_2, v_2 = 0$  with spectrum

$$\omega_{\mathbf{k}\pm} = \frac{1}{2} \left( \epsilon_{\mathbf{k}} + \lambda \pm \sqrt{(\epsilon_{\mathbf{k}} - \lambda)^2 + 4v_{1\mathbf{k}}^2} \right).$$
(4.52)

corresponding to Kondo lattice effect in channel 1, and

•  $J_2 > J_1, v_1 = 0$ , with dispersion

$$\omega_{\mathbf{k}\pm} = \frac{1}{2} \left( \epsilon_{\mathbf{k}} - \lambda \pm \sqrt{(\epsilon_{\mathbf{k}} + \lambda)^2 + 4v_{2\mathbf{k}}^2} \right).$$
(4.53)

corresponding to a Kondo lattice effect in channel 2.

The two normal phases are always unstable with respect to formation of the composite paired state at sufficiently low temperature.

We have calculated the superconducting transition temperature,  $T_c$  as a function of the ratio  $J_2/J_1$ , and Figure 4.6 shows the results of a model calculation, in which the band structure of the conduction electrons is derived from the 3D tight binding model:

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y + \cos k_z) - \mu \tag{4.54}$$



Figure 4.6: Phase diagram for a two-channel Kondo lattice, computed in the symplectic large-N limit for tetragonal symmetry, where spin is exchanged via channels  $\Gamma_1 = \Gamma_7^+$  and  $\Gamma_2 = \Gamma_7^-$ . The x-axis co-ordinate is the parametric variable  $x = 2(J_2/J_2)/(1+J_2/J_1)$  running from x = 0 to x = 2, corresponding to  $J_2/J_1$  running from zero to infinity, as labeled. Temperature is measured in units of the maximum Kondo temperature of the two channels  $T_0 = \max(T_{K1}, T_{K2})$ . Two Fermi liquids of different symmetry develop in the regions of small and large  $J_2/J_1$ , separated by a common region of composite-pairing, delineated by the gray area. The red-point denotes the location of the single-impurity quantum critical point that develops when the two channels are degenerate. In the lattice, this point is avoided through the development of composite pairing.

where  $\mu$  is the chemical potential. Our choice of form factors is dictated by the corresponding crystal structure of the PuCoGa<sub>5</sub>, where we select  $\Phi_{1\hat{k}} = \Phi_{\Gamma_7^+ k}$  for the electrons in channel one and  $\Phi_{2\hat{k}} = \Phi_{\Gamma_7^- k}$  for the holes in channel two. As we lower the temperature, the superconducting instability develops in the weaker channel. The critical temperature for the composite pairing instability is determined from equations (4.51) by putting  $v_2 = 0^+$ . From the third equation with logarithmic accuracy we have  $\log(T_{K1}/T_c) \simeq 1/J_2$  which yields

$$T_c \simeq \sqrt{T_{K1} T_{K2}}.\tag{4.55}$$

signaling a maximum  $T_c$  for  $J_1 \simeq J_2$ .

It is instructive to contrast the phase diagrams of the SU(N) and symplectic large N limits. In the former, there is a single quantum phase transition that separates the heavy electron Fermi liquids formed via a Kondo effect about the strongest channel. In the symplectic treatment, coherence develops between the channels, immersing the two-channel quantum critical point beneath a superconducting dome. The Cooper channel in the heavy-electron normal state guarantees that the secondary screening channel is always marginally relevant in the lattice, as first speculated in ref. [122]. This is, to our knowledge, the first *controlled* mean-field theory in which the phenomenon of "avoided criticality" gives rise to superconductivity.

### 4.2.4 Landau theory of composite pairing

The qualitative aspects of the symplectic large N phase diagram are simply illustrated within a Landau theory valid in the vicinity of  $J_1 = J_2^{1}$ . Here, we again take the simplified two dimensional example, in the vicinity of  $J_1 = J_2$  and at temperatures just below  $T_c \simeq \sqrt{T_{K1}T_{K2}}$ . Proximity to the transition point guarantees the smallness of the hybridization, V and pairing field,  $\Delta$  and justifies the Landau expansion in these quantities. In this region, the Landau free energy,  $F[\mathcal{V}_1, \mathcal{V}_2] = F_0 + F_L$  divides into a single impurity term,  $F_0$  that preserves the channel symmetry and a lattice term  $F_L$  containing terms that violate channel conservation and drive superconductivity.

To obtain this Landau expansion, we again take the path integral form of the mean-field partition function,

$$\mathcal{Z} = \int \mathcal{D}[f, c, \lambda, \mathcal{V}] e^{-NS[f, c, \lambda, \mathcal{V}]},$$
$$NS[f, c, \lambda, \mathcal{V}] = \int_{0}^{\beta} d\tau \sum_{\mathbf{k}, \alpha > 0} \tilde{c}_{\mathbf{k}\alpha}^{\dagger} (\partial_{\tau} + \epsilon_{\mathbf{k}} \tau_{3}) \tilde{c}_{\mathbf{k}\alpha} + \sum_{j, \alpha > 0} \tilde{f}_{j\alpha}^{\dagger} (\partial_{\tau} + \lambda \tau_{3}) \tilde{f}_{j\alpha} + \sum_{j, \Gamma} H_{\Gamma}(j),$$
(4.56)

where  $H_{\Gamma}$  is given in equation (4.36), and we consider the translationally invariant saddle point.

<sup>&</sup>lt;sup>1</sup>This section was primarily written by Maxim Dzero, and is included for completeness.

Note that we have *not* fixed the gauge, and this Landau theory is completely gauge invariant. We can now integrate out the fermionic fields, which yields the following effective action written explicitly in terms of the  $\mathcal{V}_{\Gamma}$ 's and bare fermionic propagators  $\hat{\mathcal{F}}_0 = [\partial_{\tau} - \lambda \tau_3]^{-1}$ ,  $\hat{\mathcal{G}}_0 = [\partial_{\tau} - \epsilon_k \tau_3]^{-1}$ :

$$NS_{eff} = \int_{0}^{\beta} d\tau \left( \frac{1}{J_{\Gamma}} \operatorname{Tr}[\mathcal{V}_{\Gamma}^{\dagger} \mathcal{V}_{\Gamma}] - \operatorname{Tr}\log[1 - \hat{\mathcal{F}}_{0} \mathcal{V}_{\Gamma}^{\dagger} \hat{\mathcal{G}}_{0} \mathcal{V}_{\Gamma}] \right).$$
(4.57)

The Landau free energy is obtained by expanding the expression under the logarithm in  $S_{eff}$  out to fourth order in  $\mathcal{V}$ . We have then evaluated the traces over momentum and imaginary time, to obtain the following expressions.

The single impurity contribution to the free energy can be written,

$$F_0 = \frac{1}{2}(t+\alpha)\operatorname{Tr}\left(\mathcal{V}_1\mathcal{V}_1^{\dagger}\right) + \frac{1}{2}(t-\alpha)\operatorname{Tr}\left(\mathcal{V}_2\mathcal{V}_2^{\dagger}\right) + \frac{U}{4}\operatorname{Tr}\left[\left(\mathcal{V}_1\mathcal{V}_1^{\dagger} + \mathcal{V}_2\mathcal{V}_2^{\dagger}\right)^2\right]$$
(4.58)

where  $t = \rho \ln \left(\frac{T}{\sqrt{T_{K1}T_{K2}}}\right)$ ,  $\alpha = \rho \ln \left(\frac{T_{K2}}{T_{K1}}\right)$  describes the channel asymmetry and  $\rho$  is the conduction electron density of states.  $F_0$  displays a local SU(2) symmetry,  $\mathcal{V}_{\Gamma} \rightarrow g\mathcal{V}_{\Gamma}$ , as well as the individual channel symmetries,  $\mathcal{V}_{\Gamma} \rightarrow h_{\Gamma}\mathcal{V}_{\Gamma}$ . This function captures the essence of a large N Kondo lattice where the channel quantum number is conserved. There is simply an instability at  $\frac{T}{T_c} = 1 + |\alpha|$  where hybridization develops in the strongest channel. The special case of  $\alpha = 0$  describes a bicritical point in the zero temperature phase diagram.

The lattice contribution to the free energy is given by:

$$F_{L} = -\eta \operatorname{Tr} \left[ P_{-} \Psi^{\dagger} P_{+} \Psi \right] = -\eta |\Delta_{2} V_{1} - \Delta_{1} V_{2}|^{2}, \qquad (\Psi = \mathcal{V}_{2}^{\dagger} \mathcal{V}_{1}).$$
(4.59)

where  $P_{\pm} = \frac{1}{2}(1 \pm \tau_3)$  and  $\eta \sim \frac{\rho}{T_K^2}$ . The diagrams giving rise to this term are shown to leading order in  $\mathcal{V}$  in Figure 4.7). This term drives the emergence of composite pairing, nestled between the heavy Fermi liquid phases for the two screening channels. When either  $J_1$  or  $J_2$  is small, this second transition temperature is exponentially suppressed, but never eliminated from the phase diagram because the Cooper channel guarantees that  $\eta$  contains a weak logarithmic dependence



Figure 4.7: Leading Feynman diagrams responsible for composite pairing in the two-channel Kondo lattice. The sum of all four diagrams (a)- (d) gives a contribution proportional to  $|\Lambda|^2 = |(V_1\Delta_2 - V_2\Delta_1)|^2$ .

which will always drive a composite instability at low enough temperatures.

## 4.3 Experimental consequences

There are several concrete consequences of composite pairing that permit our ideas to be compared with experiment:

Crystal fields determine the gap symmetry. When an electron scatters between the Γ = Γ<sup>±</sup><sub>7</sub> channels, it scatters between the | ± 3/2⟩ ↔ | ∓ 5/2⟩ states, and in so doing picks up l = 4 units of angular momentum via spin-orbit scattering. The corresponding order parameter then acquires the symmetry of an orbital state with l = 4, and the corresponding order parameter thus has g- wave symmetry, with eight nodal surfaces, as shown in Figure 4.5. The symmetry of this gap is independent of the microscopic details, and purely set by the tetragonal crystalline environment of the magnetic ions.

2. Upturn in the NMR. In the approach to the composite ordering transition, the local moments must correlate between sites, and this manifests itself through the development of an enhancement of the NMR relaxation rate. For those systems with maximal T<sub>c</sub>, the NMR relaxation rate in the normal state is predicted to contain a term derived from the interference between the two screening channels, proportional to the product <sup>1</sup>/<sub>T1T</sub> ∝ J<sub>1</sub>(T)J<sub>2</sub>(T) of the temperature-renormalized Kondo coupling constants. At the maximum T<sub>c</sub>, where J<sub>1</sub> ~ J<sub>2</sub>, this gives rise to an upturn in the NMR relaxation rate <sup>1</sup>/<sub>T1T</sub> ∝ [ln<sup>2</sup>(T/T<sub>c</sub>) + π<sup>2</sup>]<sup>-1</sup>, a result in accord with recent measurements on PuCoGa<sub>5</sub> [177] shown in Figure 4.8, but which has yet to be tested in NpPd<sub>5</sub>Al<sub>2</sub>. The NMR relaxation rate can be calculated as a 1/N correction to the mean-field theory, and is discussed in Appendix 4C.



Figure 4.8: Upturn in the NMR relaxation rate created by the co-operative interference of the Kondo effect in the two channels at different sites, for the extreme case of maximum  $T_c$ , where  $J_1 = J_2$  (Blue line), compared with measured NMR relaxation rate in  $PuCoGa_5$  [177] (yellow points). Inset shows Feynman diagram used to compute this contribution, where dotted lines describe the f-fermions, blue lines describe conduction electrons propagating between sites and the curly lines describe the Kondo interaction in the particle-hole (red) and particle-particle (blue) channels at different sites. Temperature is measured in units of the transition temperature  $T_c$ .

- 3. Andreev reflection. The main driver for this mechanism of heavy fermion superconductivity is Andreev reflection off quenched magnetic moments. Conventional Andreev reflection involves the direct transfer of an electron from the probe into the pair condensate of the conduction sea. The conventional BTK theory of Andreev reflection [178] predicts that such processes are severely suppressed by the large mismatch between the probe and heavy electron group velocities. However, in a heavy electron system, an electron can also "co-tunnel" into the Kondo lattice a process well-known in magnetic quantum dots, whereby the electron flips a localized spin as it tunnels into the material [179]. In a composite paired superconductor, these processes will result in the direct absorption of the electron into the condensate of composite pairs, giving rise to an enhanced contribution to the Andreev tunnel current with a Fano resonant structure.
- 4. Internal Proximity effect. When the Kondo ions in the superconductor are substituted by Kondo ions with a larger coupling constant, the robust nature of the gap symmetry will protect the superconductor against pair-breaking, and is expected to lead to an internal proximity effect, where the Andreev reflection off the substituted impurities enhances the superconducting  $T_c$ . This effect requires an overlap between the gap functions of the two different ions, but this is guaranteed by crystal symmetry, providing the same screening channels are operative for both ions. Based on this line of argument, we expect that Pu doping of  $NpPd_5Al_2$  will lead to an enhancement of the superconducting  $T_c$ .

The direct transition from Curie paramagnetism to superconductivity in  $PuCoGa_5$  and  $NpPd_5Al_2$ suggests that these materials are composite pair superconductors close to the  $J_1 = J_2$  point of maximum  $T_c$ . Our work currently leaves open the question of the link between  $NpPd_5Al_2$  and  $PuCoGa_5$  and other actinide and cerium systems of similar tetragonal structure, including  $PuRhGa_5$ [80], and the CeMIn<sub>5</sub> superconductors [83, 77, 180]. Each of these systems develops superconductivity, but magnetic susceptibility measurements indicate that the f-moments are more completely quenched at the superconducting transition. We are tempted to suggest that that these systems are examples of composite pairing in the parameter range where  $J_2/J_1$  is smaller, and further away from the maximum transition temperature. Strong Andreev reflections have recently been observed in the tetragonal Ce 115 heavy electron superconductors, a phenomenon that could be associated with co-tunneling into the composite pair condensate [181]. However, at the same time, superconductivity in the cerium systems clearly develops in close proximity to antiferromagnetism, so we can not rule out antiferromagnetic spin fluctuations as the predominant pairing mechanism in these cases, a matter we discuss in detail in the next chapter.

## **Appendix 4A: Composite pairing**

The SU(2) invariant order parameter of the composite paired state is  $\mathcal{V}_2^{\dagger}\mathcal{V}_1$ . We shall show that this matrix is equal to the amplitudes for composite pairing and composite density wave formation using a path integral approach. Here, it proves useful to employ the following matrix representation for the conduction and f-fields at each site j

$$F_{j} = \begin{pmatrix} f_{j}^{T} \\ f_{j}^{\dagger} \hat{\epsilon}^{T} \end{pmatrix} = \begin{pmatrix} f_{j1} & f_{j-1} & \dots \\ f_{j-1}^{\dagger} & -f_{j1}^{\dagger} & \dots \end{pmatrix}, \qquad \Psi_{\Gamma j} = \begin{pmatrix} \psi_{\Gamma j} \\ \psi_{\Gamma j}^{T} \\ \psi_{\Gamma j}^{\dagger} \hat{\epsilon}^{T} \end{pmatrix} = \begin{pmatrix} \psi_{\Gamma j1} & \psi_{\Gamma j-1} & \dots \\ \psi_{\Gamma j-1}^{\dagger} & -\psi_{\Gamma j1}^{\dagger} & \dots \end{pmatrix}$$
(4.60)

whose columns are made up of Nambu spinors. In the following we drop the site index, j. This notation can be used to recast the hybridization terms in a more compact form.

$$\frac{1}{2}\sum_{\alpha}\tilde{\psi}_{\Gamma\alpha}\mathcal{V}_{\Gamma}f_{\alpha} = \frac{1}{2}\mathrm{Tr}\left[\Psi_{\Gamma}^{\dagger}\mathcal{V}_{\Gamma}^{\dagger}F\right] = -\frac{1}{2}\mathrm{Tr}\left[U_{\Gamma}\mathcal{V}_{\Gamma}^{\dagger}\right],\tag{4.61}$$

where  $U_{\Gamma} = F \Psi_{\Gamma}^{\dagger}$  is a two-dimensional matrix operator. Adding a source term  $\eta \mathcal{V}_2^{\dagger} \mathcal{V}_1$ , the decoupled interaction Hamiltonian assumes the form

$$H_{K}[\eta] = -\frac{1}{2} \sum_{\Gamma} \left( \operatorname{Tr} \left[ U_{\Gamma} \mathcal{V}_{\Gamma}^{\dagger} \right] + \text{H.c.} \right) + \frac{1}{2} \operatorname{Tr} \left[ \mathcal{V}_{\Gamma} \begin{pmatrix} \frac{N}{J_{1}} & 2\eta \\ 2\bar{\eta} & \frac{N}{J_{2}} \end{pmatrix} \mathcal{V}_{\Gamma'}^{\dagger} \right].$$

After carrying out the Gaussian integral over  $\mathcal{V}_{\Gamma}$ , we expand  $H_K[\eta]$  to first order in  $\eta$ ,

$$H_K[\eta] = -\frac{J_{\Gamma}}{2N} \operatorname{Tr}\left(U_{\Gamma} U_{\Gamma}^{\dagger}\right) + \frac{J_1 J_2}{N^2} \operatorname{Tr}\left[\eta U_2^{\dagger} U_1 + \operatorname{H.c}\right]$$

Differentiating with respect to  $\eta$  then gives  $\langle \mathcal{V}_2^{\dagger} \mathcal{V}_1 \rangle = \frac{J_1 J_2}{N^2} U_2^{\dagger} U_1 = \frac{J_1 J_2}{N^2} : \left[ \Psi_2 F^{\dagger} F \Psi_1^{\dagger} \right] :$ . Using the identity :  $F^{\dagger} F := \mathbf{S} \cdot \sigma_N^T$ , which can be found by inserting the symplectic-N representations and expanding, we obtain

$$\mathcal{V}_{2}^{\dagger}\mathcal{V}_{1} = -\frac{J_{1}J_{2}}{N^{2}} \begin{pmatrix} \psi_{1}^{\dagger}(\boldsymbol{\sigma}_{N}\cdot\mathbf{S})\psi_{2} & \psi_{1}^{\dagger}(\boldsymbol{\sigma}_{N}\cdot\mathbf{S})\epsilon\psi_{2}^{\dagger} \\ \psi_{1}\epsilon^{T}(\boldsymbol{\sigma}_{N}\cdot\mathbf{S})\psi_{2} & \psi_{1}\epsilon^{T}(\boldsymbol{\sigma}_{N}\cdot\mathbf{S})\epsilon\psi_{2}^{\dagger} \end{pmatrix}.$$
(4.62)

# Appendix 4B: Dispersion in the presence of strong spin-orbit coupling

To develop a mean-field theory in the presence of spin-orbit scattering, we need to diagonalize the the conduction electron Green's function. The eigenvalues are determined by the condition

$$\det[\omega \underline{1} - \mathcal{H}(\mathbf{k})] = 0$$

If we integrate out the f-electrons, this becomes

$$det[\omega \underline{1} - \mathcal{H}(\mathbf{k})] = (\omega^2 - \lambda^2)^2 det[\mathcal{G}(\kappa)^{-1}] = (\omega^2 - \lambda^2)^2 det[\omega - \epsilon_{\mathbf{k}} \tau_3 - \Sigma(\kappa)]$$

Now since  $\Sigma(\kappa) \propto \frac{1}{\omega^2 - \lambda^2}$ , it is convenient to factor this term out of the determinant, so that

$$det[\omega \underline{1} - \mathcal{H}(\mathbf{k})] = (\omega^2 - \lambda^2)^{-2} det[(\omega^2 - \lambda^2)\mathcal{G}(\kappa)^{-1}]$$

Now

$$(\omega^2 - \lambda^2)\mathcal{G}(\kappa)^{-1} = \omega(A + D(\boldsymbol{\sigma} \cdot \mathbf{n_k})\tau_2) - B\tau_3 + C\tau_1$$
(4.63)

$$A = \omega^{2} - \lambda^{2} - v_{\mathbf{k}+}^{2}$$

$$B = \epsilon_{\mathbf{k}}(\omega^{2} - \lambda^{2}) + \lambda v_{\mathbf{k}-}^{2}$$

$$C = 2\lambda v_{1\mathbf{k}}v_{2\mathbf{k}}c_{\mathbf{k}}$$

$$D = 2v_{1\mathbf{k}}v_{2\mathbf{k}}s_{\mathbf{k}}$$
(4.64)

and  $v^2_{\mathbf{k}\pm}=v^2_{1\mathbf{k}}\pm v^2_{2\mathbf{k}}.$ 

If we project the Hamiltonian into states where  $(\mathbf{n_k} \cdot \boldsymbol{\sigma}) = \pm \mathbf{1}$ , we can replace  $A + D(\boldsymbol{\sigma} \cdot \mathbf{n_k})\tau_2 \rightarrow A \pm D\tau_2$ , i.e

$$\det[\omega \underline{1} - \mathcal{H}(\mathbf{k})] = \prod_{\pm} \frac{\det[\omega(A \pm D\tau_2) - B\tau_3 + C\tau_1]}{(\omega^2 - \lambda^2)}$$
(4.65)

The presence of the  $\omega^2 - \lambda^2$  terms in the denominator results from integrating out the f-electrons. In actual fact, there are no zeros of the determinant at  $\omega = \pm \lambda$ , and the  $\omega^2 - \lambda^2$  denominators in these expressions act to factor out the false zeros  $\omega = \pm \lambda$  in the numerator that have been introduced by integrating out the f-electrons. If we now expand the numerator:

$$\det[\omega(A \pm D\tau_2) - B\tau_3 + C\tau_1] = [\omega^2 A^2 - \omega^2 D^2 - B^2 - C^2]$$
  
=  $\omega^2 \left[ (\omega^2 - \lambda^2 - v_+^2)^2 - (2v_{1\mathbf{k}}v_{2\mathbf{k}}s_{\mathbf{k}})^2 \right] - \left[ \epsilon_{\mathbf{k}}(\omega^2 - \lambda^2) + \lambda v_-^2 \right]^2 - \left[ 2\lambda v_{1\mathbf{k}}v_{2\mathbf{k}}c_{\mathbf{k}} \right]^2 (4.66)$ 

Notice that we get the same result for both  $\pm D$ . We know that there is a factor  $(\omega^2 - \lambda^2)$  in this expression, so we can write

$$\det[\omega(A \pm D\tau_2) - B\tau_3 + C\tau_1] = (\omega^2 - \lambda^2) \left[\omega^4 - 2\omega^2 \alpha_{\mathbf{k}} + \gamma_{\mathbf{k}}^2\right]$$
(4.67)

By a direct expansion of this expression and a comparison of terms with (4.66), we are able to

confirm that this factorization works, with

$$\alpha_{\mathbf{k}} = v_{\mathbf{k}+}^{2} + \frac{1}{2}(\lambda^{2} + \epsilon_{\mathbf{k}}^{2})$$
  

$$\gamma_{\mathbf{k}}^{2} = (\epsilon_{\mathbf{k}}\lambda - v_{\mathbf{k}-}^{2})^{2} + (2v_{1\mathbf{k}}v_{2\mathbf{k}}c_{\mathbf{k}})^{2}$$
(4.68)

Thus

$$\det[\omega \underline{1} - \mathcal{H}(\mathbf{k})] = \left[\omega^4 - 2\omega^2 \alpha_{\mathbf{k}} + \gamma_{\mathbf{k}}^2\right]^2$$
(4.69)

The surviving yet crucial effect of the spin-flip scattering is entirely contained in the  $c_k$  factor in  $\gamma_k$ . The Bogoliubov quasiparticles in the composite paired state preserve their Kramer's degeneracy, with dispersion given by

$$\omega_{\mathbf{k}\pm} = \sqrt{\alpha_{\mathbf{k}} \pm (\alpha_{\mathbf{k}}^2 - \gamma_{\mathbf{k}}^2)^{1/2}},$$

as described in section 4.2.3.

## Appendix 4C: NMR relaxation rate

One of the precursor effects of co-operative interference between the two conduction channels is an increase in the NMR relaxation rate just above the transition temperature<sup>2</sup>. The NMR relaxation rate is determined by

$$\mathcal{R} \equiv \frac{1}{T_1 T} = -\frac{I^2}{2\pi} \lim_{\omega \to 0} \frac{\mathrm{Im} K^R_{+-}(\omega)}{\omega}, \qquad (4.70)$$

where I is the hyperfine coupling constant,  $\omega$  is the NMR frequency and  $K_{+-}^{R}(\omega)$  is the Fourier transform of the retarded correlation function of the electron spin densities at the nuclear site:

$$K_{+-}^{R}(\omega) = -i \int_{0}^{\infty} \langle [\hat{S}_{+}(\mathbf{0},t), \hat{S}_{-}(\mathbf{0},0)] \rangle e^{i\omega t} dt$$
(4.71)

At the mean field level  $(N \rightarrow \infty)$ , the NMR relaxation rate follows a Korringa law.

Corrections to Korringa relaxation appear in the  $1/N^2$  corrections to the mean field. To simplify

<sup>&</sup>lt;sup>2</sup>This section was written by Maxim Dzero, and is included for completeness

our discussion, we assume that the Kondo exchange constants are almost degenerate  $J_1 \sim J_2$ . In the approach to the superconducting transition, at  $T > T_c$ , in principle, we need to examine the effects of fluctuations in the hybridization and pairing amplitudes in both channel one and two. The anomalous NMR effect comes from composite pair fluctuations, and as such are driven by the interference between hybridization fluctuations in one channel and pair fluctuations in the other, and we restrict our attention to these corrections. The simplified Hamiltonian is then  $H = H_c + H_0 + H_2$ with

$$H_{0} = \sum_{\mathbf{k}} \frac{2}{J_{1}} \bar{V}_{\mathbf{k}} \hat{V}_{\mathbf{k}} + \frac{2}{J_{2}} \bar{\Delta}_{\mathbf{k}} \Delta_{\mathbf{k}},$$

$$H_{2} = \sum_{\mathbf{k},\mathbf{q};\sigma} \left( \phi_{1\hat{\mathbf{k}}} f^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} V_{\mathbf{q}} c_{\mathbf{k}\sigma} + \phi_{2\hat{\mathbf{k}}} \tilde{\sigma} c^{\dagger}_{\mathbf{k}\sigma} \Delta_{\mathbf{q}} f^{\dagger}_{\mathbf{q}-\mathbf{k},-\sigma} + \text{H.c.} \right)$$

$$(4.72)$$

and  $H_c$  describes the conduction electrons. We ignore fluctuations in the constraint fields, which do not couple to the fluctuations in  $\Delta$  and V to quadratic order. For simplicity, we take the form factors to be diagonal in spin space. Our goal is to compute the corrections to the f-spin correlator due to the channel interference terms, which will be proportional to  $\phi_{1\hat{k}}^*\phi_{2\hat{k}}$ .

The relaxation rate will be governed by the f-spin correlations:

$$K_{ff}(\vec{x};\tau) = -\langle \hat{T}_{\tau} \hat{f}_{\uparrow}^{\dagger}(\vec{x},\tau) \hat{f}_{\downarrow}(\vec{x},\tau) \hat{f}_{\downarrow}^{\dagger}(0,0) \hat{f}_{\uparrow}(0,0) e^{-\int_{0}^{\beta} \hat{H}_{2}(\tau) d\tau} \rangle_{c}, \qquad (4.73)$$

where  $\langle ... \rangle_c$  denotes the connected Green's function obtained by perturbatively expanding the timeordered exponential in the high-temperature state where the f-electrons and conduction electrons are decoupled at the mean-field level. The leading contribution to the temperature dependence of the relaxation rate is governed by the diagram in Figure 4.9 which describes the effect of *inter-site* scattering associated with an electron switching from one symmetry channel to another as it hops from site to site. To write down an analytic expression for the diagram, we employ the Matsubara correlation functions for the f- and c- electrons together with the correlation functions of the slave fields  $K_V(\vec{r}, \tau) = -\langle \hat{T}_{\tau} \hat{V}(\vec{r}, \tau) \hat{V}^{\dagger}(0, 0) \rangle$  and  $K_{\Delta}(\vec{r}, \tau) = -\langle \hat{T}_{\tau} \hat{\Delta}(\vec{r}, \tau) \hat{\Delta}^{\dagger}(0, 0) \rangle$ . Contrary to the single channel effect, this contribution enhances the screening of the local spins rather then suppressing it. To compute the relaxation rate, we must include the renormalization of the slave boson propagators due to Kondo screening. These propagators are:

$$\mathcal{K}_{V}(\vec{p};i\Omega) = \left[\frac{1}{J_{1}} + \Pi_{V}(i\Omega)\right]^{-1}, \quad \mathcal{K}_{\Delta}(\vec{p};i\Omega) = \left[\frac{1}{J_{2}} + \Pi_{\Delta}(i\Omega)\right]^{-1}, \quad (4.74)$$

where  $\Pi_{V,\Delta}(i\Omega)$  are the polarization bubbles associated with hybridization and pair fluctuations. The analytic expression for the diagram reads:

$$\frac{T^3}{N^2} \sum_{i \in i\Omega_V, i\Omega_\Delta} \sum_{q, p, k_V, k_\Delta} G_f(p - k_V) G_f(p + q - k_V) \mathcal{K}_V(k_V) 
\times G_c(p+q) G_c(p) \mathcal{K}_\Delta(k_\Delta) G_f(k_\Delta - p - q) G_f(k_\Delta - p),$$
(4.75)

where we employ the four-vector notation  $p = (\vec{p}, i\omega)$  and have absorbed the form factors into the conduction electron propagators. The Matsubara frequency summations can be performed by employing the spectral function representation for the correlators in expression (4.75). For example,

$$G_{f,c}(\vec{p};i\omega) = \int_{-\infty}^{\infty} \frac{d\varepsilon}{\pi} \frac{\rho_{f,c}(\vec{p},\varepsilon)}{i\omega - \varepsilon},$$
(4.76)

where  $\rho_{f,c}(\vec{p},\varepsilon)$  are the corresponding spectral functions. In the high temperature phase, V and  $\Delta$  have zero expectation values and the fluctuation propagators are independent of momentum  $K_{V,\Delta}(\vec{p};i\Omega) = K_{V,\Delta}(i\Omega)$ . The resulting expression for the relaxation rate can be compactly written as follows

$$\frac{1}{T_1 T} \simeq \frac{1}{N^2} \int_{-\infty}^{\infty} W_{fc}(\omega) \mathcal{K}_{\Delta}(\omega) \mathcal{K}_{V}(-\omega) \frac{d\omega}{2\pi}, \qquad (4.77)$$

where  $W_{fc}(\omega)$  is proportional to  $\rho_f(\omega)\rho_c(\omega)$ . The integral (4.77) is dominated by energies near the Fermi surface. Finally, by approximating the slave boson functions with  $\mathcal{K}_{V,\Delta}(\omega) \sim J_{1,2}/\log[(T - C_{V,\Delta})]$   $i\omega)/T_K$  [182] we obtain the following estimate for the relaxation rate

$$\frac{1}{T_1 T} \sim \frac{1}{N^2} \frac{1}{\log^2(T/T_K) + \pi^2},\tag{4.78}$$

Our result for the relaxation rate shows an upturn in  $(T_1T)^{-1}$  with decrease in temperature, in agreement with experimental data of Curro *et al.* [177], shown in Figure 4.8.



Figure 4.9: Channel interference contribution to the NMR relaxation rate originating from the interaction of nuclear moments with f-spins in the normal state. Solid lines are the conduction band propagators, wiggly lines are the propagators  $K_V$  and  $K_{\Delta}$  of the slave fields for the channel one and two correspondingly. The dashed lines are the f-electron propagators.

# **Chapter 5**

# Tandem Pairing and the Cerium 115s

### 5.1 Introduction

In a superconductor, zero resistance results from the formation of a condensate of pairs of quasiparticles called "Cooper pairs". Although the quasiparticle is a composite object, involving a bare electron screened by a cloud of spin and charge fluctuations, it behaves as a point-like particle inside the Cooper pair, provided the quasiparticles are well-formed at the superconducting transition. However, in many strongly interacting materials, quasiparticles are ill-formed at the superconducting transition, giving the Cooper pair a non-trivial internal structure. The 115 family of heavy fermion superconductors [77, 83, 180, 79, 80, 81] provide an extreme case of this phenomenon, where quasiparticle formation, through the screening of local magnetic moments by mobile electrons, coincides with the onset of superconductivity. Here, we examine the internal structure of the heavy fermion condensate, showing that it necessarily involves two bosonic entities: a d-wave pair of quasiparticles on neighboring lattice sites, condensed in tandem with a composite pair of electrons bound to a local moment, residing within a single unit cell. These two components draw upon the antiferromagnetic and Kondo screening interactions to cooperatively enhance the superconducting transition temperature, explaining the multiple superconducting domes seen in the 115 phase diagram [9]. We show that tandem condensate is electrostatically active, with a small electric quadrupole moment that couples to strain. This accounts for the linear enhancement of the transition temperature with the c/a ratio [183] and is predicted to lead to a shift in the NQR frequency of the nuclei of surrounding ions that can be used to test the validity of the theory.

Over the past decade, the 115 family of superconductors, CeMIn<sub>5</sub> [77, 83, 180], PuMGa<sub>5</sub> [79, 80], and NpPd<sub>5</sub>Al<sub>2</sub> [81], (M= {Co,Rh,(Ir)}) has attracted great interest as a research platform for

the interplay of Kondo physics, magnetism and superconductivity. These highly tunable, layered felectron materials are descendants of the cubic antiferromagnet CeIn<sub>3</sub>. Since the original discovery of superconductivity under pressure at  $T_c$ =0.2K in CeIn<sub>3</sub> [73], the transition temperature has risen by two decades, up to 2.3K in the Ce 115 materials [83], and then 18.5K in PuCoGa<sub>5</sub> [79]. The pairing mechanism that drives this remarkable rise in  $T_c$  is an outstanding mystery which may offer clues relevant to higher  $T_c$  transition metal superconductors.

The abundance of magnetism in the phase diagram has led to a consensus that spin fluctuations drive the superconductivity in the Ce 115s [66, 73, 74], explaining the enhancement of  $T_c$  as MIn<sub>2</sub> layers are added to cubic CeIn<sub>3</sub>. CeRhIn<sub>5</sub> is a canonical example, where moderate pressure reveals a superconducting dome as the Néel temperature,  $T_N$  vanishes [77, 184]. However, there are certain difficulties with this picture, for example, further pressure [185] or Ir doping on the Rh site [186, 9] leads to a second dome, where spin fluctuations are weaker [187]. Furthermore, the highest transition temperatures are found in the actinide 115s, which show no signs of magnetism.



Figure 5.1: Local moments are seen in the Curie-Weiss susceptibilities:  $\text{CeCoIn}_5(T_c = 2.3K)$  [63] and NpPd<sub>5</sub>Al<sub>2</sub>( $T_c = 4.9K$ ) [81] are reproduced and rescaled by  $\chi(T_c)$  to show their similarity (data below  $T_c$  not shown).

One of the common, unexplained features of this family of superconductors is the presence of unquenched local moments at the superconducting transition temperature (Figure 5.3(a)). In a typical heavy fermion superconductor, the local moments quench to form a *Pauli paramagnet*  $(\chi(T) \sim \chi_0)$  prior to the development of superconductivity; this is the situation in spin fluctuation mediated superconductors, which pair pre-formed f-electrons. Yet four of the six 115 superconductors: PuCoGa<sub>5</sub> [79], NpPd<sub>5</sub>Al<sub>2</sub> [81] and Ce{Co,Ir}In<sub>5</sub> [83, 180] exhibit a Curie-Weiss susceptibility  $\chi(T) \sim 1/(T + T_{CW})$  down to  $T_c$ . The disappearance of the Curie-Weiss component in the Knight shift below  $T_c$  [188] and a concomitant loss of spin entropy  $\Delta S \sim 0.3R \log 2$  [79, 81, 83, 180], indicate that in these systems, the local moments quench simultaneously with the development of superconductivity.



Figure 5.2: (a) High pressure studies on CeRhIn<sub>5</sub> show two connected superconducting domes(reproduced from Muramatsu *et al.* [185]). (b) Two domes are also seen in a doping study tuning continuously between CeMIn<sub>5</sub> for M = (Co, Rh, In) (reproduced from Sarrao and Thompson [189]).

These observations led us to propose in Chapter 4 that the actinide 115s are *composite pair* superconductors [176]. In a one-channel Kondo lattice, the heavy Fermi liquid is composed of composite fermions created by binding an electron to a spin flip:  $f_{\uparrow}^{\dagger} \sim c_{\downarrow}^{\dagger}S_{+}$ . In the presence of a second screening channel, a heavy Cooper pair forms by combining *two* electrons with a spin flip to form a composite pair,

$$\Lambda_C = \langle N | c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger} S_+ | N+2 \rangle, \tag{5.1}$$

where  $c_{1,2}^{\dagger}$  create electrons in two orthogonal Kondo screening channels [122, 190]. This condensate develops an Andreev component to the resonant Kondo scattering, and this drives superconductivity.

However, composite pairing alone cannot account for the importance of magnetism in the Ce 115 phase diagram.

We are led by these conflicting observations to propose a model for the 115 materials where the composite and magnetic mechanisms work in tandem to drive superconductivity. Composite pairing originates from two channel Kondo impurities, while magnetic pairing emerges from antiferromagnetically coupled Kondo impurities. These two systems are equivalent at criticality in the dilute limit [92], and we argue that this connection persists to the lattice superconducting state concealing a common quantum critical point (QCP) [89].



Figure 5.3: A tandem pair contains a superposition of magnetic and composite pairing, both with d-wave symmetry. The magnetic pair (left) contains f-electrons at neighboring sites, while the composite pair (right) is made up of a spin flip and two conduction electrons. The unit cell is denoted by dotted lines, with dots indicating the local moment sites.

### 5.2 Internal structure of a heavy fermion pair

To understand the interplay between magnetic and composite pairing, we examine the internal structure of a heavy fermion pair. In a Kondo lattice, the heavy quasiparticles are a linear combination  $a^{\dagger}_{\mathbf{k}\uparrow} = u_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow} + v_{\mathbf{k}}f^{\dagger}_{\mathbf{k}\uparrow}$ , where  $(c^{\dagger})$  creates a mobile conduction electron and  $(f^{\dagger})$  creates a localized spin [191]. The superconducting wavefunction is a coherent state

$$|\Psi\rangle = P_G \exp(\Lambda^{\dagger})|0\rangle, \qquad (5.2)$$

where  $\Lambda^{\dagger} = \sum_{\mathbf{k}} \Delta_k (a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow})$  creates a d-wave pair of quasiparticles and  $P_G$  is the Gutzwiller projection operator ensuring that the f-occupation at each lattice site is one. Acting the Gutzwiller projector on the f-electron field reveals its internal structure as a composite between a conduction electron and a spin flip at a given site j,  $P_G f^{\dagger}_{j\uparrow} \sim (c^{\dagger}_{j\downarrow} S_+) P_G$ .

The pairing field  $\Lambda^\dagger$  contains three terms

$$\Lambda^{\dagger} = \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}\uparrow}^{\dagger} & , f_{\mathbf{k}\uparrow}^{\dagger} \end{pmatrix} \begin{bmatrix} \Delta_{\mathbf{k}}^{e} & \Delta_{\mathbf{k}}^{C} \\ \Delta_{\mathbf{k}}^{C} & \Delta_{\mathbf{k}}^{M} \end{bmatrix} \begin{pmatrix} c_{-\mathbf{k}\downarrow}^{\dagger} \\ f_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} = \Psi_{e}^{\dagger} + \Psi_{C}^{\dagger} + \Psi_{M}^{\dagger}.$$
(5.3)

The diagonal terms, with  $\Delta_{\mathbf{k}}^{e} = u_{\mathbf{k}}^{2} \Delta_{\mathbf{k}}$  and  $\Delta_{\mathbf{k}}^{M} = v_{\mathbf{k}}^{2} \Delta_{\mathbf{k}}$  create f- and conduction electron pairs. A d-wave pair of f-electrons is an inter-site operator, taking the form

$$\Psi_M^{\dagger} = \sum_{i,j} \Delta^M(\mathbf{R}_{ij}) \left[ (c_{i\uparrow}^{\dagger} S_{i-}) (c_{j\downarrow}^{\dagger} S_{j+}) \right]$$
(5.4)

outside the Gutzwiller projection. However, if we expand the off-diagonal terms in real space,

$$\Psi_C^{\dagger} = \sum_{i,j} \Delta^C(\mathbf{R}_{ij}) \left[ c_{i\uparrow}^{\dagger} c_{j\uparrow}^{\dagger} S_{j-} \right]$$
(5.5)

where  $\Delta^C(\mathbf{R}) = \sum_{\mathbf{k}} (u_{\mathbf{k}}v_{\mathbf{k}}\Delta_{\mathbf{k}})e^{i\mathbf{k}\cdot\mathbf{R}}$ , we find a composite pair formed between a triplet pair of conduction electrons and a spin flip [190, 122, 176]. Unlike its diagonal counterparts, which are necessarily inter-site, composite pairs are compact objects formed from pairs of orthogonal Wannier states surrounding a *single local moment* (Figure 5.3).

Magnetic interactions will favor the inter-site component of the pairing, while the two-channel Kondo effect will favor the composite intra-site component. However, both components will always be present in the superconducting Kondo lattice. If the product of the Kondo screening channels has a d-wave symmetry, the composite and magnetic order parameters necessarily couple linearly to one another, a process that we will show enhances the transition temperature over a large region of the phase diagram, providing a natural explanation for both the actinide and Ce 115s.

### 5.3 The two channel Kondo-Heisenberg model

To treat these two pairing mechanisms simultaneously, we introduce the two channel Kondo-Heisenberg model,

$$H = H_c + H_{K1} + H_{K2} + H_M (5.6)$$

and solve it in the symplectic-N limit [190]. There are four terms,

$$H_c = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \quad H_M = J_H \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$
(5.7)

$$H_{K\Gamma} = J_{\Gamma} \sum_{j} \psi_{j\Gamma a}^{\dagger} \vec{\sigma}_{ab} \psi_{j\Gamma b} \cdot \vec{S}_{j}.$$
(5.8)

where  $\vec{S}_j$  is the local moment on site j, and  $\psi_{j\Gamma}$  is the Wannier state representing a conduction electron on site j with symmetry  $\Gamma$ ,

$$\psi_{j\Gamma a} = \sum_{\mathbf{k}} \Phi_{\Gamma \mathbf{k} a b} c_{\mathbf{k} b} \mathrm{e}^{i\mathbf{k} \cdot \mathbf{R}_{j}},\tag{5.9}$$

where the form factor  $\Phi_{\Gamma kab}$  is only diagonal in the spin indices in the absence of spin-orbit. Microscopically, the two orthogonal Kondo channels,  $J_{\Gamma}$  arise from virtual fluctuations from the ground state doublet to excited singlets, where the two channels correspond to adding and removing an electron, respectively. The Ce  $4f^1$  state is split by tetragonal symmetry into three Kramer's doublets, where  $\Gamma_7^+$  is the ground state doublet [192, 193], so we may summarize the virtual valence fluctuations with:

$$4f^{0}(\cdot) \stackrel{\Gamma_{7}^{+}}{\rightleftharpoons} 4f^{1}(\Gamma_{7}^{+}) \stackrel{\Gamma_{6}}{\rightleftharpoons} 4f^{2}(\Gamma_{7}^{+} \otimes \Gamma_{6}).$$
(5.10)

Requiring the composite pairing to resonate with the d-wave magnetic pairing [181] uniquely selects

 $\Gamma_7^+ \otimes \Gamma_6$  as the lowest doubly occupied state, as this combination leads to d-wave composite pairing [190]. To illustrate the basic physics, a simplified two dimensional model is sufficient, where the d-wave composite pair now comes from the combination of s-wave hybridization in channel one and d-wave hybridization in channel two [194, 195]. The magnetism is included as an explicit RKKY interaction,  $J_H$  between neighboring local moments  $\langle ij \rangle$ , generated by integrating out electron in bands far from the Fermi surface [64]. Treating the magnetism as a Heisenberg term leads to a two band version of resonating valence bond (RVB) superconductivity [23], where the local moments form valence bonds which "escape" into the conduction sea through the Kondo hybridization to form charged, mobile Cooper pairs [196].

To solve this model, we use a fermionic spin representation,  $\vec{S}_j = f_j^{\dagger} \vec{\sigma} f_j$ ; symplectic-N maintains the time-reversal properties of SU(2) in the large N limit by using the symplectic Pauli matrices  $\vec{\sigma}$  to construct the spin Hamiltonians [190],

$$H_{K\Gamma}(j) = -\frac{J_{\Gamma}}{N} \left[ (\psi_{j\Gamma}^{\dagger} f_j) (f_j^{\dagger} \psi_{j\Gamma}) + (\psi_{j\Gamma}^{\dagger} \epsilon^{\dagger} f_j^{\dagger}) (f_j \epsilon \psi_{j\Gamma}) \right]$$
  

$$H_M(ij) = -\frac{J_H}{N} \left[ (f_i^{\dagger} f_j) (f_j^{\dagger} f_i) + (f_i^{\dagger} \epsilon^{\dagger} f_j^{\dagger}) (f_j \epsilon f_i), \right]$$
(5.11)

where  $\epsilon$  is the large N generalization of  $i\sigma_2$ . Each quartic term can be decoupled by a Hubbard-Stratonovich field, leading to normal,  $V_{\Gamma} \propto \langle c_{\Gamma}^{\dagger} f \rangle$  and anomalous,  $\Delta_{\Gamma} \propto \langle c_{\Gamma}^{\dagger} \epsilon f^{\dagger} \rangle$  hybridization in each Kondo channel, and particle-hole,  $h_{ij} \propto \langle f_i^{\dagger} f_j \rangle$  and pairing,  $\Delta_{ij}^H \propto \langle f_i^{\dagger} \epsilon f_j^{\dagger} \rangle$  terms for the spin liquid, where  $\langle \cdots \rangle$  represents a thermal expectation value. This Hamiltonian possesses an SU(2) gauge symmetry,  $f \longrightarrow uf + v\epsilon^{\dagger} f^{\dagger}$ , which we use to eliminate  $\Delta_1$ , and composite pair superconductivity occurs when  $V_1\Delta_2$  is nonzero[?]. We calculate the mean field values of these fields using the saddle point approximation, which becomes exact as  $N \to \infty$ . The lowest energy solutions involve only pairing fields in the magnetic and second Kondo channels, giving rise to only three nonzero Hubbard-Stratonovich fields,  $V_1$ ,  $\Delta_2$  and  $\Delta_H$ [?]. We take  $\Delta_H$  to be d-wave in the plane, so that  $\Delta_k^H \equiv \Delta_H(\cos k_x - \cos k_y)$ ; in this simple model,  $\Phi_1 = 1$  and  $\Phi_2 = (\cos k_x - \cos k_y)$ . Using the Nambu notation,  $\tilde{c}_k^{\dagger} = (c_k^{\dagger}, \epsilon c_{-k})$ ,  $\tilde{f}_k^{\dagger} = (f_k^{\dagger}, \epsilon f_{-k})$ , and defining  $\mathcal{V}_k = V_1 \Phi_{1\mathbf{k}} \tau_3 + \Delta_2 \Phi_{2\mathbf{k}} \tau_1$ , the mean field Hamiltonian can be concisely written as

$$H = \sum_{k} \left( \begin{array}{c} \tilde{c}_{k}^{\dagger} & \tilde{f}_{k}^{\dagger} \end{array} \right) \left[ \begin{array}{c} \epsilon_{k} \tau_{3} & \mathcal{V}_{k}^{\dagger} \\ \mathcal{V}_{k} & \lambda \tau_{3} + \Delta_{Hk} \tau_{1} \end{array} \right] \left( \begin{array}{c} \tilde{c}_{k} \\ \tilde{f}_{k} \end{array} \right) \\ + N \left( \frac{V_{1}^{\dagger} V_{1}}{J_{1}} + \frac{\Delta_{2}^{\dagger} \Delta_{2}}{J_{2}} + \frac{4\Delta_{H}^{2}}{J_{H}} \right),$$
(5.12)

where  $\lambda$  is the Lagrange multiplier enforcing the constraint  $n_f = 1$ . The mean field Hamiltonian can be diagonalized analytically. Upon minimizing the free energy, we obtain four equations for  $\lambda$ ,  $V_1$ ,  $\Delta_2$ , and  $\Delta_H$ . Solving these numerically, and searching the full parameter space of  $J_2/J_1$ ,  $J_H/J_1$  and T to find both first and second order phase transitions, we find four distinct phases,

- A light Fermi liquid with free local moments when all parameters are zero, at high temperatures.
- A heavy Fermi liquid when either  $V_1$  or  $\Delta_2$  are finite, with symmetry  $\Gamma$ , below  $T_{K\Gamma}$ .
- A spin liquid state decoupled from a light Fermi liquid when  $\Delta_H$  is finite, below  $T_{SL}$ . There is no long range magnetic order due to our fermionic spin representation [123].
- A tandem superconducting ground state with V<sub>1</sub>, Δ<sub>2</sub> and Δ<sub>H</sub> all finite, below T<sub>c</sub>, as shown in Figure 5.4.

A qualitative understanding of this tandem pairing can be obtained within a simple Landau expansion. For  $T \sim T_c \ll T_{K1}$ ,  $\Phi \equiv \Delta_2$  and  $\Psi \equiv \Delta_H$  will be small, and the free energy can be expressed as

$$F = \alpha_1 (T_{c1} - T) \Psi^2 + \alpha_2 (T_{c2} - T) \Phi^2 + 2\gamma \Psi \Phi + \beta_1 \Psi^4 + \beta_2 \Phi^4 + 2\beta_i \Psi^2 \Phi^2$$
(5.13)

 $\alpha_{1,2}$ ,  $\beta_{1,2,i}$  and  $\gamma$  are all functions of  $\lambda$  and  $V_1$  and can be calculated exactly in the mean field limit. The linear coupling of the two order parameters,  $\gamma = \partial^2 F / \partial \Delta_2 \partial \Delta_H$  is always nonzero in the



Figure 5.4: The superconducting transition temperature as the amounts of magnetic,  $J_H$  and second channel,  $J_2$  couplings are varied. A slice at  $T = T_{K1}$  shows the regions of the spin liquid and Fermi liquids, and the orange ellipse is a path illustrating how materials could tune the relative coupling strengths (see Figure 5.5). The phase diagram was calculated in a simple two dimensional model with channel one s-wave and channel two d-wave ( $n_c = .75$ ). The transition is first order for  $J_H/J_1 > 4$ , but otherwise second order.

heavy Fermi liquid, leading to an enhancement of the transition temperature,

$$T_c = \frac{T_{c1} + T_{c2}}{2} + \sqrt{\left(\frac{T_{c1} - T_{c2}}{2}\right)^2 + \frac{\gamma^2}{\alpha_1 \alpha_2}}.$$
(5.14)

For  $\beta_1\beta_2 > \beta_i^2$ , the two order parameters are only weakly repulsive, leading to smooth crossovers from magnetic to composite pairing under the superconducting dome [197].

# 5.4 Experimental consequences

Experimentally,  $CeMIn_5$  can be continuously tuned from M = Co to Rh to Ir [9]. While  $CeRhIn_5$  is a canonical example of a magnetically paired superconductor, where moderate pressure reveals a superconducting dome as the Néel temperature vanishes [77], further pressure [185] or Ir doping on

the Rh site [9] leads to a second dome, where spin fluctuations are weaker [187]. We assume that the changing chemical pressure varies the relative strengths of the Kondo and RKKY couplings, so that doping traces out a path through the phase diagram like the one in Figure 5.5, chosen for its similarities to CeMIn<sub>5</sub>. While different paths may lead to one, two or three superconducting domes, by maintaining the same Fermi liquid symmetry throughout ( $T_{K1} > T_{K2}$ ), we are restricted to one (magnetic only) or two (magnetic and tandem) domes. In real materials, weak disorder will decrease  $T_c$  for non-stoichiometric compounds, and antiferromagnetism will appear for  $T_{SL}/T_{K1}$ sufficiently large. It requires much more fine tuning to obtain a superconductor when only one pairing mechanism is operating, explaining why Yb superconductors, where the  $4f^{13} \rightleftharpoons 4f^{12}$  are greatly suppressed in relation to  $4f^{13} \rightleftharpoons 4f^{14}$  are much harder to obtain than Ce superconductors in which the two channels have similar strengths.

Conventional superconductivity is electrostatically neutral, in that the development of a condensate does not change the underlying charge distribution. By contrast, tandem pairing is electrostatically active and redistributes charge, leading to an electric quadrupole moment. The transition temperature of the 115 superconductors is known to increase linearly with the lattice c/a ratio [183], conventionally attributed to decreasing dimensionality. Our theory suggests an alternative interpretation: in a condensate with a quadrupole moment,  $Q_{zz} \propto \Psi_C^2$ , which couples linearly to the tetragonal strain,  $\Delta F \propto -Q_{zz}u_{tet}$ , we can rewrite the second term in the Landau free energy (5.13) as  $\alpha_2[T - (T_{c2} + \lambda u_{tet})]\Psi_C^2$ . This coupling naturally accounts for the linear increase in  $T_c$ . The development of a condensate quadrupole moment should be also detectable as a shift of the nuclear quadrupole resonance (NQR) frequency at the nuclei of surrounding ions.

The link between f-electron valence and the Kondo effect is well established [199], but tandem pairing introduces a new element to this relationship. Changes in the charge distribution around the Kondo ion can be read off from its coupling to the changes in the chemical potential,  $\Delta \rho(x) =$  $|e|\delta H/\delta \mu(x)$  where H is the pairing Hamiltonian (12). The sensitivity of the Kondo couplings to the chemical potential is obtained from a Schrieffer-Wolff transformation of a two-channel Anderson model, which gives  $J_{\Gamma}^{-1} = \Delta E_{\Gamma}/V_{\Gamma,0}^2$ . Here,  $V_{\Gamma,0}$  is the bare hybridization in channel  $\Gamma$ , and



Figure 5.5: A possible experimental path through the phase diagram in Figure 5.4, chosen for its similarity to the Ce 115 doping phase diagram [9]. The transition temperatures for superconductivity ( $T_c$  in solid blue), spin liquid ( $T_{SL}$  in dotted red), and Fermi liquid ( $T_{K1}$  in dashed orange and  $T_{K2}$  in dot-dashed white) are plotted for comparison. Temperatures are scaled by  $T_{K1}$ , which may itself vary as one moves around the phase diagram [198]. While we always find a superconducting ground state, due to our choice of a fermionic spin representation, real materials will have an antiferromagnetic ground state for  $T_{SL}/T_{K1}$  sufficiently large.

 $\Delta E_{\Gamma}$  are the charge excitation energies of the magnetic moment. With a shift in  $\mu \to \mu + \delta \mu(x)$ ,  $\delta J_{\Gamma}^{-1} = \pm |\Phi_{\Gamma}(x)|^2 \delta \mu(x) / V_{\Gamma,0}^2$ , where  $|\Phi_{\Gamma}(x)|^2$  are the full spin-orbit crystal field charge densities. The sign is positive for  $J_1$  and negative for  $J_2$  because they involve fluctuations to the empty and doubly occupied states, respectively:  $f^0 \stackrel{\Gamma_1}{\rightleftharpoons} f^1 \stackrel{\Gamma_2}{\rightleftharpoons} f^2$ . Differentiating (3.22) with respect to  $\delta \mu(x)$ , the change in the charge distribution will be:

$$\Delta \rho(x) = |e| \left[ \left( \frac{V_1}{V_{1,0}} \right)^2 |\Phi_1(x)|^2 - \left( \frac{\Delta_2}{V_{2,0}} \right)^2 |\Phi_2(x)|^2 \right],$$
(5.15)

where  $V_1$  and  $\Delta_2$  are the hybridizations in channels 1 and 2, which together make up the composite

order parameter. For equal channel strengths, the total charge is constant, and the f-ion will develop equal hole densities in  $\Gamma_7^+$  and electron densities in  $\Gamma_6$ , leading to a positive change in the electric field gradient,  $\partial E_z/\partial z \propto (T_c - T) > 0$  at the in-plane In sites that will appear as a small shift in the NQR frequencies growing abruptly below  $T_c$  (see Figure 6.53).



Figure 5.6: Predicted NQR frequency shift,  $\Delta \nu_{NQR}$  in CeMIn<sub>5</sub> at the high symmetry indium nucleus. The inset shows the relative locations of the indiums in-, In(1) and out-of-plane, In(2).  $\Delta \nu_{NQR}$  measures the change in the electric field gradient (EFG) due to the onset of superconductivity. For equal channel strengths, the total charge of the f-ion remains unity, but the increasing occupations of the empty and doubly occupied sites cause holes to build up with symmetry  $\Gamma_7^+$ (orange) and electrons with symmetry  $\Gamma_6$  (blue). The change in charge distribution and resulting electric fields are shown above in a slice along the [110] direction (the dashed line in the inset). The positive EFG,  $\partial E_z/\partial z$  at the In(1) site will lead to a sharp positive shift in  $\nu_{NQR}$  starting at  $T_c$ .

A small superconducting shift should also appear in the f-electron valence, observable with corelevel X-ray spectroscopy. The valence shift is obtained by integrating (5.15):  $\Delta n_f(T) \propto \Psi_C^2 \propto (T_c - T)$ , as  $\Psi_C \propto \Delta_2$  when  $J_1 > J_2$ . While the development of Kondo screening leads to a gradual valence decrease through  $T_K$ , as it is a crossover scale, the development of superconductivity is a phase transition, leading to a sharp mean-field increase of the valence beginning at  $T_c$ . Observation of sharp shifts at  $T_c$  in either the NQR frequency or the valence would constitute an unambiguous confirmation of the electrostatically active tandem condensate.

# Appendix 5A: Diagonalizing the Hamiltonian in the presence of spin-orbit coupling

In the presence of spin-orbit coupling, the mean-field Hamiltonian is an  $8 \times 8$  matrix, and requires a little more effort to diagonalize. This diagonalization has already been done in the absence of magnetic pairing,  $\Delta_{Hk}$  in Appendix 4B. The eigenvalues of the mean field Hamiltonian are determined by

$$\det[\omega \mathbf{1} - \mathcal{H}_k] = 0 \tag{5.16}$$

where  $\mathcal{H}_k$  is given by

$$\begin{pmatrix} \epsilon_k \tau_3 & \mathcal{V}^{\dagger} \\ \mathcal{V} & \lambda \tau_3 + \Delta_{Hk} \tau_1 \end{pmatrix}$$
(5.17)

with  $\mathcal{V}^{\dagger} = V_1 \Phi_{1k}^{\dagger} + \Delta_2 \Phi_{2k}^{\dagger}$ , where  $\Phi_{\Gamma k}^{\dagger} = \phi_{\Gamma k} U_k^{\dagger}$  is proportional to a 2x2 unitary matrix, discussed in detail in Chapter 4. After integrating out the f-electrons, we obtain,

$$\det[\omega \mathbf{1} - \mathcal{H}_k] = (\omega^2 - \lambda^2 - \Delta_{Hk}^2)^2 \det[\mathcal{G}_k^{-1}]$$
(5.18)

where  $\mathcal{G}_k$  is the full conduction electron Green's function,

$$\mathcal{G}_{k}^{-1} = \omega \mathbf{1} - \epsilon_{k} \tau_{3} - \Sigma_{k} \text{ and } \Sigma_{k} = \frac{\mathcal{V}^{\dagger}(\omega \mathbf{1} + \lambda \tau_{3} + \Delta_{Hk} \tau_{1})\mathcal{V}}{\omega^{2} - \lambda^{2} - \Delta_{Hk}^{2}}.$$
(5.19)

Since  $\Sigma_K \propto (\omega^2 - \lambda^2 - \Delta_{Hk}^2)^{-1}$ , we can factor  $(\omega^2 - \lambda^2 - \Delta_{Hk}^2)^2$  out of the determinant,

$$\det[\omega \mathbf{1} - \mathcal{H}_k] = (\omega^2 - \lambda^2 - \Delta_{Hk}^2)^{-2} \det[(\omega^2 - \lambda^2 - \Delta_{Hk}^2)\mathcal{G}_k^{-1}]$$
(5.20)

which can be written as

$$(\omega^2 - \lambda^2 - \Delta_{Hk}^2)\mathcal{G}_k^{-1} = \omega A\mathbf{1} - B\tau_3 + C\tau_1 + D\tau_2,$$

where

$$A = \omega(\omega^2 - \lambda^2 - \Delta_{Hk}^2) - Tr \mathcal{V}^{\dagger}(\omega \mathbf{1} + \lambda \tau_3 + \Delta_{Hk} \tau_1) \mathcal{V} \mathbf{1}$$
(5.21)

$$B = (\omega^2 - \lambda^2 - \Delta_{Hk}^2)\epsilon_k + Tr\mathcal{V}^{\dagger}(\omega\mathbf{1} + \lambda\tau_3 + \Delta_{Hk}\tau_1)\mathcal{V}\tau_3$$
(5.22)

$$C = -Tr\mathcal{V}^{\dagger}(\omega \mathbf{1} + \lambda \tau_3 + \Delta_{Hk}\tau_1)\mathcal{V}\tau_1$$
(5.23)

$$D = -Tr \mathcal{V}^{\dagger}(\omega \mathbf{1} + \lambda \tau_3 + \Delta_{Hk} \tau_1) \mathcal{V} \tau_2$$
(5.24)

By evaluating the traces, we find

$$A = \omega(\omega^2 - \lambda^2 - \Delta_{Hk}^2) - \omega V_+^2$$
(5.25)

$$B = (\omega^2 - \lambda^2 - \Delta_{Hk}^2)\epsilon_k + \lambda V_-^2 - 2\Delta_{Hk}V_{1k}\Delta_{2k}\cos(\zeta_k/2)$$
(5.26)

$$C = +2\lambda V_{1k}\Delta_{2k}\cos(\zeta_k/2) - \Delta_{Hk}V_-^2$$
(5.27)

$$D = +2\omega V_{1k} \Delta_{2k} (\vec{n} \cdot \vec{\sigma}) \sin(\zeta_k/2)$$
(5.28)

where we have defined  $V_{\pm}^2=V_{1k}^2\pm\Delta_{2k}^2, V_{1k}=V_1\phi_{1k}, \Delta_{2k}=\Delta_2\phi_{2k}$ , and

$$\cos(\zeta_k/2) = Tr[\Phi_{1k}^{\dagger}\Phi_{2k} + \Phi_{2k}^{\dagger}\Phi_{1k}]/(\phi_{1k}\phi_{2k})$$
$$i(\vec{n}\cdot\vec{\sigma})\sin(\zeta_k/2) = Tr[\Phi_{1k}^{\dagger}\Phi_{2k} - \Phi_{2k}^{\dagger}\Phi_{1k}]/(\phi_{1k}\phi_{2k}), \qquad (5.29)$$

which we will further simplify as  $c_k = \cos(\zeta_k/2)$  and  $s_k = \sin(\zeta_k/2)$ , and we will project the Hamiltonian into states where  $\vec{n} \cdot \vec{\sigma} = \pm 1$ , so that the determinant can be simply written,

$$det[A\mathbf{1} - B\tau_3 + C\tau_1 + D\tau_2] = A^2 - B^2 - C^2 - D^2$$
  
=  $\omega^2 [(\omega^2 - \lambda^2 - \Delta_{Hk}^2 - V_+^2)^2 - (2V_{1k}\Delta_{2k}s_k)^2]$   
-  $(\epsilon_k(\omega^2 - \lambda^2 - \Delta_{Hk}^2) + \lambda V_-^2 - 2\Delta_{Hk}V_{1k}\Delta_{2k}c_k)^2 - (2\lambda V_{1k}\Delta_{2k}c_k - \Delta_{Hk}V_-^2)^2 (5.30)$ 

 $(\omega^2 - \lambda^2 - \Delta_{Hk}^2)$  can now be factored out from the overall expression. The result should be

$$\det[A\mathbf{1} - B\tau_3 + C\tau_1 + D\tau_2] = (\omega^2 - \lambda^2 - \Delta_{Hk}^2)(\omega^4 - 2\omega^2\alpha_k + \gamma_k^2), \tag{5.31}$$

and from this we find

$$\alpha_k = \frac{\lambda^2 + \epsilon_k^2 + \Delta_{Hk}^2}{2} + V_{k+}^2, \quad \gamma_k^2 = (\epsilon_k \lambda - V_{k-}^2)^2 + (2V_{1k}\Delta_{2k}c_k + \epsilon_k \Delta_{Hk})^2.$$
(5.32)

Just as in the absence of magnetic pairing, all the effects of spin-flip scattering are contained in the one cosine term. The linear coupling between  $V_{1k}\Delta_{2k}c_k$  and  $\epsilon_k\Delta_{Hk}$  is clear.
# **Chapter 6**

# Symplectic Anderson models

### 6.1 Introduction

One of the major focuses of this dissertation has been to understand the origin of unconventional superconductivity in the 115 family of heavy fermion superconductors. This family has attracted great interest for the unusual transition directly from Curie paramagnetism into heavy fermion superconductivity, which suggests that the spins play a more direct role in the superconducting mechanism than previously believed, but also for the remarkable rise in the transition temperature between the cerium ( $T_c = 2.3K$  for CeCoIn<sub>5</sub>) and the more mixed valent actinide 115s, where PuCoGa<sub>5</sub> ( $T_c = 18.5K$ ) is the highest temperature heavy fermion superconductor. In Chapter 4, we proposed that the actinide 115s are *composite pair superconductors*, where the superconductivity is a local phenomena involving the condensation of bound states between local moments and conduction electrons in two orthogonal Kondo channels,

$$\Lambda_j = \langle \psi_{1j\uparrow}^{\dagger} \psi_{2j\uparrow}^{\dagger} S_{-}(j) \rangle, \tag{6.1}$$

where  $\psi_{1,2}^{\dagger}$  create local Wannier states of conduction electrons with two different symmetries. Near the point of channel degeneracy, composite pairing can explain the presence of local moments down to the transition temperature, however, magnetic pairing clearly plays an important role in the cerium 115s, and in Chapter 5, we discussed how magnetic and composite pairing can work in tandem to increase the transition temperature and avoid the fine-tuning problem of channel degeneracy. The magnetic and composite order parameters are indistinguishable at the macroscopic level, but composite pairing has unique electrostatic properties, and the formation of composite pairs appears to redistribute the f-electron charge within the unit cell, which should be experimentally detectable. Thus far, we have only studied composite pairing within the two channel Kondo model, which cannot access these charge degrees of freedom directly. To rigorously address the charge aspects of composite pairing, in this chapter we introduce the two channel Anderson model and solve it in the symplectic-N limit. This model not only allows us to properly treat the charge degrees of freedom, but also to illuminate the effects of valence fluctuations on the superconductivity, which are especially important for the actinide 115s, PuMGa<sub>5</sub> (M = Co,Rh) [79, 80] and NpPd<sub>5</sub>Al<sub>2</sub> [81].



Figure 6.1: Virtual charge fluctuations of a two channel Anderson impurity, where the addition and removal of an f-electron occur in channels of two different crystal field symmetry,  $\Gamma_1$  and  $\Gamma_2$ . The ground state is a Kramer's doublet, while the excited states are singlets. In general, we will neglect the excited crystal field doublet,  $|\Gamma_2 : \alpha\rangle$ . We show the corresponding valence states of Ce<sup>3+</sup> (4*f*<sup>1</sup>) ions and their 5f hole analogue, Pu<sup>3+</sup> (5*f*<sup>5</sup>).

To study composite pairing in mixed valent compounds, we introduce the two channel Anderson model. This model describes strongly correlated f-ions with a doublet ground state,  $|\Gamma_1 \pm \rangle$  whose valence can fluctuate either by losing or gaining an electron,

$$f^0 + e^- \leftrightarrows f^1 \leftrightarrows f^2 + h^+. \tag{6.2}$$

There are three relevant atomic multiplets: the empty state,  $|0\rangle$ , which is necessarily a singlet, the Kramers doublet,  $|\Gamma_1\pm\rangle$ , and a doubly occupied state, which we assume to be a singlet containing

f-electrons in two orthogonal symmetries,

$$|2\rangle \equiv |\Gamma_2 \otimes \Gamma_1\rangle_s = \frac{1}{\sqrt{2}} \sum_{\sigma=\pm 1} \operatorname{sgn}(\sigma) f^{\dagger}_{\Gamma_2 \sigma} f^{\dagger}_{\Gamma_1 - \sigma} |0\rangle.$$
(6.3)

These states are shown in Figure 6.1, and are described by the atomic Hamiltonian,

$$H_a(j) = E_0 X_{00}(j) + E_2 X_{22}(j) + \sum_{\sigma} \epsilon_f X_{\sigma\sigma}(j),$$
(6.4)

where the X's are the Hubbard operators  $X_{00} = |0\rangle \langle 0|$ ,  $X_{22} = |2\rangle \langle 2|$ , and  $X_{\sigma\sigma} = |\sigma\rangle \langle \sigma|$ , which are projectors for the local atomic basis. These f-electrons coexist with a bath of non-interacting conduction electrons,  $H_c = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$ , and these two species will hybridize in two different channels, as

$$H_V(j) = V_1 \psi_{1j\sigma}^{\dagger} X_{0\sigma}(j) + \text{h.c.} + V_2 \psi_{2j\sigma}^{\dagger} \tilde{\sigma} X_{-\sigma 2}(j) + \text{h.c.}, \qquad (6.5)$$

where  $\psi_{\Gamma j\sigma}$  are Wannier states representing a conduction electron in symmetry  $\Gamma$  on site j. We have employed the Hubbard operators,  $X_{0\sigma} = |0\rangle\langle\sigma|$  and  $X_{2\sigma} = |2\rangle\langle\sigma|$  as projected annihilation operators to ensure the absence of any doubly occupied states besides  $|2\rangle$ , for example,  $|\Gamma_1 \otimes \Gamma_1\rangle$ will be eliminated. In this sense, our two channel Anderson model,

$$H = H_c + \sum_{j} H_a(j) + \sum_{j} H_V(j)$$
(6.6)

is the combination of two infinite-U Anderson models in the two different channels. Here we have adopted the notation of Ce atoms, whose ground state is a  $4f^1$  doublet, but this formalism applies equally well to Pu  $5f^5$  atoms, which are hole analogues of Ce:  $|0\rangle \equiv |5f^6\rangle$  represents the half-filled J = 5/2 level,  $|\sigma\rangle \equiv |5f^5 : \sigma\rangle$  represents one hole in this half-filled level and  $|2\rangle \equiv |5f^4\rangle$  contains two holes.

In order to develop a large N Anderson model capturing composite pairing, we must maintain the time-reversal properties of the physical electrons in the large N limit. The defining feature of SU(2) spins is that they invert under time-reversal,  $\mathbf{S} \to \theta \mathbf{S} \theta^{-1} = -\mathbf{S}$ . Maintaining this property as we generalize to large N is essential to the survival of Cooper pairs, and corresponds to generalizing SU(2) spins to symplectic, SP(N) spins:

$$S_{\alpha\beta} = f^{\dagger}_{\alpha}f_{\beta} + \tilde{\alpha}\tilde{\beta}f_{-\alpha}f^{\dagger}_{-\beta}$$
  

$$\alpha \in \{-N/2, ..., -1, 1, ..., N/2\}, \text{ and } \tilde{\alpha} = \operatorname{sgn}(\alpha).$$
(6.7)

The symplectic nature of these spins is responsible for the appearance of composite pairing in the symplectic-N two channel Kondo model, and so to create a symplectic Anderson model, we must ensure that the spin flip operators,  $S_{\alpha\beta}$  are symplectic spins. The Hubbard operators must therefore satisfy the anti-commutation relations,

$$\{X_{0\alpha}, X_{\beta 0}\} = S_{\alpha\beta} + \left(X_{00} + \frac{X_{\gamma\gamma}}{N}\right)\delta_{\alpha,\beta},\tag{6.8}$$

where  $S_{\alpha\beta}$  are the traceless forms of the Hubbard operators,  $X_{\alpha\beta}$ . We show in Section 6.2 that a proper symplectic slave boson representation of the Hubbard operators requires the introduction of *two* slave bosons to describe a single channel:

$$X_{0\alpha} = b_1^{\dagger} f_{\alpha} + a_1^{\dagger} \tilde{\alpha} f_{-\alpha}^{\dagger}$$
  

$$X_{00} = b_1^{\dagger} b_1 + a_1^{\dagger} a_1.$$
(6.9)

As we shall demonstrate, these symplectic Hubbard operators maintain the neutrality of the singly occupied state, which manifests itself as an invariance of the Anderson Hamiltonian with respect to a local SU(2) gauge symmetry associated with the particle-hole transformation,  $f_{\sigma} \rightarrow \cos \theta f_{\sigma} + \operatorname{sgn}(\sigma) \sin \theta f_{-\sigma}^{\dagger}$  [140]. This representation was originally introduced in a mean-field treatment of the t - J model by Wen and Lee [129], and we shall show that these Hubbard operators maintain this gauge symmetry for all N. Here, we focus on composite pairing, and the key result is that the

amount of composite pairing can be written in a simple gauge-invariant form as

$$\Delta_{\rm SC} \propto \langle X_{02} \rangle \propto \langle \psi_{1j\uparrow}^{\dagger} \psi_{2j\uparrow}^{\dagger} S_{-}(j) \rangle, \tag{6.10}$$

where the Hubbard operator  $X_{02} = |0\rangle\langle 2|$  mixes the empty and doubly occupied states. We show that there will be a charge response in the composite-paired superconducting state, as the charge in the *f*-orbitals rearranges to accommodate the mixing, and predict that such a rearrangement will result in the modified electric field gradients felt by the nuclei of the surrounding In atoms, which should be detectable by as a sharp shift in the nuclear quadrupolar resonance (NQR) frequency below the superconducting transition. The magnitude and sign of this shift in CeCoIn<sub>5</sub> can be estimated quantitatively.

This chapter is organized as follows. First we review the single-channel Anderson problem and discuss the previous SU(N) results, before introducing the symplectic Hubbard operators in section 6.2 and demonstrating that the symplectic-N and SU(N) large N limits are identical for a single channel. We then generalize this formalism to the case of two channels in Section 6.3 and show how composite pairing naturally appears as a mixing of the empty and doubly occupied states. The mean-field solution is presented in Section 6.4, in which we show how the superconducting transition temperature increases with increasing mixed valence. In Section 6.5, we calculate the charge distribution of the f-orbitals in the state with composite pairing and predict a shift in the NQR frequency at  $T_c$ . Finally, section 6.6 discusses the implications for the finite-U Anderson model and examines the broader implications of our results.

### 6.1.1 The infinite-U Anderson model and Hubbard operators

The Anderson model combines weakly interacting conduction electrons and localized, strongly interacting f-electrons, coexisting at the same lattice sites,

$$H = H_c + H_f + H_{mix}, ag{6.11}$$

where the first term describes free conduction electrons and the second is an atomic Hamiltonian with a strong on-site Coulomb repulsion,

$$H_c = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \quad H_f = \sum_i \epsilon_f f^{\dagger}_{i\sigma} f_{i\sigma} + U_f \hat{n}_{fi\uparrow} \hat{n}_{fi\downarrow}.$$
(6.12)

These two species mix quantum mechanically through a hybridization term [95],

$$H_{mix} = V \sum_{i} c_{i\sigma}^{\dagger} f_{i\sigma} + \text{h.c.}, \qquad (6.13)$$

where we have taken the hybridization to be isotropic. In the limit of large U, electrons hopping on and off the f-atom are strongly restricted by the high energy cost of double occupancy. The infinite-U Anderson model is a low energy approximation of the full Anderson model in this limit, where the doubly occupied states are eliminated. A proper treatment of this model requires the introduction of *Hubbard operators* to project out any doubly occupied states [98]. These operators,  $X_{ab} = |a\rangle\langle b|$ , act within the space  $|a\rangle = |0, \uparrow, \downarrow\rangle$ , where the diagonal Hubbard operators,  $X_{aa}$  are projection operators, satisfying the completeness relation,

$$X_{00} + \sum_{\sigma} X_{\sigma\sigma} = 1, \tag{6.14}$$

and obeying bosonic commutation relations. The off-diagonal Hubbard operators,  $X_{\sigma 0}$  and  $X_{0\sigma}$  are projected creation/annihilation operators, which obey the anti-commutation relations,

$$\{X_{\sigma 0}, X_{\sigma' 0}\} = X_{\sigma \sigma'} + X_{00}\delta_{\sigma, \sigma'}.$$
(6.15)

Together, we say that the Hubbard operators satisfy a *graded Lie algebra* that is bosonic for the projection operators and spin flips, and fermionic for the projected creation and annihilation operators.

The hybridization and atomic Hamiltonians may be rewritten with these Hubbard operators [99],

$$H_{mix} = V \sum_{i} c_{i\sigma}^{\dagger} X_{0\sigma}(i) + \text{h.c.}, \quad H_a = |\epsilon_f| \sum_{i} X_{00}(i), \quad (6.16)$$

where here we measure the energies from the f-level, so that the energy of the empty state,  $E_0 = -\epsilon_f > 0$ .

Since Hubbard operators, like spins, do not obey canonical commutation relations, they cannot be treated directly within quantum field theory, but they may be represented as bilinears of fermions and bosons. In the usual slave boson approach [100, 101], a boson,  $b^{\dagger}$  is introduced to represent the empty state, two fermions,  $f_{\sigma}^{\dagger}$  are introduced to represent the singly occupied spin states:

$$\begin{aligned} |0\rangle &= b^{\dagger} |\Omega\rangle \\ |\sigma\rangle &= f^{\dagger}_{\sigma} |\Omega\rangle, \end{aligned}$$
 (6.17)

where  $|\Omega\rangle$  is an unphysical vacuum state containing no fermions or bosons. This representation separates the electron into two components: charged, but spinless holons and neutral spinons, which now have the potential to move separately. It can be checked explicitly that the projected hopping operators,

$$X_{0\sigma} = b^{\dagger} f_{\sigma}, \tag{6.18}$$

satisfy the Hubbard algebra, (6.15). The projector into the empty state,  $X_{00} = b^{\dagger}b$  counts the number of bosons and the constraint of no double occupancy fixing the total number of particles,  $n_b + n_f = 1$  can be enforced at each site by employing a Lagrange multiplier,  $\lambda_i$ . This constraint eliminates all but the three physical atomic states (6.17), and because the constraint commutes with the Anderson Hamiltonian, the physical and nonphysical states do not mix. As these Hubbard operators are invariant under a local U(1) gauge transformation,  $b_i \rightarrow b_i e^{i\theta_i}$ ,  $f_{i\sigma} \rightarrow f_{i\sigma} e^{i\theta_i}$  [127, 128], they are known as U(1) slave bosons.

The mean field solution of the infinite-U Anderson is obtained by replacing  $b_i$  and  $\lambda_i$  by their

uniform expectation values,  $\langle b \rangle$  and  $\lambda$ . The resulting Hamiltonian is quadratic in the fermions and can be solved exactly. This mean field limit becomes exact as the number of spin components, N = 2j + 1 goes to infinity. In the mean field theory,  $\langle b \rangle^2$  not only represents the occupancy of the empty state, but it also plays the role of the Kondo hybridization, V. As the conduction and f-electrons hybridize, the valence of the f-electron,  $n_f = 1 - \langle b \rangle^2$  decreases from unity [199]. The lattice Kondo temperature indicates when b first develops an expectation value,

$$T^* = \frac{\Delta}{\pi} e^{-E_0^*/\Delta} \tag{6.19}$$

where  $\Delta = \pi V^2$  is the hybridization width, and  $E_0^* = |\epsilon_f| - \frac{\Delta}{\pi} \log \frac{\Delta}{D}$  shows how the f-level,  $\epsilon_f$  renormalizes. When  $E_0^* < 0$ ,  $T_K$  is no longer limited by  $\Delta/\pi$  and grows all the way to the conduction electron bandwidth, D for sufficiently small  $E_0$ . Here, it is no longer reasonable to think about local moments hybridizing to form a heavy Fermi liquid - the local moments never form and the state will always be a light Fermi liquid.

Let us take a moment to ask: what large N limit does this approach encode? The anti-commutator of these Hubbard operators gives  $S_{\alpha\beta} = f^{\dagger}_{\alpha}f_{\beta}$ , the well-known form of SU(N) spins. It is no wonder then, that this approach contains no superconductivity in the large N limit.

### 6.2 Symplectic Hubbard operators

As we generalize the number of spin components from 2 to N, we must maintain a well-defined time-reversal operation ( $\theta$ ). Correctly incorporating time-reversal symmetry allows the formation of Cooper pairs, which pair an electron and its time-reversed twin and thus enables the development of superconductivity. We have previously shown that composite pairing is contained in the symplectic-N limit of the two channel Kondo model (Chapter 4), which maintains the time-inversion properties of spins in the large N limit by using symplectic spins,

$$S_{\alpha\beta} = f_{\alpha}^{\dagger} f_{\beta} + \tilde{\alpha} \tilde{\beta} f_{-\alpha} f_{-\beta}^{\dagger}.$$
(6.20)

In order to develop composite pairing within a large N Anderson model, we need to introduce a set of Hubbard operators that maintain time-reversal symmetry in the large N limit. The Hubbard operators describe both the charge,  $X_{0\alpha}$  and spin,  $X_{\alpha\beta}$  fluctuations subject to the constraint of no double occupancy. To maintain time-reversal symmetry, these spin fluctuations must be symplectic spins,  $S_{\alpha\beta}$ . Starting from a spin state  $|\sigma\rangle$ , hopping an electron off and then back on should give rise to a spin flip, and this condition defines the Hubbard operators within a single channel, where the projected hopping operators anti-commute,

$$\{X_{0\alpha}, X_{\beta 0}\} = S_{\alpha\beta} + \left(X_{00} + \frac{X_{\gamma\gamma}}{N}\right)\delta_{\alpha,\beta}.$$
(6.21)

The traceless forms of the Hubbard operators,  $S_{\alpha\beta} = X_{\alpha\beta} - \frac{X_{\gamma\gamma}}{N}\delta_{\alpha\beta}$  are the symplectic spins, satisfying the SP(N) commutation relations. As in previous work [167], we use slave bosons and fermionic spinors to represent these Hubbard operators. Satisfying the symplectic Hubbard algebra, (6.21) and thus preserving the symplectic symmetry of the spins requires the introduction of *two* slave bosons,

$$X_{0\alpha} = b_1^{\dagger} f_{\alpha} + a_1^{\dagger} \tilde{\alpha} f_{-\alpha}^{\dagger}$$
  

$$X_{00} = b_1^{\dagger} b_1 + a_1^{\dagger} a_1.$$
(6.22)

At this point, one might wonder why we would want to exchange the elegant simplicity of the original Hubbard operators,  $X_{ab} = |a\rangle\langle b|$  for this profusion of slave bosons. The answer is that, while the original Hubbard operators appear simple, treating them is not [99], due to their non-canonical anti-commutation algebra, (6.21). Introducing the slave boson representation allows us to represent these complicated operators in terms of canonical bosons and fermions. Doubling the number of slave bosons preserves the symplectic character of the spins and we shall see that this encodes the hard-to-enforce Gutzwiller projection as a more mathematically tractable SU(2) gauge symmetry.

In the fermionic spin representation of SP(N), the preservation of time-reversal comes hand

in hand with the neutrality of the spins under charge conjugation. Symplectic spins thus possess a continuous particle-hole symmetry, which can be seen most naturally by introducing the generalized pair creation operators,

$$\Psi^{\dagger} = \frac{1}{2} \sum_{\alpha} \tilde{\alpha} f^{\dagger}_{\alpha} f^{\dagger}_{-\alpha} = \sum_{\alpha > 0} f^{\dagger}_{\alpha} f^{\dagger}_{-\alpha}, \qquad (6.23)$$

which allow us to construct the isospin vector,  $\vec{\Psi} = (\Psi_1, \Psi_2, \Psi_3) = \tilde{f}^{\dagger}_{\alpha} \vec{\tau} \tilde{f}_{\alpha}$ , where

$$\Psi_{1} = \left(\Psi^{\dagger} + \Psi\right), \quad \Psi_{2} = -i\left(\Psi^{\dagger} - \Psi\right)$$
  

$$\Psi_{3} = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{\alpha} - f_{-\alpha} f_{-\alpha}^{\dagger} = n_{f} - N/2, \quad (6.24)$$

and  $n_f = \sum_{\alpha} f_{\alpha}^{\dagger} f_{\alpha}$  is the number of fermions. The isospin vector was shown in section 2.5.1 to commute with symplectic spins,  $\left[\vec{\Psi}, S_{\alpha\beta}\right] = 0$ , which indicates that the symplectic spins possess an SU(2) gauge symmetry: a continuous particle-hole symmetry that allows us to redefine the spinon,  $f_{\alpha} \rightarrow u f_{\alpha} + v \tilde{\alpha} f_{-\alpha}^{\dagger}$ . This symmetry is reflected in the requirement of two types of bosons, as the empty state does not distinguish between zero and two fermions, and thus requires two bosons to keep track of the two ways of representing the empty state,  $b_1^{\dagger} |\Omega\rangle$  and  $a_1^{\dagger} f_1^{\dagger} f_1^{\dagger} |\Omega\rangle = a_1^{\dagger} \Psi^{\dagger} |\Omega\rangle$ , where  $|\Omega\rangle$  is the vacuum. Of course, there is only one physical empty state, as becomes clear when we restrict these Hubbard operators to the physical subspace. In order to faithfully represent the symplectic spins, the sum of the spin and charge fluctuations must be fixed,  $\vec{S}^2 + \vec{\Psi}^2 = \frac{N}{2}(\frac{N}{2} +$ 2) [190]. While in the pure spin model, this constraint is enforced by setting  $\vec{\Psi} = 0$ , here we must equate our two types of charge fluctuations, by setting

$$Q_{3} = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{\alpha} - N/2 + b_{1}^{\dagger} b_{1} - a_{1}^{\dagger} a_{1} = 0$$

$$Q_{+} = \sum_{\alpha>0} f_{\alpha}^{\dagger} f_{-\alpha}^{\dagger} + b_{1}^{\dagger} a_{1} = 0$$

$$Q_{-} = \sum_{\alpha>0} f_{-\alpha} f_{\alpha} + a_{1}^{\dagger} b_{1} = 0.$$
(6.25)

 $\vec{Q}$  commutes with the Hamiltonian, so the physical subspace will not mix with any unphysical subspaces. It is clear from this constraint that  $b_1$  and  $a_1$  have opposite gauge charges, and the only

gauge invariant states satisfying the constraint (for N = 2) are,

$$|\alpha\rangle = f_{\alpha}^{\dagger}|\Omega\rangle$$
  

$$|0\rangle = \left(b_{1}^{\dagger} + a_{1}^{\dagger}\Psi^{\dagger}\right)|\Omega\rangle.$$
(6.26)

The constraint reflects the neutrality of the spins under charge conjugation:  $Q_3$  conserves the total particle number, and prevents doubly occupancy, while  $Q_{\pm}$  kills any states with s-wave pairs on-site.

These Hubbard operators can be written more compactly by using the Nambu notation,

$$X_{0\alpha} = B_1^{\dagger} \tilde{f}_{\alpha}, \ X_{00} = B_1^{\dagger} B_1$$
  
where  $B_1^{\dagger} = \left( b_1^{\dagger}, \ a_1^{\dagger} \right), \ \text{and} \ \tilde{f}_{\alpha} = \left( \begin{array}{c} f_{\alpha} \\ \tilde{\alpha} f_{-\alpha}^{\dagger} \end{array} \right).$  (6.27)

The constraint becomes  $\vec{Q} = B_1^{\dagger} \vec{\tau} B_1 + \tilde{f}_{\alpha}^{\dagger} \vec{\tau} \tilde{f}_{\alpha} = 0$ . For N = 2, we recognize these Hubbard operators as the SU(2) slave bosons introduced by Wen and Lee in the context of the t - J model [129]. Here, it becomes clear that the SU(2) structure not an ad-hoc construction, but rather a consequence of the symplectic symmetry present in both the symplectic-N Kondo and Anderson models for all N. This symmetry can be physically interpreted as the result of valence fluctuations in the presence of a particle-hole symmetric spin.

The most important consequence of this gauge symmetry is the absence of superconductivity in the single channel infinite U Anderson model,

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + E_0(b^{\dagger}_{1j}b_{1j} + a^{\dagger}_{1j}a_{1j}) + V_1 \sum_j \psi^{\dagger}_{1j\sigma}(b^{\dagger}_1 f_\sigma + a^{\dagger}_1 \tilde{\sigma} f^{\dagger}_{-\sigma}) + \text{h.c.}$$
(6.28)

The new hybridization term,  $a_1^{\dagger}\psi_{1\sigma}^{\dagger}\tilde{\sigma}f_{-\sigma}^{\dagger}$  appears to pair the conduction electrons and "f-electrons", however, the SU(2) symmetry allows the f-spinon to be redefined to eliminate this pairing,  $b_1^{\dagger}f_{\alpha} + a_1^{\dagger}f_{-\alpha}^{\dagger}\tilde{\alpha} \rightarrow b_1^{\prime\dagger}f_{\alpha}^{\prime}$ , recovering the usual U(1) slave boson Hamiltonian discussed in the introduction.

### 6.3 The two channel Anderson model

We now turn to the two channel Anderson model, where the two channels involve charge fluctuations to the empty and doubly occupied states taking place in orthogonal symmetry channels. The symmetry of the channels is determined by the crystal fields, and we assume that the ground state of the atom is a Kramer's doublet,  $|\Gamma_1\pm\rangle$ . For Ce<sup>3+</sup>, a 4f<sup>1</sup> ion, the valence fluctuations will be:  $f^0 \Rightarrow f^1 \Rightarrow f^2$ . The empty state,  $|0\rangle \equiv |f^0\rangle$  is trivially a singlet, and we choose the doubly occupied state to be a singlet formed from electrons in two orthogonal channels,

$$|2\rangle \equiv |f^2\rangle = \tilde{\alpha} f^{\dagger}_{\Gamma_1,\alpha} f^{\dagger}_{\Gamma_2-\alpha} |0\rangle, \qquad (6.29)$$

where  $\Gamma_2$  is an excited crystal field doublet. In the finite-U Anderson model, these two symmetry channels are the same, but here Hund's rules force the second electron to be placed in an orthogonal orbital to the first. This physics is what enables the development of composite pairing, and what gives it a nodal superconducting gap.

The local atomic Hamiltonian at site j can be expressed in terms of Hubbard operators,

$$H_a(j) = E_0 X_{00}(j) + E_2 X_{22}(j), (6.30)$$

where the X's are the Hubbard operators  $X_{00} = |0\rangle\langle 0|$  and  $X_{22} = |2\rangle\langle 2|$ , and we measure the energies from the f-electron level, so that  $E_0 = -\epsilon_f$  and  $E_2 = U_{12} + \epsilon_f$  are both positive, where  $U_{12}$  is the Hubbard U for the  $|f^2\rangle$  state. Here, we ignore the excited crystal field doublet as it does not play an important role in the Kondo physics. These f-electrons hybridize with a bath of conduction electrons in two different channels

$$H_{V}(j) = \sum_{j} V_{1} \psi_{1j\sigma}^{\dagger} X_{0\sigma}(j) + \text{h.c.} + V_{2} \psi_{2j\sigma}^{\dagger} \tilde{\sigma} X_{-\sigma 2}(j) + \text{h.c.}$$
(6.31)

 $X_{0\sigma} = |0\rangle\langle\sigma|$  and  $X_{2\sigma} = |2\rangle\langle\sigma|$  are the projected hopping operators between the singly occupied

state and empty or doubly occupied states, respectively. We have chosen to hide the angular momentum dependence the Wannier states representing a conduction electron with symmetry  $\Gamma$  on site j,

$$\psi_{\Gamma j\sigma} = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \left[\Phi_{\Gamma \mathbf{k}}\right]_{\sigma\sigma'} c_{\mathbf{k}\sigma'}, \qquad (6.32)$$

where the crystal field form-factors  $[\Phi_{\Gamma \mathbf{k}}]_{\sigma\sigma'} = \langle k\Gamma\sigma' | \mathbf{k}\sigma \rangle$  are proportional to unitary matrices.

We now introduce a second set of symplectic-N Hubbard operators for the second channel,

$$X_{2\alpha} = b_2^{\dagger} f_{\alpha} - a_2^{\dagger} \tilde{\alpha} f_{-\alpha}^{\dagger}, \ X_{22} = b_2^{\dagger} b_2 + a_2^{\dagger} a_2.$$
(6.33)

These operators have the same form as for the first channel, except that we are free to choose the sign of  $a_2$ , and have chosen the negative sign to preserve continuity with the results from the two channel Kondo model. They can again be written more compactly by using the Nambu notation,

$$X_{2\alpha} = B_2^{\dagger} \tilde{f}_{\alpha}, \ X_{22} = B_2^{\dagger} B_2 \text{ with } B_2^{\dagger} = \left(b_2^{\dagger}, \ -a_2^{\dagger}\right).$$
(6.34)

 $B_2^{\dagger}$  represents the creation of electrons and will have an opposite electromagnetic charge to  $B_1^{\dagger}$ , but since both  $B_{1,2}^{\dagger}$  remove particles from the singly occupied state, they have the same gauge charge.  $b_2^{\dagger}$  and  $a_2^{\dagger}$ , of course, have opposite gauge charges, as is again seen in the doubly occupied state,

$$|2\rangle = \left(b_2^{\dagger} - a_2^{\dagger}\Psi^{\dagger}\right)|\Omega\rangle \tag{6.35}$$

These two algebras intersect, as they describe the same spin fluctuations, and the constraint becomes,

$$\vec{Q} = B_1^{\dagger} \vec{\tau} B_1 + B_2^{\dagger} \vec{\tau} B_2 + \tilde{f}_{\alpha}^{\dagger} \vec{\tau} \tilde{f}_{\alpha} = 0,$$
(6.36)

where the two channels come in with the same sign because they have the same gauge charge -  $Q_3$  conserves the total particle number, not the electromagnetic charge. The intersection of these two



Figure 6.2: The six states in the physical Hilbert space of the two channel Anderson model. For N = 2, there are ground state and excited crystal field doublets, and the empty and doubly occupied singlets. The arrows indicate the Hubbard operators that move between states in the Hilbert space.

algebras gives rise to an extra doublet,

$$|\Gamma_2\alpha\rangle = \left(b_1^{\dagger}a_2^{\dagger} + b_2^{\dagger}a_1^{\dagger}\right)f_{\alpha}^{\dagger}|\Omega\rangle, \qquad (6.37)$$

which we interpret as the excited crystal field doublet because it is reached by destroying a  $\Gamma_1$  electron from the doubly occupied state, leaving behind the  $\Gamma_2$  electron. However,  $X_{00}$  and  $X_{22}$  are no longer projectors in this enlarged Hilbert space, as neither of them kill the new doublet. Even though we have not explicitly included the excited crystal field doublet in our Hamiltonian, this doublet automatically has the energy,  $E_0 + E_2$ . If we wish to adjust the energy of this state as a free parameter,  $\Delta_{CEF}$ , we must add the quartic term,

$$\left[\Delta_{CEF} - (E_0 + E_2)\right] \left(b_1^{\dagger} a_2^{\dagger} + a_1^{\dagger} b_2^{\dagger}\right) \left(b_1 a_2 + a_1 b_2\right), \tag{6.38}$$

to the atomic Hamiltonian (6.30). We choose to omit this term, making the extra doublet the highest energy state in the problem, and it should have little effect on the low energy physics of interest. In

fact, as we shall see later, this term vanishes for the superconducting state, but acts as an attractive term for uniform composite density waves.

In addition to an extra state, there are two additional operators,

$$X_{02} = \{X_{0\alpha}, X_{\alpha 2}\} = B_1^{\dagger} B_2 = b_1^{\dagger} b_2 - a_1^{\dagger} a_2$$
  
$$X_{\Gamma_1 \alpha; \Gamma_2 \beta} = -\{X_{0\alpha}, X_{2\beta}\} = \left(b_1^{\dagger} a_2^{\dagger} + a_1^{\dagger} b_2^{\dagger}\right) \tilde{\alpha} \delta_{\alpha, -\beta}.$$
 (6.39)

Both of these operators mix states within the Hilbert space when they acquire an expectation value.  $X_{\Gamma_1\alpha;\Gamma_2\beta}$  mixes the ground state and excited crystal field doublets, which we shall later show corresponds to the development of a uniform composite density wave. This mixing is similar to the ordered state mixing ground state and excited singlets proposed for URu<sub>2</sub>Si<sub>2</sub> [200]. On the other hand,  $X_{02} = |0\rangle\langle 2|$  mixes the empty and doubly occupied states. In this sense, composite pairing resembles an intra-site version of negative-U pairing, where the ground state tends to contain a mixture of empty and doubly occupied sites [201]. Here, instead of s-wave pairing, which is forbidden by the large, positive U, the pairs will be d-wave.

### 6.4 The large N two channel Anderson model

We are now able to write the symplectic-N two channel Anderson model in terms of the symplectic Hubbard operators,

$$H = \sum_{\mathbf{k}} \epsilon_k c_{\mathbf{k}\alpha}^{\dagger} c_{\mathbf{k}\alpha} + \sum_j E_0 B_1^{\dagger}(j) B_1(j) + E_2 B_2^{\dagger}(j) B_2(j) + \frac{V_1}{\sqrt{N/2}} \sum_j \psi_{1j\alpha}^{\dagger} B_1^{\dagger}(j) \tilde{f}_{j\alpha} + \text{h.c.} + \frac{V_2}{\sqrt{N/2}} \sum_j \psi_{2j\alpha}^{\dagger} \tilde{\alpha} \tilde{f}_{j-\alpha}^{\dagger} B_2(j) + \text{h.c.}$$
(6.40)

In order to keep the Hamiltonian extensive in N, we have rescaled the hybridization terms by  $(N/2)^{-1/2}$ , so that they recover the correct N = 2 form, (6.31). This rescaling involves the implicit assumption that the slave bosons  $B_{\Gamma}$  will be of order  $\sqrt{N}$ , which will be true in the large N limit. As N gets large, there are still only two flavors of bosons, and for the bosons to have any

contribution in the large N limit, they must be condensed.

In order to write down a translationally invariant Hamiltonian, we assume that the expectation values of the slave bosons will be uniform, which allows us to write down the Hamiltonian in momentum space. To simplify this step, we drop the spin-orbit dependence of the Wannier functions, and instead assume that the form factors are spin-diagonal,  $\psi_{\Gamma j\alpha} = \sum_{\mathbf{k}} c_{\mathbf{k}\alpha} \phi_{\Gamma \mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j}$ . This allows us to absorb the momentum dependence of the form-factors into the hybridizations by defining  $V_{\Gamma \mathbf{k}} = \frac{V_{\Gamma}}{\sqrt{N/2}} \phi_{\Gamma \mathbf{k}}$ . To obtain the d-wave symmetry which arises naturally from the spin-orbit form factors, we must explicitly make  $V_{1k}V_{2k}$  d-wave. The full spin-orbit dependence can be restored in a similar manner to that discussed in Appendix 4B for the two channel Kondo model. The Hamiltonian is,

$$H = \sum_{\mathbf{k}} \left( \epsilon_k c_{\mathbf{k}\alpha}^{\dagger} c_{\mathbf{k}\alpha} + V_{1\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} B_1^{\dagger} \tilde{f}_{\mathbf{k}\alpha} + V_{2\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} \tilde{\alpha} \tilde{f}_{\mathbf{k}-\alpha}^{\dagger} B_2 + h.c. \right)$$
  
+ $\mathcal{N}_s \left( E_0 B_1^{\dagger} B_1 + E_2 B_2^{\dagger} B_2 \right)$  (6.41)

The SU(2) constraint is implemented with a vector of Lagrange multipliers,  $\vec{\lambda}$ ,

$$\vec{\lambda} \cdot \left( \sum_{\mathbf{k}} \tilde{f}^{\dagger}_{\mathbf{k}\alpha} \vec{\tau} \tilde{f}^{\dagger}_{\mathbf{k}\alpha} + B_1^{\dagger} \vec{\tau} B_1 + B_2^{\dagger} \vec{\tau} B_2 \right), \tag{6.42}$$

where we have also assumed that  $\vec{\lambda}$  is translationally invariant, enforcing the constraint on average. This approximation becomes exact in the large N limit. The final step is to rewrite the Hamiltonian with Nambu spinors in the compact form,

$$H = \sum_{\mathbf{k}} \left( \tilde{c}_{\mathbf{k}\alpha}^{\dagger} \ \tilde{f}_{\mathbf{k}\alpha}^{\dagger} \right) \left( \begin{array}{c} \epsilon_{\mathbf{k}} \tau_3 & V_{1\mathbf{k}} \mathcal{A}_1^{\dagger} + V_{2\mathbf{k}} \mathcal{A}_2^{\dagger} \\ V_{1\mathbf{k}} \mathcal{A}_1 + V_{2\mathbf{k}} \mathcal{A}_2 & \vec{\lambda} \cdot \vec{\tau} \end{array} \right) \left( \begin{array}{c} \tilde{c}_{\mathbf{k}\alpha} \\ \tilde{f}_{\mathbf{k}\alpha} \end{array} \right) \\ + \left[ E_0 B_1^{\dagger} B_1 + E_2 B_2^{\dagger} B_2 + \vec{\lambda} \cdot \left( B_1^{\dagger} \vec{\tau} B_1 + B_2^{\dagger} \vec{\tau} B_2 \right) \right], \quad (6.43)$$

where we have collected the slave bosons into the SU(2) matrices,

$$\mathcal{A}_{1}^{\dagger} = \begin{pmatrix} b_{1}^{\dagger} & a_{1}^{\dagger} \\ a_{1} & -b_{1} \end{pmatrix}, \quad \mathcal{A}_{2}^{\dagger} = \begin{pmatrix} a_{2} & b_{2} \\ b_{2}^{\dagger} & -a_{2}^{\dagger} \end{pmatrix}.$$
(6.44)

These matrices transform under the SU(2) gauge symmetry as  $\mathcal{A}_{\Gamma} \to g\mathcal{A}_{\Gamma}$  (where g is an SU(2) matrix), so that the product

$$\mathcal{A}_{2}^{\dagger}\mathcal{A}_{1} = \begin{pmatrix} b_{1}a_{2} + b_{2}a_{1} & a_{1}^{\dagger}a_{2} - b_{1}^{\dagger}b_{2} \\ b_{2}^{\dagger}b_{1} - a_{2}^{\dagger}a_{1} & b_{2}^{\dagger}a_{1}^{\dagger} + a_{2}^{\dagger}b_{1}^{\dagger} \end{pmatrix}$$
(6.45)

is gauge invariant. In chapter 4, we encountered a similar set of matrices for the two channel Kondo model,  $\mathcal{V}_{\Gamma} = \begin{pmatrix} V_{\Gamma} & \Delta_{\Gamma}^{\dagger} \\ \Delta_{\Gamma} & -V_{\Gamma}^{\dagger} \end{pmatrix}$ , and the off-diagonal elements of the product  $\mathcal{V}_{2}^{\dagger}\mathcal{V}_{1}$  were identified with composite pairing:  $\langle \psi_{1}^{\dagger}(\boldsymbol{\sigma}_{N} \cdot \mathbf{S})i\sigma_{2}\psi_{2}^{\dagger}\rangle$ , where  $\boldsymbol{\sigma}_{N}$  are the symplectic generalization of the Pauli matrices. In the Kondo limit,  $E_{0}, E_{2} \gg \pi \rho V^{2}$ , a Schrieffer-Wolff transformation takes  $b_{1} \rightarrow V_{1}$ ,  $a_{1} \rightarrow \Delta_{1}, b_{2} \rightarrow \Delta_{2}$  and  $a_{2} \rightarrow V_{2}$ , which allows us to identify the off-diagonal components of  $\mathcal{A}_{2}^{\dagger}\mathcal{A}_{1}$  with composite pairing. This identification is why we have taken the negative sign of  $a_{2}$  in the definition of the Hubbard operators. More generally, the components of  $\mathcal{A}_{2}^{\dagger}\mathcal{A}_{1}$  can be identified with the state mixing operators,

$$\mathcal{A}_{2}^{\dagger}\mathcal{A}_{1} = \begin{pmatrix} X_{\Gamma_{1}\Gamma_{2}} & -X_{02} \\ X_{20} & X_{\Gamma_{2}\Gamma_{1}} \end{pmatrix}, \qquad (6.46)$$

which confirms the identification of  $\langle X_{02} \rangle$  with composite pairing, and implies that the composite pair state will contain an admixture of the empty and doubly occupied states.

### 6.4.1 The mean field solution

In order to examine the effects of mixed valence on the superconductivity, we examine the mean field solution of the composite pair state in the symplectic-N limit. The bosons are replaced by their expectation values,  $B_{\Gamma} \rightarrow \langle B_{\Gamma} \rangle \sim O(\sqrt{(N)})$ , and the Hamiltonian (6.43) becomes quadratic in the

fermions, which may be integrated out exactly. We use the SU(2) gauge symmetry to eliminate the  $a_1$  boson, and now the composite pair state is defined by the nonzero expectation value of  $\langle b_1^{\dagger}b_2 \rangle$ . If the  $a_2$  boson were to acquire an expectation value, it would lead to a uniform composite density wave solution, which is generally unstable to the composite pair solution. The resulting free energy can be rewritten in terms of our mean field parameters, where we replace  $\langle b_{\Gamma} \rangle / \sqrt{N/2}$  with  $b_{\Gamma}$  for clarity, (however keep in mind that these have lost their dynamics),

$$F = -NT \sum_{\mathbf{k}\pm} \log 2 \cosh \frac{\beta \omega_{k\pm}}{2} + \frac{NN_s}{2} \left[ b_1^2 (E_0 + \lambda) + b_2^2 (E_2 + \lambda) \right].$$
(6.47)

 $\mathcal{N}_s$  is the number of sites, and the dispersion of the heavy electrons is given by  $\omega_{k\pm}$  and  $-\omega_{k\pm}$ , where  $\omega_{k\pm} = \sqrt{\alpha_k \pm \Gamma_k}$ , and

$$\alpha_{k} = b_{+}^{2} + \frac{1}{2}(\epsilon_{\mathbf{k}}^{2} + \lambda_{3}^{2}), \ \Gamma_{\mathbf{k}} = \sqrt{\alpha_{k}^{2} - \gamma_{k}^{2}}$$
  
$$\gamma_{k}^{2} = \left[\epsilon_{\mathbf{k}}\lambda_{3} - b_{-}^{2}\right]^{2} + \left[2V_{1\mathbf{k}}b_{1}V_{2\mathbf{k}}b_{2}\right]^{2}.$$
(6.48)

We have also defined  $b_{\pm}^2 = V_{1\mathbf{k}}^2 b_1^2 \pm V_{2\mathbf{k}}^2 b_2^2$ . In a nodal composite pair superconductor, the  $\vec{\lambda}$  constraint reduces to  $\lambda_3$ , as the  $\lambda_1$  constraint acts as a Coulomb pseudo-potential [111] eliminating s-wave pairing, and it is unnecessary when we choose  $V_{1\mathbf{k}}V_{2\mathbf{k}}$  to give nodal superconductivity. However, if we were to treat the finite U model, where  $V_{1k} = V_{2k}$ , this constraint is essential to eliminate the appearance of a false s-wave superconducting phase.

The mean field parameters are determined by minimizing the free energy with respect to  $b_1$ ,  $b_2$ ,  $\lambda_3$  and  $\lambda_1$ . To understand their implications, we first present the mean field equations in real space,

$$\langle b_{1j} \rangle = \frac{V_1^2}{E_0} \langle f_{j\alpha}^{\dagger} \psi_{1j\alpha} \rangle$$

$$\langle b_{2j} \rangle = \frac{V_2^2}{E_2} \langle \tilde{\alpha} f_{j-\alpha} \psi_{2j\alpha} \rangle$$

$$\langle f_{j\alpha}^{\dagger} f_{j\alpha} \rangle = N/2 - \langle b_{1j} \rangle^2 - \langle b_{2j} \rangle^2$$

$$\langle \tilde{\alpha} f_{j\alpha}^{\dagger} f_{j-\alpha}^{\dagger} \rangle = 0.$$

$$(6.49)$$

These equations bear a strong resemblance to the two channel Kondo equations, where  $\langle b_1 \rangle$  plays the role of the hybridization,  $V_1$  in channel one, while  $\langle b_2 \rangle$  plays the role of the pairing field,  $\Delta_2$ in channel two; here the hybridizations are explicitly identified as the magnitude of the valence fluctuations to the empty and doubly occupied states.  $n_f$  is no longer fixed to N/2 and instead decreases as hybridization and pairing develop.

To calculate the phase diagram, we return to the momentum space picture, and derive the three equations relevant for composite pair superconductivity with a nodal order parameter. For simplicity, we replace  $\langle b_1 \rangle$  and  $\langle b_2 \rangle$  with  $b_1$  and  $b_2$ . The first equation imposes the constraint  $Q_3 = 0$ , fixing  $n_f = N/2 - b_1^2 - b_2^2$ , while the next two equations determine the magnitude of the valence fluctuations to the empty and doubly occupied states, respectively:

$$\sum_{\pm} \int_{\mathbf{k}} \frac{\tanh \frac{\beta \omega_{\mathbf{k}\pm}}{2}}{2\omega_{\mathbf{k}\pm}} \left\{ \begin{pmatrix} \lambda \\ 2V_{1k}^2 \\ 2V_{2k}^2 \end{pmatrix} \pm \frac{A}{\Gamma_k} \right\} = \begin{pmatrix} b_1^2 + b_2^2 \\ 2(E_0 + \lambda) \\ 2(E_2 + \lambda) \end{pmatrix}, \quad (6.50)$$

where

$$A = \begin{pmatrix} \lambda \alpha_k + \epsilon_{\mathbf{k}} \left[ b_-^2 - \lambda \epsilon_{\mathbf{k}} \right] \\ V_{1\mathbf{k}}^2 (\epsilon_{\mathbf{k}} + \lambda)^2 \\ V_{2\mathbf{k}}^2 (\epsilon_{\mathbf{k}} - \lambda)^2 \end{pmatrix}.$$
 (6.51)

In addition to these three equations, we must also fix the total electromagnetic charge in the system by keeping the total number of conduction electrons plus physical f-electrons constant. Notice that the number of physical f-electrons,  $\tilde{n}_f = N/2 - b_1^2 + b_2^2$  counts the electrons in both the singly and doubly occupied states, and differs from the occupation of the spin states,  $n_f = N/2 - b_1^2 - b_2^2$ by  $2b_2^2$ . These equations can be solved numerically for a simple two-dimensional model where we take  $V_{1k} = V$  and  $V_{2k} = V (\cos k_x - \cos k_y)$ , and take the conduction electron dispersion,  $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$ , where  $\mu$  is adjusted to fix the total charge,  $\tilde{n}_f + n_c$ . This model contains three non-trivial phases:

• For  $E_0 < E_2$ , a heavy Fermi liquid develops at  $T_1^*$ , where  $b_1$  becomes nonzero with the



Figure 6.3: This phase diagram for the two channel Anderson model, showing the transition temperatures as we vary  $E_0/E_2$ , is qualitatively identical to that of the two channel Kondo model. Here, we have fixed  $n_c + \tilde{n}_f = 1.8$ , and adjusted  $V_2$  so that  $T_1^* = T_2^*$  when  $E_2 = E_0$ .

symmetry,  $\Gamma_1$  of the ground state doublet. The f-electron valence will be less than N/2, and these results will be identical to the infinite-U Anderson model discussed in the introduction.

- For E<sub>2</sub> > E<sub>0</sub>, a heavy Fermi liquid develops at T<sup>\*</sup><sub>2</sub>, where b<sub>2</sub> becomes nonzero. This Fermi liquid will have the symmetry, Γ<sub>2</sub> of the excited doublet, and the f-electron valence will be larger than N/2. Again, these results should be identical to the appropriate infinite-U Anderson model.
- However, beginning at  $T_c$ , there will be a phase of d-wave composite pairing, where  $b_1b_2$  is nonzero.  $T_c$  is maximal at  $E_0 = E_2$ , where the high temperature state of free spins transitions directly into the composite pair superconductor. As superconductivity is driven by the Cooper channel in the heavy electron normal states, the ground state will always be superconducting. The f-electron valence will generally differ from N/2, with nonzero contributions of both  $f^0$ and  $f^2$ .

We show a phase diagram in Figure 6.3 obtained by varying  $E_0/E_2$ , which is qualitatively identical to that of the two channel Kondo model for varying  $J_2/J_2$ : there is a superconducting dome with maximal  $T_c$  for  $E_0/E_2 = 1$ . We could equally well have varied  $V_2/V_1$ . What is new is what happens to this phase diagram if we fix  $E_0/E_2$  and change their overall scale, which is equivalent to changing the degree of mixed valence. We show these results in Figure 6.4, where we plot  $T_c$ against the occupancy of the singly occupied state,  $n_f$ ; as expected,  $T_c$  increases with increasing mixed valence, following the trend of the Kondo temperature at the maximal  $T_c$ , and explaining the increase in  $T_c$  between CeCoIn<sub>5</sub> and PuCoGa<sub>5</sub>.



Figure 6.4: The degree of mixed valence can be quantified by the occupation of the singly occupied doublet,  $n_f = N/2 - b_1^2 - b_2^2$ . Here, we plot the maximum  $T_c = T_1^* = T_2^*$  (for  $E_0 = E_2$ ), which increases monotonically with the degree of mixed valence.  $T_c$  is scaled by  $\Delta = \pi V_1^2$ , and we have fixed  $n_c + \tilde{n}_f = 1.8$  in units of N/2.

### 6.5 Charge Redistribution

As the development of composite pairing mixes the empty and doubly occupied states, each develops a non-zero occupation, and it is interesting to examine how the charge density changes. The link between the f-electron charge, and the development of the Kondo effect in the one-channel Anderson model was explored by Gunnarsson and Schoenhammer [199], who showed that the f-electron valence,  $\tilde{n}_f$  decreases gradually with temperature through the Kondo crossover,  $\tilde{n}_f = 1 - b_1^2(T)$ (for N = 2). The mixing of the empty and doubly occupied states adds a new element to this relationship, and the consideration of real, non-s-wave hybridizations allows us to explore the higher angular momentum components of the charge distribution. The charge density can be written,  $\hat{\rho}(\mathbf{x}) = \hat{\psi}^{\dagger}_{\alpha}(\mathbf{x})\hat{\psi}_{\alpha}(\mathbf{x})$ , where  $\hat{\psi}^{\dagger}_{\alpha}(\mathbf{x})$  creates a physical electron of spin  $\alpha$  at  $\mathbf{x}$ . An electron at  $\mathbf{x}$  exists in a superposition of the orbitals  $\Gamma_1$  and  $\Gamma_2$  at nearby lattice sites j,

$$\hat{\psi}_{\alpha}(\mathbf{x}) = \sum_{j} \left[\Phi_{1}\right]_{\alpha\beta} \left(\mathbf{x} - \mathbf{R}_{j}\right) f_{1j\beta} + \left[\Phi_{2}\right]_{\alpha\beta} \left(\mathbf{x} - \mathbf{R}_{j}\right) f_{2j\beta},\tag{6.52}$$

where we have reintroduced the spin-orbit form factor,  $[\Phi_{\Gamma}]_{\alpha\beta}$  in order to model real materials. The charge density of an f-electron located at the origin in channel  $\Gamma$  is  $\rho_{\Gamma}(\mathbf{x}) = \text{Tr}|\Phi_{\Gamma}(\mathbf{x})|^2 R(\mathbf{x})$ , where  $R(\mathbf{x})$  is the radial function for the f-electron, and  $|\Phi_{\Gamma}(\mathbf{x})|^2$  is a diagonal matrix. If we assume that the overlap of electrons at neighboring sites is negligible, the total charge density has three terms,

$$\hat{\rho}(\mathbf{x}) = \sum_{j} \rho_{1}(\mathbf{x} - \mathbf{R}_{j}) f_{1j\beta}^{\dagger} f_{1j\beta} + \rho_{2}(\mathbf{x} - \mathbf{R}_{j}) f_{2j\beta}^{\dagger} f_{2j\beta} + \left[ \Phi_{1}^{\dagger} \Phi_{2} \right]_{\alpha\beta} (\mathbf{x} - \mathbf{R}_{j}) f_{1j\alpha}^{\dagger} f_{2j\beta} + \text{h.c.}$$
(6.53)

We have kept the spin indices of  $\left[\Phi_1^{\dagger}\Phi_2\right]_{\alpha\beta}$ , as it may not be diagonal in spin space. In terms of the Hubbard operators, we can identify,

$$f_{1j\beta}^{\dagger}f_{1j\beta} = X_{22}(j) + n_f(j)$$
  

$$f_{2j\beta}^{\dagger}f_{2j\beta} = X_{22}(j)$$
  

$$f_{1j\alpha}^{\dagger}f_{2j\beta} = X_{\Gamma_1\alpha\Gamma_2\beta}(j).$$
(6.54)

The third term only acquires an expectation value only in the composite density wave state, which mixes the two crystal field states, shifting charge from  $\Gamma_1$  to  $\Gamma_2$ . In the heavy Fermi liquid and superconducting states,  $a_2 = 0$ , and we may use the constraint to rewrite  $f_{1j\beta}^{\dagger}f_{1j\beta} = N/2 - X_{00}(j)$ . The charge distribution then becomes,

$$\hat{\rho}(\mathbf{x}) = \sum_{j} \rho_1(\mathbf{x} - \mathbf{R}_j) \left[ \frac{N}{2} - X_{00}(j) \right] + \rho_2(\mathbf{x} - \mathbf{R}_j) X_{22}(j).$$
(6.55)

Integrating this charge density around a single site gives us the f-electron valence,  $\tilde{n}_f = N/2 - b_1^2 + b_2^2$ , which we show as a function of T in Figure 6.5 for different  $E_2/E_0$ . In the large N limit, both the transition into the heavy Fermi liquid, at  $T^*$  and into the superconductor, at  $T_c$  are second order phase transitions. The former is an artifact of the large N limit, and for any finite N the transition into the heavy Fermi liquid is a crossover, however, the sharp shift in  $\tilde{n}_f$  at the superconducting transition temperature survives for all N, and should be observable experimentally with core-level valence spectroscopy. The observation of such a shift would clearly indicate the presence of composite pairing.



Figure 6.5: The f-electron valence,  $\tilde{n}_f$  changes as the Kondo effect and composite pair superconductivity develop. Two examples are shown - the black curve has  $E_0 = E_2$ , and here  $T_c = T_K$ , however, channel one dominates at lower temperatures, causing the valence to decrease. For the gray curve,  $T_c < T_K$  and a sharp shift in the valence is seen at  $T_c$ , where the previously increasing valence begins to decrease.

Now we explore the quadrupole charge component. As superconductivity develops, the occupation of the doubly occupied state acquires an expectation value, leading to an increase in the  $\Gamma_2$ charge density. This redistribution of the f-electron charge results in a quadrupole moment associated with superconductivity, which has an indirect effect on the superconducting transition temperature through its linear coupling to strain, leading to a linear dependence of  $T_c$  on the tetragonal strain, c/a. Such a linear increase of  $T_c$  with c/a has been observed in both the Ce and Pu 115s, although it is conventionally attributed to dimensionality effects [183]. The quadrupole moment of the composite condensate provides an alternate explanation. This quadrupole moment can also be measured directly through nuclear quadrupole resonance (NQR), and hence we discuss the real materials in detail, estimating the magnitude of the NQR frequency shift. Again, since the development of superconductivity is a phase transition, the quadrupole moment changes sharply at  $T_c$ , leading to electric field gradients around the f-lattice sites, which in turn lead to a shift in the nuclear quadrupole resonance frequency,  $\Delta \nu_{NQR}$  at the nuclei of the nearby atoms.

To make contact with potential experiments, we examine CeMIn<sub>5</sub> in more detail. <sup>115</sup>In atoms have a nuclear moment I = 9/2, which results in a quadrupole moment,  $Q = 8.3 \times 10^{-29} m^2$ , which makes them "NQR active" [202]. The symmetry of the ground state doublet is  $\Gamma_7^+$  [192], whose angular dependence is given by,

$$|\Phi_{\Gamma_7^+}|^2(\theta,\phi) = \frac{3}{16}\sin^2\theta \left[11 + 6\cos 2\xi + 5\cos 2\theta(1 + 2\cos 2\xi) + 2\sqrt{5}\cos 4\phi\sin^2\theta\sin 2\xi\right],$$
(6.56)

where  $\xi$  is a crystal-field parameter depending on the microscopic details. It can be measured with inelastic neutron scattering, and we set  $\xi \approx .25$  for CeCoIn<sub>5</sub> [192]. We take the excited doublet to be  $\Gamma_2 = \Gamma_6$ , whose angular dependence is,

$$|\Phi_{\Gamma_6}|^2(\theta,\phi) = \frac{3}{32} \left[ 12\cos 2\theta + 5(3+\cos 4\theta) \right].$$
(6.57)

We can now use the real charge distributions of the two orbitals to estimate the magnitude of the electric field gradient,  $V_{ab} = -\partial E_a/\partial x_b$ , where

$$\rho_{\Gamma}(\mathbf{x}) = |\Phi_{\Gamma}|^2(\theta, \phi) R(r).$$
(6.58)

R(r) is the 4f radial function,

$$R(r) = \frac{1}{96\sqrt{35}} \left(\frac{Z^{3/2}r}{2a_B}\right)^3 \exp\left(-\frac{Zr}{4a_B}\right).$$
 (6.59)

9

 $a_B = 0.53$ Å is the Bohr radius, and  $Z = r_{Ce}/6\sqrt{10}$  is adjusted so that the atomic radius is that of Ce<sup>3+</sup>,  $\langle r \rangle = 0.115$ Å[203].



Figure 6.6: The crystal structure of  $CeCoIn_5$ , indicating the high symmetry In(1) sites and lower symmetry In(2) sites.

The NQR frequency measures the electric field gradients at two different indium sites in the crystal: the in-plane, high symmetry In(1) sites, which sit in the center of a square of Ce atoms, and the out-of-plane In(2) sites, which are above and in-between two Ce atoms. We focus on the high symmetry In(1) atoms because here  $V_{zz}$  is the only contribution to the NQR frequency [204],

$$\nu_{NQR} = \frac{3eV_{zz}Q}{2hI(2I-1)}$$
 Hz, (6.60)

while the In(2) site will have an asymmetry contribution,  $\eta = V_{xx} - V_{yy}$ .

$$V_{zz}^{\Gamma}(\mathbf{x}, \mathbf{R}_j) = \frac{q}{4\pi\epsilon_0} \int_{\mathbf{x}'} \rho_{\Gamma}(\mathbf{x}' - \mathbf{R}_j) \left[ \frac{3(z - z')^2}{|\mathbf{x} - \mathbf{x}'|^5} - \frac{1}{|\mathbf{x} - \mathbf{x}'|^3} \right].$$
 (6.61)

Summing over the eight neighboring Ce sites is sufficient to estimate the magnitude of the NQR shift, where we use the lattice constants of CeCoIn<sub>5</sub>, a = 4.6Å, and c = 7.4Å[83]. We find the electric field gradients for a charge q in channel  $\Gamma$  to be,

$$V_{zz}^{7+}(\mathbf{x} = In(1)) = -7q \times 10^{19} \text{V/m}^2$$
  
$$V_{zz}^6(\mathbf{x} = In(1)) = -q \times 10^{20} \text{V/m}^2.$$
 (6.62)

For equal channel strengths, the total charge of the f-ion remains unity, and the increasing occupations of the empty and doubly occupied sites cause holes to build up with symmetry  $\Gamma_7^+$  and electrons with symmetry  $\Gamma_6$ . If the channels are not equal, the valence of f-ion will not be fixed, and we would have to consider charge coming from the conduction electrons. We now introduce x(T)as the temperature dependent occupation of the empty/doubly occupied states,  $x(T) = \langle b_1^2 \rangle = \langle b_2^2 \rangle$ , which is proportional to  $T_c - T$  just below  $T_c$ , allowing us to write

$$x(T) = x_0 \frac{T_c - T}{T_c},$$
(6.63)

where  $x_0$  is the ground state occupation of the empty/doubly occupied states. In terms of  $x_0$ , the superconducting NQR frequency shift will be,

$$\Delta \nu_{NQR}(T) = 25x_0 \frac{(T_c - T)}{T_c} \text{kHz.}$$
(6.64)

A reasonably large value of  $x_0 = 0.05$  will lead to an admittedly small shift in  $\nu_{NQR}$  with a slope of  $\approx +5kHz/K$ , beginning precisely at  $T_c$ . If this shift can be distinguished, it would be an unambiguous signal of composite pairing.

### 6.6 Conclusions

Our two-channel Anderson model treatment has shown that composite pairing is the low energy consequence of valence fluctuations in two competing symmetry channels, which manifests itself

as a mixing of the empty and doubly occupied states,

$$\Delta_{SC} \propto \langle |0\rangle \langle 2| \rangle. \tag{6.65}$$

Composite pairing is primarily a local phenomena, where the pairing occurs within a single unit cell. The mixing is reminiscent of an *intra-atomic* negative-U pairing with a d-wave symmetry, although, amazingly it occurs in a model with only repulsive interactions. Here, it is really the atomic physics of the f-ions, tuned by their local chemical environment that drives the superconductivity. Such chemically driven d-wave pairing is a fascinating direction for exploring higher temperature superconductors in the even more mixed valent 3d superconductors, as the strength of the composite pairing increases monotonically with increasing valence fluctuations, accounting for the difference in transition temperatures between the cerium and the actinide 115 superconductors.

The redistribution of charge due to the mixing of empty and doubly occupied states provides a promising direction to experimentally test for composite pairing in the 115 superconductors, which should appear as a sharp redistribution of charge associated with the superconducting transition. Both monopole (f-valence) and quadrupole (electric field gradients) charge effects should be observable, with core-level X-ray spectroscopy or as a shift in the NQR frequency at surrounding nuclei, respectively. We predict a shift with slope +5kHz/K in the NQR frequency of In(1) nuclei in CeCoIn<sub>5</sub>.

Deriving these results in an exact, controlled mean field solution has required the introduction of symplectic Hubbard operators, which maintain the time-reversal properties of SU(2) electrons in the large N limit. It is possible to use these Hubbard operators to develop a dynamical mean field theory treatment of the two-channel Anderson lattice, enabling us to examine composite pairing for N = 2.

In addition to the two-channel Anderson model, the development of symplectic-Hubbard operators allows a controlled treatment of the finite-U Anderson model, which is potentially useful as an impurity solver for dynamical mean field theory. We identify the finite-U model as a special case of our two channel model when the electron and hole fluctuations occur in the same symmetry channel,  $\Gamma_1 = \Gamma_2$ . In the large N limit, this model simply gives a Fermi liquid solution identical to that of the infinite-U model, once the SU(2) gauge invariance is used to eliminate the false appearance of s-wave superconductivity. However, the 1/N corrections to this mean field limit will differ, and an interesting future direction is to use the Gaussian fluctuations to examine the charge fluctuation side peaks.

### Appendix 6A: Full mean field solution

In the main text, we have focused on the superconducting solution, and additionally assumed that the  $\lambda_1$  condition enforcing the absence of on-site pairing will be unnecessary due to the d-wave gap. For completeness, we present here the full mean field equations for uniform solutions - allowing uniform composite density wave solutions in addition to superconductivity. The free energy is given by,

$$F = -NT \sum_{\mathbf{k}\pm} \log 2 \cosh \frac{\beta \omega_{\mathbf{k}\pm}}{2} + \mathcal{N}_s \left[ b_1^2 (E_0 + \lambda_3) + b_2^2 (E_2 + \lambda_3) + a_2^2 (E_2 - \lambda_3) - 2\lambda_1 b_2 a_2 \right],$$
(6.66)
where  $\omega_{\mathbf{k}\pm} = \sqrt{\alpha_k \pm \sqrt{\alpha_k^2 - \gamma_k^2}}$ , and

$$\alpha_{k} = (V_{1\mathbf{k}}b_{1} + V_{2\mathbf{k}}a_{2})^{2} + (V_{2\mathbf{k}}b_{2})^{2} + \frac{1}{2}(\epsilon_{\mathbf{k}}^{2} + \lambda_{3}^{2} + \lambda_{1}^{2})$$
  

$$\gamma_{k}^{2} = [\epsilon_{\mathbf{k}}\lambda_{3} - (V_{1\mathbf{k}}b_{1} + V_{2\mathbf{k}}a_{2})^{2} + (V_{2\mathbf{k}}b_{2})^{2}]^{2} + [2(V_{1\mathbf{k}}b_{1} + V_{2\mathbf{k}}a_{2})V_{2\mathbf{k}}b_{2} - \epsilon_{\mathbf{k}}\lambda_{1}]^{2}(6.67)$$

The mean field equations are found by minimizing the free energy with respect to  $\lambda_3$ ,  $\lambda_1$ ,  $b_1$ ,  $b_2$ , and  $a_2$  and are nearly identical to the two channel Kondo equations, except that  $n_f \neq 1$ . For simplicity

we replace  $\langle x \rangle$  with x. The five mean field equations are given by,

$$\sum_{\pm} \int_{\mathbf{k}} \frac{\tanh \frac{\beta \omega_{\mathbf{k}\pm}}{2}}{2\omega_{\mathbf{k}\pm}} \left\{ \begin{pmatrix} \lambda_{3} \\ \lambda_{1} \\ 2(V_{1\mathbf{k}}b_{1} + V_{2\mathbf{k}}a_{2})V_{1\mathbf{k}} \\ 2(V_{1\mathbf{k}}b_{1} + V_{2\mathbf{k}}a_{2})V_{2\mathbf{k}} \\ 2V_{2\mathbf{k}}b_{2} \end{pmatrix} \pm \frac{A}{\Gamma_{k}} \right\} = \begin{pmatrix} b_{1}^{2} + b_{2}^{2} - a_{2}^{2} \\ -2a_{2}b_{2} \\ 2b_{1}(E_{0} + \lambda_{3}) \\ 2b_{2}\lambda_{1} + 2a_{2}(E_{2} - \lambda_{3}) \\ 2a_{2}\lambda_{1} + 2b_{2}(E_{2} + \lambda_{3}) \end{pmatrix}, \quad (6.68)$$

where

$$A = \begin{pmatrix} \lambda_{3}\alpha_{k} + \epsilon_{k} \left[ (V_{1k}b_{1} + V_{2k}a_{2})^{2} - V_{2k}^{2}b_{2}^{2} - \lambda_{3}\epsilon_{k} \right] \\ \lambda_{1}\alpha_{k} + \epsilon_{k} \left[ 2V_{2k}b_{2}(V_{1k}b_{1} + V_{2k}a_{2}) - \epsilon_{k}\lambda_{1} \right] \\ (V_{1k}b_{1} + V_{2k}a_{2}) \left[ (\epsilon_{k} + \lambda_{3})^{2} + \lambda_{1}^{2} \right] V_{1k} + 2V_{2k}V_{1k}b_{2}\epsilon_{k}\lambda_{1} \\ (V_{1k}b_{1} + V_{2k}a_{2}) \left[ (\epsilon_{k} + \lambda_{3})^{2} + \lambda_{1}^{2} \right] V_{2k} + 2V_{2k}^{2}b_{2}\epsilon_{k}\lambda_{1} \\ 2(V_{1k}b_{1} + V_{2k}a_{2})V_{2k}\epsilon_{k}\lambda_{1} + V_{2k}^{2}b_{2} \left[ (\epsilon_{k} - \lambda_{3})^{2} + \lambda_{1}^{2} \right] \end{pmatrix}.$$
(6.69)

These can be solved numerically, and generally the composite density wave states will be unstable to composite pair superconductivity, although there may be exceptions for special dispersions near the Kondo insulator regime, which we have not explored.

# **Chapter 7**

# The symplectic t-J model

### 7.1 Introduction

Most strongly correlated superconductors, aside from the heavy fermions, arise upon doping strongly correlated magnets. This basic phase diagram is captured by the t - J model, which describes the low energy physics of a one-band Hubbard model where U is so large that double-occupancy is essentially eliminated. The hopping term cannot be simply treated in terms of free electrons, and must instead be represented with Hubbard operators, which act to add and remove spins from a site while respecting the constraint of no double occupancy.

$$H = -\sum_{ij} t_{ij} \left[ X_{\sigma 0}(i) X_{0\sigma}(j) + \text{h.c.} \right] + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j.$$
(7.1)

By defining symplectic Hubbard operators, we can generalize symplectic-N to treat the t-J model. The anti-commutator of two distinct Hubbard operators corresponds to a spin flip operator, and symplectic-N ensures the consistency of the spin and charge fluctuations by insisting that these spin-flips are symplectic spins. This representation requires the introduction of two types of slave bosons, and we show that it generalizes the SU(2) slave boson approach of Wen and Lee [129] to the large N limit. To illustrate the differences between the symplectic-N limit and previous mean field treatments, we examine the  $t - J_2$  model, motivated in part by the iron-pnictide superconductors, which are widely believed to have an  $s_{\pm}$  superconducting order parameter: a 45 degree rotation of the extended s-wave order parameter considered for the  $t - J_1$  model [164]. While d-wave order parameters automatically avoid double occupancy, the effect of Coulomb repulsion on  $s_{\pm}$ superconductors depends strongly on the Fermi surface configurations. Previous strongly correlated approaches have neglected this Coulomb repulsion altogether. Symplectic-N not only includes this Coulomb repulsion, but also allows the nodes of the  $s_{\pm}$  gap to adjust to eliminate any on-site pairing.

### 7.1.1 Brief overview of the iron-based superconductors

The discovery, in March 2008, of a new family of high temperature superconductors based on ironarsenic [205], rather than copper-oxygen planes, and with transition temperatures up to 56K [206], attracted a huge amount of experimental and theoretical attention [108, 109]. Now that the dust has settled a bit, let us make a brief (and therefore incomplete) summary of the relevant physics of these iron-based superconductors.

As with the cuprates, there are several families of iron-pnictide superconductors: the "1111" family,  $RFeAs(O_{1-x}F_x)$  were the first to be discovered [205] and contain  $Gd_{1-x}Th_xFeAsO$ , which has the highest transition temperature,  $T_c = 56K$  [206]; the intermetallic "122" family,  $AFe_2As_2$  (A = Ba,Sr,Ca) are easier to synthesize, but have lower transition temperatures [207, 208]; while the simplest, "11" family, Fe(Se,Te) shows that arsenic may be replaced by another pnictogen [209, 210]. These families share several key characteristics,

- Electronic structure: The parent compounds are semi-metallic, with two (or more) hole pockets near the Γ = (0,0) point and two electron pockets at the M = (π, π) point [211], as shown in Figure 7.1(a). While the cuprates are described by a one-band Hubbard model, here all five iron d-orbitals are important. While many of the Fermi surfaces have a two dimensional character, these materials are more three dimensional than the cuprates.
- Magnetism: The magnetism of these materials has a dual character: part localized and part itinerant [212]. From the localized point of view, superexchange paths through the arsenics generate a  $J_1 - J_2$  Heisenberg model [110, 200], with  $J_2 > J_1/2$  large enough to stabilize the collinear antiferromagnetic state shown in Figure 7.1(b). The same state arises in the itinerant picture due to Fermi surface nesting, however the experimentally determined magnetic moments are much smaller than those predicted in the itinerant picture [212], suggesting that the formation of the moments may be local, but their ordering is itinerant, or perhaps indicating the importance of frustration.

- How strong are the correlations?: There is no consensus on the strength of the correlations. On the side of strong correlations is the argument that the parent compounds are bad metals, with a large resistivity at room temperature, ρ(300K) ~ .5mΩcm suggesting that these are intermediate between weakly correlated metals and strongly correlated Mott insulators [110, 152, 213]. A relatively strong Hund's coupling, J<sub>H</sub> can also help tune these materials towards more localized behavior [200, 214]. However, on the weakly correlated first principles calculations [215, 216, 217], and the large resistivities may be attributable to poor sample quality. Both strongly and weakly correlated theoretical approaches obtain similar phase diagrams.
- Symmetry of the superconducting gap: The order parameter is known to be a spin-singlet [218], but its momentum dependence is still unresolved. The observation of c-axis Josephson currents rules out a d-wave gap [219], leaving two s-wave possibilities, either uniform (s<sub>++</sub>) or with opposite signs on the hole and electron Fermi surfaces (s<sub>±</sub>)[215]. Some experiments (e.g.-ARPES [220]) find nodeless gaps, while others (e.g.-penetration depth [221]) find line or point nodes; these depend on the material, and sometimes the sample. The s<sub>±</sub> gap shown in Figure 7.1(b) may have "accidental nodes," depending on the Fermi surface, which are not guaranteed by symmetry. Both strongly [110, 222, 223] and weakly correlated [215, 224, 225, 226, 227, 228] theoretical approaches suggest the s<sub>±</sub> gap structure, as superconductivity mediated by repulsive interactions with characteristic wavevector Q = (π, 0), generally requires the order parameter to change sign as, Δ<sub>k+Q</sub> = -Δ<sub>k</sub> [109].

We shall take the point of view that these are moderately correlated materials, with weakly and strongly correlated approaches providing complementary pictures. In this chapter, we address the basic question of how strong correlations affect an  $s_{\pm}$  superconductor by examining a simple, one-band t - J model. While this model will never provide a detailed description of the five-band real materials, it can capture the competition between d-wave and s-wave superconductivity, and the effect of the Coulomb repulsion.



Figure 7.1: (a) The basic building block of all the iron-based superconductors is the iron-arsenic plane, shown here. The irons order antiferromagnetically, with a collinear structure favored by the  $J_1 - J_2$  model. (b) A schematic two-dimensional slice through the Brillouin zone shows the generic Fermi surface structure of these materials, which typically have two or more hole pockets around the  $\Gamma = (0,0)$  point and two electron pockets around the  $M = (0,\pi) = (\pi,0)$  point. The  $s_{\pm}$ order parameter changes sign between the electron and hole Fermi surfaces (positive gap regions shown in white, negative regions in gray). The two Fermi surfaces are roughly connected by the  $\mathbf{Q} = (\pi, 0)$  ordering vector, which characterizes both the magnetic and  $s_{\pm}$  superconducting orders. (c) A schematic phase diagram showing how the metallic, antiferromagnetic spin density wave order of the parent compounds yields to superconductivity with either hole or electron doping.

### **7.1.2** t - J model and the Coulomb pseudopotential

On-site pairing is disfavored by the Coulomb pseudopotential, which will cost a bare energy, UN(0), which is, by definition, the average of the Coulomb repulsion,  $V(\mathbf{r}_i - \mathbf{r}_j) = e^2/|\mathbf{r}_i - \mathbf{r}_j|$  over the Fermi sea. However, in the weak coupling limit, where we assume the pairing is mediated by the exchange of a boson with characteristic frequency  $\omega_B$ , the time scale of the pairing is much longer than that of the Coulomb repulsion. In other words, while the effective electron-electron interaction is attractive, it is also retarded, meaning the electrons like to be in the same place, but at different

times, while the Coulomb repulsion is a nearly instantaneous repulsion of two electrons at the same place *and* time. The Coulomb pseudopotential is therefore renormalized [111],

$$\mu^* = \frac{N(0)U}{1 + N(0)U \log \frac{E_F}{\omega_B}}$$
(7.2)

to weak coupling. If  $T_c \propto \omega_B \exp(-1/\lambda)$ , the attractive interaction is reduced by  $\lambda \to \lambda - \mu^*$ , which is usually too weak to destroy superconductivity in the weak coupling limit. In BCS superconductivity, the bosons exchanged are phonons, and the Debye frequency,  $\omega_D \ll E_F$  [14]. However, in more strongly correlated superconductors, the two time scales are of the same order, and the Coulomb pseudopotential can drastically affect the superconductivity. Strongly correlated examples, like the cuprate and heavy fermion superconductors, avoid this problem by developing a d-wave gap, where the pairing with a positive gap is exactly cancelled out by that with a negative gap, as guaranteed by the d-wave symmetry. This choice of gap neutralizes the Coulomb pseudopotential. However, the iron-based superconductors are widely believed to have an  $s_{\pm}$  gap, where the amount of cancellation between positive and negative gap regions is not protected by symmetry, and depends strongly on the Fermi surfaces. When this cancellation is incomplete,  $\mu^*$  reduces  $T_c$  and it is extremely important to consider this effect when mapping out the phase diagram, as it affects the relative stability of s- and d-wave superconducting phases. These effects have been incorporated in the weakly correlated solutions [224, 225, 227, 109], but not yet in the strongly correlated approaches.

Here, we take the strongly correlated limit,  $U \to \infty$  to eliminate double occupancy, which corresponds to taking  $\mu^* \to \infty$ . The Heisenberg model, discussed in Chapter 3 describes the insulating half-filled limit of the t - J model, but generally holes (n < 1) or electrons (n > 1) will hop around in an antiferromagnetic background. As doubly occupied states must be avoided, the hopping is *not* that of free electrons. Rather, it is *projected hopping*, described by the t - J model,

$$H = -\sum_{ij} t_{ij} \left[ X_{\sigma 0}(i) X_{0\sigma}(j) + \text{h.c.} \right] + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j.$$
(7.3)



Figure 7.2: (Left) In the d-wave gap, the cancellation of the superconducting order parameter over the Fermi surface is guaranteed by symmetry, as the positive (blue) regions will exactly cancel the negative (white) regions. (Right) However, in the  $s_{\pm}$  superconducting gap, the amount of cancellation is extremely sensitive to the Fermi surface.

The t - J model is an effective low energy Hamiltonian obtained from the Hubbard model by a canonical transformation similar to the Schrieffer-Wolff transformation [112], and proposed as the relevant model for the cuprate superconductors by Anderson [23]. The Hubbard operators,  $X_{ab} = |a\rangle\langle b|$ , where  $|a\rangle = |0\rangle$ ,  $|\sigma\rangle$  ensure that only empty sites, or holes can hop (or for n > 1that electrons can only hop from doubly occupied sites to singly occupied sites). Here,  $X_{\sigma 0}$  are projected hopping operators, and they satisfy the anti-commutation relations,

$$\{X_{\sigma 0}, X_{0\sigma'}\} = S_{\sigma\sigma'} + \left(X_{00} + \frac{X_{\tau\tau}}{2}\right)\delta_{\sigma\sigma'},\tag{7.4}$$

where  $S_{\sigma\sigma'}$  flips the spin;  $S_{\sigma\sigma'}$  is the traceless form of the Hubbard operator  $X_{\sigma\sigma'}$ , and  $X_{00}$  is a projection operator into the empty state.

Exact solutions of the t - J model are unavailable in more than one dimension, and the typical approach is to write down a mean field solution using the slave boson approach [229, 165, 129, 230, 231], which divides the electron into charged, but spinless holons and neutral spinons. The most

common choice is the U(1) slave boson representation,

$$X_{\sigma 0} = f_{\sigma}^{\dagger} b, \tag{7.5}$$

so-called because it is invariant under U(1) gauge transformations. However, mean field solutions will in general lose some of the properties of the full model, and may not maintain the  $\mu^* \to \infty$ limit. One way to generate mean-field solutions is to extend the SU(2) spin group of the t - Jmodel to some N component group. When incorporating a large N treatment of the hopping term, one must be careful that the two terms are consistent: that the charge fluctuations described by the t term generate the spin fluctuations in the Heisenberg term. Examining the U(1) slave bosons, we find that they give rise to SU(N) spin fluctuations,

$$\{X_{\alpha 0}, X_{0\beta}\} = \underbrace{f_{\alpha}^{\dagger} f_{\beta}}_{\mathrm{SU(N)spins}} + b^{\dagger} b \delta_{\alpha \beta}, \tag{7.6}$$

and the large N limit of the SU(N) t - J model can be written,

$$H_{SU(N)} = -\sum_{\langle ij\rangle} \frac{t_{ij}}{N} f_{i\alpha}^{\dagger} b_i b_j^{\dagger} f_{j\alpha} + \sum_{ij} \frac{J_{ij}}{N} \left( f_{i\alpha}^{\dagger} f_{j\alpha} \right) \left( f_{j\beta}^{\dagger} f_{i\beta} \right).$$
(7.7)

Decoupling the J term will yield a dispersion for the spinons, but no pairing. There is no superconductivity in this large N limit. In fact, our introduction of symplectic Hubbard operators provides the first consistent, superconducting large N solution of the t - J model.

### **7.2** The symplectic t - J model

A superconducting large N limit requires a proper definition of time-reversal, as Cooper pairs can only form between time-reversed pairs of electrons. As we have shown in Chapter 2, the inversion of spins under time-reversal is equivalent to symplectic symmetry, and the only way to preserve
time-reversal in the large N limit is to use symplectic spins,

$$S_{\alpha\beta} = f_{\alpha}^{\dagger} f_{\beta} - \tilde{\alpha} \tilde{\beta} f_{-\beta}^{\dagger} f_{-\alpha}, \qquad (7.8)$$

where  $\alpha$  ranges from -N/2 to N/2 and  $\tilde{\alpha} = \text{sgn}(\alpha)$ . Here we use the fermionic representation because we are interested in the doped spin liquid states that become superconductors. In most mean field treatments of the t - J model, the electron is separated into charged holons and spin 1/2 spinons. Either the holon or the spinon may be taken to be bosonic; both representation are exact for N = 2, but the bosonic holon condenses to give coherent Fermi liquids and superconductors in the mean-field limit, and this is the usual choice to treat superconductivity, although it cannot describe antiferromagnetism. First, we will briefly discuss the fermionic representation of the symplectic Heisenberg model,

$$H_{spin} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j = -\sum_{ij} \frac{J_{ij}}{N} \left[ (f_{i\alpha}^{\dagger} f_{j\alpha}) (f_{j\beta}^{\dagger} f_{i\beta}) + (\tilde{\alpha} f_{i\alpha}^{\dagger} f_{j-\alpha}^{\dagger}) (\tilde{\beta} f_{j\beta} f_{i-\beta}) \right], \quad (7.9)$$

and how it differs from the bosonic approach discussed in Chapter 3. The most important property of this large N limit is the SU(2) symmetry of the symplectic spins: a continuous particle-hole symmetry derived from the neutrality of the symplectic spins,  $f_{\alpha} \rightarrow u f_{\alpha} + v \tilde{\alpha} f_{-\alpha}^{\dagger}$ . This symmetry was first noticed by Affleck *et al.* [140] for the SU(2) Heisenberg model, but here we see that it is present for all N. The quartic terms may be decoupled as before,

$$\frac{J_{ij}}{N}\vec{S}_i \cdot \vec{S}_j = \bar{\chi}_{ij}f_{j\beta}^{\dagger}f_{i\beta} + \bar{\Delta}_{ij}\tilde{\beta}f_{j\beta}f_{i-\beta} + \text{h.c.} + \frac{N}{J_{ij}}\left(|\Delta_{ij}|^2 + |\chi_{ij}|^2\right), \tag{7.10}$$

where both  $\chi$  and  $\Delta$  are SP(N) singlets. In the bosonic Heisenberg model discussed in Chapter 3, the particle-hole,  $h_{ij} = b_{i\alpha}^{\dagger}b_{j\alpha}$  and particle-particle,  $\Delta_{ij} = \tilde{\alpha}b_{i\alpha}^{\dagger}b_{j-\alpha}^{\dagger}$  enter into the Hamiltonian with different signs  $(-h^2/J + \Delta^2/J)$  and represent different physics: h indicates ferromagnetism, while  $\Delta$  indicates antiferromagnetism. However, in the fermionic model, both  $\chi^2$  and  $\Delta^2$  enter with the same sign: both represent antiferromagnetism, and they may be transformed into one another by the SU(2) gauge symmetry. The Hamiltonian can be written compactly in terms of Nambu spinors,  $\tilde{f}^{\dagger} = (f^{\dagger}_{\alpha}, \tilde{\alpha}f_{-\alpha}),$ 

$$H_{spin} = \sum_{ij} \tilde{f}_{i}^{\dagger} U_{ij} \tilde{f}_{j} + \frac{N}{J_{ij}} \left( |\Delta_{ij}|^{2} + |\chi_{ij}|^{2} \right)$$
(7.11)

where  $U_{ij}$  is an SU(2) matrix,

$$U_{ij} = \begin{pmatrix} -\chi_{ij} & \Delta_{ij} \\ \bar{\Delta}_{ij} & \bar{\chi}_{ij} \end{pmatrix}.$$
 (7.12)

The SU(2) gauge transformation becomes  $\tilde{f}_i \to g_i \tilde{f}_i$  and  $U_{ij} \to g_i^{\dagger} U_{ij} g_j$ , where  $g_i$  is an SU(2) matrix. The mean field theory for the fermionic square lattice Heisenberg model has been discussed extensively [38, 140, 231], and we just summarize the results here, as the  $J_2$  states of interest are a 45° rotation of these states. While there appear to be many Ansatzes for mean field spin-liquid states, the SU(2) symmetry means that many of these are identical [140, 231]. For example, the s-wave ( $\Delta_{ij} = \Delta$ ) and d-wave ( $\Delta_x = -\Delta_y = \Delta$ ) pairing Ansatzes are gauge equivalent not only to each other, but also to the uniform  $\chi$  phase, while the s + id-wave superconductor ( $\Delta_x = -i\Delta_y = \Delta$ ) is gauge equivalent to the  $\pi$ -flux phase,  $\chi_{ij} = e^{i\pi/4}\chi$ . The ground state for this model is not actually a spin-liquid at all, but a spin-Peierls state that breaks translational symmetry and generates a spin gap  $\propto J$  in addition to the charge gap  $\propto U$  [38]. For larger dopings, the spin-Peierls phase gives way to one of the spin liquid phases. The fermionic representation cannot really capture the ground state of the square Heisenberg lattice anyway, which is not a spin-liquid nor a spin-Peierls state, but rather a long range ordered antiferromagnet. These uniform Ansatzes will, however, be reasonable for the moderate dopings that give rise to superconductivity.

Introducing doping means introducing a small number of mobile empty states. When an electron hops on and off a site, it can flip the spin of the site, and consistency requires that these spin flips be symplectic as well,

$$\{X_{\alpha 0}, X_{0\beta}\} = S_{\alpha\beta} + \left(X_{00} + \frac{X_{\gamma\gamma}}{N}\right)\delta_{\alpha\beta},\tag{7.13}$$

where  $S_{\alpha\beta}$  is a symplectic spin. When we represent the Hubbard operators with slave bosons, the



Figure 7.3: Charge fluctuations, where an electron hops off,  $X_{0\sigma}$  and then on again,  $X_{\sigma'0}$  generate spin fluctuations,  $X_{\sigma\sigma'}$ . In order to have a consistent large N limit, the spin group of these spin fluctuations must be the same as the spins described by the Heisenberg term.

symplectic projected creation operators take the following form,

$$X_{\alpha 0} = f_{\alpha}^{\dagger} b + \tilde{\alpha} f_{-\alpha} a. \tag{7.14}$$

Symplectic symmetry requires the introduction of *two* slave bosons to reflect the neutrality of the spin, and we recognize these Hubbard operators as the SU(2) slave boson approach introduced by Wen and Lee [129]. However, here the SU(2) symmetry appears for all N, as a consequence of the time-inversion properties of symplectic spins. The Nambu notation,  $B^{\dagger} = (b^{\dagger}, a^{\dagger})$  simplifies the expressions, as  $X_{\alpha 0} = \tilde{f}^{\dagger}_{\alpha} B$  and the hopping term of symplectic-N t - J model can be written,

$$H_{t} = -\sum_{ij} \frac{t_{ij}}{N} \left( \tilde{f}_{i\alpha}^{\dagger} B_{i} B_{j}^{\dagger} \tilde{f}_{j\alpha} + \text{h.c.} \right)$$
  
$$= -\sum_{ij} \frac{t_{ij}}{N} \left[ \left( f_{i\alpha}^{\dagger} b_{i} + \tilde{\alpha} f_{i-\alpha} a_{i} \right) \left( f_{j\alpha} b_{j}^{\dagger} + \tilde{\alpha} f_{j-\alpha}^{\dagger} a_{j}^{\dagger} \right) + \text{h.c.} \right].$$
(7.15)

To restrict the spin and charge fluctuations to the physical subspace, this Hamiltonian must be supplemented by the constraint,  $\vec{S}_j^2 + \vec{\Psi}_j^2 = N/2(N/2+2)$  is fixed, where  $\vec{\Psi}_j = \tilde{f}_{j\alpha}^{\dagger} \vec{\tau} \tilde{f}_{j\alpha}$  is the isospin vector (see Chapter 2 for more details). Setting the two types of charge fluctuations equal to one another,  $B^{\dagger}\vec{\tau}B=-\vec{\Psi}$  requires an SU(2) constraint at every site,

$$b_{j}^{\dagger}b_{j} - a_{j}^{\dagger}a_{j} + f_{j\alpha}^{\dagger}f_{j\alpha} = N/2$$
  

$$b_{j}^{\dagger}a_{j} + \tilde{\alpha}f_{j\alpha}^{\dagger}f_{j-\alpha}^{\dagger} = 0$$
  

$$a_{j}^{\dagger}b_{j} + \tilde{\alpha}f_{j-\alpha}f_{j\alpha} = 0.$$
(7.16)

Under this constraint, there is only a single, physical empty state, which is

$$|0\rangle = \left(b^{\dagger} + a^{\dagger}\Psi^{\dagger}\right)|\Omega\rangle, \qquad (7.17)$$

for N = 2. The physical interpretation of these terms becomes clearer if we pick a particular gauge. Since we only have two flavors of bosons and N flavors of fermions, the only way the bosons can contribute in the large-N limit is to condense. As the bosons condense at all temperatures, the only possible states are Fermi liquids and superconductors. While this situation is clearly unphysical, and will be resolved with 1/N corrections, it does allow us to fix the gauge in a particularly simple way by setting a = 0 and condensing only the b bosons.  $\langle b \rangle$  must be fixed to Nx/2 because the bosons carry all the charge in the system, Nx/2, where the factor of N/2 makes the doping extensive in N. In this gauge, the constraint simplifies to,

$$f_{j\alpha}^{\dagger} f_{j\alpha} = \frac{N(1-x)}{2}$$
$$\tilde{\alpha} f_{j\alpha}^{\dagger} f_{j-\alpha}^{\dagger} = 0$$
$$\tilde{\alpha} f_{j-\alpha} f_{j\alpha} = 0, \qquad (7.18)$$

which is enforced by a trio of Lagrange multipliers  $\vec{\lambda} = (\lambda_3, \lambda_+, \lambda_-)$ . The first term is clearly recognizable as Luttinger's theorem. When we fix the gauge, we see that symplectic-N is identical to U(1) slave bosons [229, 165, 230], except for the important additional constraints eliminating s-wave pairing. For the d-wave superconductors, like the cuprates, that have been the main focus of previous t-J model studies, these constraints are satisfied automatically, and at the mean-field level, there is no difference between the symplectic-N limit and many of the previously considered uncontrolled mean field theories. How the symplectic 1/N corrections change this phase diagram is an interesting open problem, especially as reducing the coherence should generate a pseudogap phase of preformed pairs between the mean-field  $T_c$  and the onset of superconducting coherence. However, for now we focus on the large N limit, where for  $s_{\pm}$  superconductors like the iron-pnictides, these additional constraints enforce the Coulomb pseudopotential,  $\mu^*$  and have an important effect on the stability of  $s_{\pm}$  superconductivity.

Once the bosons are condensed, and the Heisenberg term decoupled, the spinon Hamiltonian is quadratic,

$$H = \sum_{ij} \tilde{f}_{i\alpha}^{\dagger} \left( -\frac{xt_{ij}}{2} \tau_3 + U_{ij} \right) \tilde{f}_{j\alpha} + \frac{N}{J_{ij}} \left( |\Delta_{ij}|^2 + |\chi_{ij}|^2 \right),$$
(7.19)

where  $\chi_{ij}$  generates a dispersion for the spinons, while  $\Delta_{ij}$  pairs them. The physical electron,  $c^{\dagger} \sim \langle b \rangle f^{\dagger}$  will hop coherently, forming a Fermi liquid when  $\Delta_{ij} = 0$  and superconducting when  $\Delta_{ij} \neq 0$ . The phase diagram is obtained by minimizing the free energy with respect to the bond variables,  $\chi_{ij}$  and  $\Delta_{ij}$ , while simultaneously enforcing the SU(2) constraint on average with the Lagrange multipliers,  $\vec{\lambda}$ . These approximations become exact in the large N limit.



Figure 7.4: Gap symmetries for the  $J_1 - J_2$  model

In general, the bond variables will take different values,  $\chi_{\eta}$  and  $\Delta_{\eta}$  on different links,  $\eta = (ij)$ . For example, in the  $J_1 - J_2$  model, we will assume  $\chi = \chi_1$  on all nearest neighbor  $(J_1)$  links and  $\chi = \chi_2$  on all next-nearest neighbor  $(J_2)$  links. When these are Fourier transformed,  $\chi_{\mathbf{k}} =$  $\sum_{\eta} \chi_{\eta} \gamma_{\eta \mathbf{k}} \equiv 2\chi_1(c_x + c_y) + 4\chi_2 c_x c_y$ , where we have defined  $c_{\zeta} = \cos k_{\zeta} a$ , and a is the lattice spacing. The pairing may be either s-wave or d-wave on a set of links,  $\eta = 1, 2$ , so we consider  $\Delta_{\mathbf{k}} = \sum_{\eta, s/d} \Delta_{\eta s/d} \delta_{\eta s/d\mathbf{k}}$ , where for the  $J_1 - J_2$  model we have the following four possibilities

$$2\Delta_{1s}(c_x + c_y) \qquad \text{Extended } s$$

$$2\Delta_{1d}(c_x - c_y) \qquad d_{x^2 - y^2}$$

$$2\Delta_{2s}(c_{x+y} + c_{x-y}) = 4\Delta_{2s}c_xc_y \qquad s_{\pm}$$

$$2\Delta_{2d}(c_{x+y} - c_{x-y}) = -4\Delta_{2d}s_xs_y \qquad d_{xy}, \qquad (7.20)$$

whose nodes are shown in Figure 7.4. Complex linear combinations of these are also possible, but tend to be unstable, so we assume both  $\chi$  and  $\Delta$  are real. The full Hamiltonian takes the form,

$$H = \sum_{\mathbf{k}} \tilde{f}_{\mathbf{k}\alpha}^{\dagger} \left( -\frac{x\epsilon_{\mathbf{k}}}{2} + U_{\mathbf{k}} + \lambda_{3}\tau_{3} + \lambda_{1}\tau_{1} \right) \tilde{f}_{\mathbf{k}\alpha} + \mathcal{N}_{s} \sum_{\eta} \frac{N}{J_{\eta}} \left( |\Delta_{\eta}|^{2} + |\chi_{\eta}|^{2} \right) - \frac{4N\mathcal{N}_{s}x\lambda_{3}}{2}$$
(7.21)

where  $\epsilon_{\mathbf{k}}$  and  $U_{\mathbf{k}}$  are the Fourier transforms of  $t_{ij}$  and  $U_{ij}$ , respectively, and  $\mathcal{N}_s$  is the number of sites.  $\lambda_1 = \frac{1}{2}(\lambda_+ + \lambda_-)$ , and  $\lambda_2 = \frac{-i}{2}(\lambda_+ - \lambda_-)$  is automatically zero if  $\Delta$  is real. This Hamiltonian can be diagonalized, and the spinons integrated out to yield the free energy,

$$F[\chi_{\eta}, \Delta_{\eta}, \lambda_{1}, \lambda_{3}] = -2NT \sum_{\mathbf{k}} \log 2 \cosh \frac{\beta \omega_{\mathbf{k}}}{2} + \mathcal{N}_{s} \sum_{\eta} \frac{4N}{J_{\eta}} \left( |\Delta_{\eta}|^{2} + |\chi_{\eta}|^{2} \right) - \frac{N\mathcal{N}_{s} x \lambda_{3}}{2},$$
(7.22)

where

$$\omega_{\mathbf{k}} = \sqrt{\alpha_{\mathbf{k}}^2 + \beta_{\mathbf{k}}^2}, \quad \text{where} \ \ \alpha_{\mathbf{k}} = \lambda_3 - \frac{x\epsilon_{\mathbf{k}}}{2} + \chi_{\mathbf{k}}, \quad \beta_{\mathbf{k}} = \lambda_1 + \Delta_{\mathbf{k}}.$$
(7.23)

This leads to the four mean field equations,

$$\frac{\partial F}{\partial \chi_{\eta}} = \int_{\mathbf{k}} \frac{\tanh \frac{\beta \omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \alpha_{\mathbf{k}} \gamma_{\eta \mathbf{k}} - \frac{4}{J_{\eta}} = 0$$
$$\frac{\partial F}{\partial \Delta_{\eta}} = \int_{\mathbf{k}} \frac{\tanh \frac{\beta \omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \beta_{\mathbf{k}} \delta_{\eta \mathbf{k}} - \frac{4}{J_{\eta}} = 0$$
$$\frac{\partial F}{\partial \lambda_{3}} = \int_{\mathbf{k}} \frac{\tanh \frac{\beta \omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \alpha_{\mathbf{k}} - x/2 = 0$$

$$\partial F/\partial \lambda_1 = \int_{\mathbf{k}} \frac{\tanh \frac{\beta \omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \beta_{\mathbf{k}} = 0,$$
 (7.24)

where  $\int_{\mathbf{k}} = \int \frac{dx}{2\pi} \int \frac{dy}{2\pi}$ . The first three mean field equations are identical to those derived for U(1) slave bosons, when the spins are decoupled into both  $\chi$  and  $\Delta$  terms [165]. However, the last equation enforces  $\mu^* \to \infty$  by forcing the average pair density over the Fermi surface to be zero,

$$\int_{\mathbf{k}} \tanh \frac{\beta \omega_{\mathbf{k}}}{2} \left( \frac{\lambda_1 + \Delta_{\mathbf{k}}}{2\omega_{\mathbf{k}}} \right) = 0.$$
(7.25)

When  $\Delta_k$  is d-wave, the integral vanishes by symmetry for  $\lambda_1 = 0$ . For the simple  $t_1 - J_1$  model, the form factors  $\epsilon_k$ ,  $\gamma_{1k}$  and  $\delta_{1sk}$ , and thus  $\omega_k$  are *all* proportional to  $c_x + c_y$ . The integral, (7.25) only vanishes when both  $\lambda_1$  and  $\Delta_{1s}$  do, completely eliminating any s-wave phase. For more complicated models,  $\lambda_1$  acts as a pair chemical potential, adjusting the gap to eliminate the onsite s-wave pairing. This adjustment costs energy and typically depresses the s-wave transition temperature.

#### 7.3 Mean field solutions

Now let us consider a few simple models in order to see this constraint in action. First, we consider the  $t_1 - J_2$  model, shown in Figure 7.5 (a), which is the simplest model containing  $s_{\pm}$  pairing. Here, the next-nearest neighbor coupling,  $J_2$  can induce either  $s_{\pm}$  or  $d_{xy}$  pairing, while the nearestneighbor hopping,  $t_1$  leads to a single large Fermi surface, with occupation 1 - x. We will restrict ourselves to hole doping, where x > 0. Both the s-wave and d-wave transition transition temperatures can be found by setting  $\Delta_{2(s,d)} = 0$  in the mean field equations, (7.24), with the appropriate form-factor. These equations are then solved for  $\lambda_1, \lambda_3, \chi$  and  $T_c$ . In order to elucidate the effects of the pair chemical potential,  $\lambda_1$ , we have done this calculation both with and without the  $\lambda_1$  constraint. Without the pair chemical potential, the solution is identical to previous U(1) slave boson mean field theories. The d-wave transition temperature is, of course, unaffected by  $\lambda_1$ , but the swave transition temperature is reduced when  $\lambda_1$  is included. However, the pair chemical potential does not completely eliminate the  $s_{\pm}$  pairing, as it does for the  $t_1 - J_1$  model. Here, it is able to



Figure 7.5: (a) The  $t_1 - J_2$  model. (b) The Fermi surface (holes shown in red) for the  $t_1 - J_2$  model at intermediate doping. In the superconducting state, the gap nodes follow the dashed lines, separating regions of positive and negative gap. (c) The superconducting transition temperatures for the  $t_1 - J_2$  model both with (solid lines) and without the  $\lambda_1$  constraint(dashed lines), for s-wave (blue) and d-wave (green) superconductivity. d-wave superconductivity is unaffected by the Coulomb repulsion, while the s-wave transition temperature is decreased. (Calculated for  $t_1/J_2 = 10$ ).

adjust the gap nodes to eliminate the Coulomb repulsion by balancing the regions of positive and negative gap, as shown in Figure 7.5(b). Given that there is only a single Fermi surface, this process necessarily introduces line nodes: lines on the three dimensional Fermi surface where the gap changes sign. Experimentally, it would be difficult to distinguish such an s-wave state from a dwave state. However, in gaining line nodes, s-wave pairing loses its usual energetic advantage over d-wave pairing: the complete gapping of the Fermi surface. Thus, there is no  $s_{\pm}$  superconductivity in the  $t_1 - J_2$  model.

To allow the possibility of a stable  $s_{\pm}$  superconducting phase, we must consider a situation with multiple Fermi surfaces. Such a Fermi surface may be obtained even within a one-band model by carefully tuning the hoppings, although the Fermi surface structure is unfortunately quite sensitive to the doping level within this one band model. For an intermediate range of dopings, the  $t_1$  –



Figure 7.6: (a) The  $t_1 - t_2 - t_3 - J_2$  model. (b) The Fermi surface (holes shown in red) for the  $t_1 - t_2 - t_3 - J_2$  model at intermediate doping, showing the two Fermi pockets. The gap nodes of the superconducting state are indicated with dashed lines. ( $t_1 = 2J_2$ ,  $t_2 = -6J_2$ , and  $t_3 = 8J_2$ ). (c) The doping phase diagram for the  $t_1 - t_2 - t_3 - J_2$  model, calculated with the  $\lambda_1$  constraint. There is a quantum phase transition between d-wave pairing (green) and s-wave pairing (blue) as doping increases and the s-wave states become fully gapped.

 $t_2 - t_3 - J_2$  model shown in Figure 7.6(a) has two hole pockets, surrounding the  $\Gamma$  and M points, respectively. Now it is possible for  $s_{\pm}$  superconductivity to gap out the two Fermi surfaces with opposite signs. We again calculate the s-wave and d-wave transition temperatures with and without the  $\lambda_1$  constraint, which yields the phase diagram shown in Figure 7.6(c). The nodal structure of the  $s_{\pm}$  state is strongly dependent on doping, through the sensitivity of the Fermi surfaces. For small x, it contains line nodes, favoring the d-wave state, but as the doping increases, the line nodes merge to become point nodes and eventually vanish. When this change occurs, s-wave superconductivity is favored over the d-wave, giving rise to a d-wave to s-wave quantum phase transition as a function of doping.

In the  $s_{\pm}$  phase, the pair chemical potential naturally generates two gaps,  $\lambda_1 \pm |\Delta|$  on the two different Fermi surfaces, as seen in some of the iron-based superconductors[109]. The difference

between the two gaps increases with the difference in Fermi surface occupation, so in a more realistic model, with one electron and one hole Fermi surface exactly balanced at half filling, we predict that the difference between the two gaps increases with doping.

These models may easily be made more complex by adding nearest-neighbor exchange,  $J_1$ , or multiple, independent bands, but these do not change the qualitative conclusions. Treating multiple bands properly requires adding a ferromagnetic Hund's coupling,  $-|J_H|\vec{S}_{\mu i} \cdot \vec{S}_{\mu' i}$  between spins in different bands,  $\mu \neq \mu'$  on the same site, and we do not yet know how to handle a ferromagnetic interaction with fermionic spinons, although the infinite  $J_H$  limit may prove a more tractable possibility. However, the current models are sufficient to illustrate the importance of incorporating the Coulomb pseudopotential for calculations on strongly correlated  $s_{\pm}$  superconductors, especially when examining the nodal structure, and are not meant to be a detailed model of the iron-pnictides.

### 7.4 Conclusions

The doped semi-metal Fermi surface structure of the iron-based superconductors favors the  $s_{\pm}$  pairing state, which retains the ability to fully gap out the Fermi surface while avoiding Coulomb repulsion by switching signs between the two Fermi surfaces. We have introduced symplectic Hubbard operators to properly treat the effect of the Coulomb pseudopotential on the superconducting states of the t - J model within a well-defined large N limit. While the Coulomb pseudopotential has been incorporated into most weakly correlated approaches to the iron-based superconductors, this work is the first time the Coulomb pseudopotential has been included in a strongly correlated model, where it is arguably more important. We find that the mean field phases contain a pair chemical potential that adjusts the nodes of the  $s_{\pm}$  gap to eliminate the Coulomb repulsion by balancing the positive and negative gap regions of the Fermi surfaces. This pair chemical potential naturally accounts for the diversity of gaps found in the iron-based superconductors: line nodes, point nodes, and multiple gaps are all present in our large N limit at different dopings.

The cuprate and iron-pnictide superconductors both have rich phase diagrams, containing incoherent strange metals and pseudogap phases, none of which can be captured within the large N limit of the symplectic-N t - J model because the bosons are always condensed. Reducing this coherence is essential to gaining a real understanding of these phase diagrams, and this reduction can be done in two ways: either by calculating the symplectic 1/N corrections to Gaussian order, or by artificially enhancing the number of bosons, K such that K/N remains finite in the large N limit, which corresponds to generalizing the isospin from SU(2) to either SU(K) or SP(K).

## References

- [1] P.W. Anderson, Science 177, 393 (1972).
- [2] B. A. Bernevig, T. L. Hughes, S.-C. Zhang, Science 314, 1757 (2006).
- [3] L.D. Landau, Sov. Phys. JETP 3, 920(1957).
- [4] D. Bohm and D. Pines, Phys. Rev. 92, 609(1953).
- [5] S. Tomonaga, Prog. in Theor. Phys. 5, 544 (1950).
- [6] J. M. Luttinger, J. of Math. Phys. 4, 1154 (1963).
- [7] H.L. Stormer, Rev. Mod. Phys. 71, 875889 (1999).
- [8] C. Nayak et al., Rev. Mod. Phys. 80, 1083 (2008).
- [9] P.G. Pagliuso *et al.*, Physica B **320**, 370(2002).
- [10] H. Takagi et al., Phys. Rev. Lett. 69, 2975(1992).
- [11] N.F. Mott, R. Peierls, Proc. Phys. Soc. London 49, 72 (1937).
- [12] N.F. Mott, Proc. Phys. Soc. London A62, 416(1949).
- [13] Y. Onuki, Y. Shimizu and T. Komatsubara, J. Phys. Soc. Jpn. 53, 1210 (1984).
- [14] J. Bardeen, L.N. Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175-1204(1957).
- [15] For a review see, for example, P. A. Lee, Rep. Prog. Phys. 71, 012501 (2008).
- [16] E. Witten, Nucl Phys. B 160, 57 (1979).
- [17] P.W. Anderson, Mater. Res. Bull. 8, 153(1973).
- [18] L. N. Cooper, Phys. Rev. 104 4: 1189 (1956).
- [19] P. W. Anderson, Phys. Rev. 115, 2 (1959).
- [20] R. Moessner and A. Ramirez, Physics Today p. 24 February, 2006.
- [21] G. Misguich, arXiv:0809.2257(2008) and references therein.
- [22] G. Misguich and C. Lhuillier, "Frustrated spin systems", H. T. Diep editor, World-Scientific (2005) and references therein.
- [23] P.W. Anderson, Science 235, 118(1987).
- [24] P.W. Anderson, G. Baskaran, Z. Zou and T. Hsu, Phys. Rev. Lett. 58, 2790(1987).
- [25] N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17 1133(1966).
- [26] P. Chandra, P. Coleman and A. I. Larkin, Phys. Rev. Lett. 64, 88 (1990).

- [27] J. Villain, J. Phys.(Paris) 38 26(1977); J. Villain, J. Phys.(Paris)41 1263(1980).
- [28] E. Shender, Zh. Eksp. Teor. Fiz. 83, 326(1982).
- [29] C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989).
- [30] T.H. Berlin and M. Kac, Phys. Rev. 86, 821(1952).
- [31] P.W. Anderson, Phys. Rev. 86, 694 (1952).
- [32] F. Dyson, Phys. Rev. 102, 1217 (1956).
- [33] S.V.Maleev, Zh. Eksp. Teor. Fiz. 33, 1010 (1957).
- [34] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. 60, 1057(1988); Phys. Rev. B 39, 2344(1989).
- [35] F.D.M. Haldane, Phys. Rev. Lett. 61, 1029(1988).
- [36] A. D'Adda, M. Lüscher, and P. Di Vecchia, Nucl. Phys. B 146, 63(1978).
- [37] I. Affleck, Phys. Rev. Lett. 54, 966(1985).
- [38] I. Affleck and J.B. Marston, Phys. Rev. B 37, 3774(1988).
- [39] Y. Ran and X.G. Wen, cond-mat/0609620v3 (2006)
- [40] M. Hermele, T. Senthil, M. P. A. Fisher, P. A. Lee, N. Nagaosa, and X.-G. Wen, Phys. Rev. B 70, 214437 (2004).
- [41] J. Schwinger, Quantum Theory of Angular Momentum, edited by L. Biedenharn and H. Van Dam (Academic, New York, 1965).
- [42] N. Read and Subir Sachdev, Phys. Rev. Lett. 66, 1773 (1991);
- [43] J. Kondo, Prog. Theo. Phys. 28, 772 (1962).
- [44] J. Kondo, Prog. Theo. Phys. 32, 37 (1964).
- [45] A.A. Abrikosov, Physics 2, 5, (1965).
- [46] H. Suhl, Phys. Rev. 38A, 515 (1965).
- [47] D.C. Langreth, Phys. Rev. 150, 516518 (1966).
- [48] P. Coleman, Handbook of Magnetism and Advanced Magnetic Materials. Edited by Helmut Kronmuller and Stuart Parkin. Vol 1: Fundamentals and Theory. John Wiley and Sons, 95-148 (2007).
- [49] A. Sumiyama et al., J. Phys. Soc. Jpn. 55, 1294 (1986).
- [50] F. Steglich et al., Phys. Rev. Lett 43, 1892(1976).
- [51] P. W. Anderson, Phys. Rev. 124, 41 (1961).
- [52] J.R. Schrieffer & P.A. Wolff, Phys. Rev. 149, 491(1966).

- [53] B. Coqblin, and J. R. Schrieffer, Phys. Rev. 185, 847 (1969).
- [54] K. G. Wilson Rev. Mod. Phys. 47, 773 (1976).
- [55] N. Andrei, K. Furuya, and J. Lowenstein, Rev. Mod. Phys 55, 331 (1983).
- [56] A. Tsvelik, and P. Wiegmann, Adv. Phys. 32, 453 (1983).
- [57] P. Nozières, Ann. Phys. Paris 10, 19 (1985).
- [58] S. Burdin, A. Georges, and D. R. Grempel, Phys. Rev. Lett 85, 1048 (2000).
- [59] T. Kasuya, Prog. Theo. Phys. 16, 45 (1956).
- [60] S. Doniach, Physica B & C **91**, 231(1977).
- [61] P. Nozières, Journal de Physique C **37**, 1(1976).
- [62] P. Nozières and A. Blandin, Journal de Physique 41, 193 (1980).
- [63] H. Shishido et al., J. Phys. Soc. Jap. 7, 162173(2002).
- [64] M.A. Ruderman & C. Kittel, Phys. Rev. 96, 99(1954); T. Kasuya, Prog. Theor. Phys. 16, 45 (1956); K. Yosida, Phys. Rev. 106, 893 (1957).
- [65] P. Gegenwart, Q. Si and F. Steglich, Nat. Phys. 4, 186 (2008).
- [66] K. Miyake, S. Schmitt-Rink and C. M. Varma, Phys. Rev. B 34, 6554 (1986).
- [67] M. T. Beal Monod, C. Bourbonnais, and V. Emery, Phys. Rev. B. 34 7716-7720, (1986).
- [68] D. J. Scalapino, D. J., E. Loh and J. E. Hirsch, Phys. Rev. B 34, 8190-8192, (1986).
- [69] Y. Kohori, T. Kohara, H. Shibai, Y. Oda, Y. Kitaoka, K. Asayama, J. Phys. Soc. Jpn. 57, 395 (1988).
- [70] G.R. Stewart, Rev. Mod. Phys 56, 755(1984).
- [71] R. Joynt and L. Taillefer, Rev. Mod. Phys. 74, 235 (2002).
- [72] C. Pfleiderer, Rev. Mod. Phys. 81, 1551 (2009).
- [73] N. Mathur *et al.*, Nature **394**,39 (1998).
- [74] P. Monthoux, and G. G. Lonzarich, Phys. Rev. B 63, 054529-054538 (2001).
- [75] P. Monthoux, and G. G. Lonzarich, Phys. Rev. B 66, 224504 (2002).
- [76] C. Petrovic *et al.*, J. Phys.: Condens. Matter **13**, L337(2001).
- [77] H. Hegger et al., Phys. Rev. Lett. 84, 4986(2000).
- [78] C. Petrovic *et al.*, Europhysics Letters **53**, 354(2001).
- [79] J. L. Sarrao et al., Nature (London) 420, 297-299 (2002).
- [80] F. Wastin, P. Boulet, J. Rebizant, E. Colineau, and G. H. Lander, J. Phys.: Condens. Matter 15, S2279-S2285 (2003).

- [81] D. Aoki *et al.*, Journal of the Physical Society of Japan, **76**, 063701-063704 (2008).
- [82] P. H. Frings, J. J. M. Franse, F. R. de Boer, and A. Menovsky, J. Magn. Magn. Mater. 31, 240 (1983).
- [83] C. Petrovic et al., J. Phys.: Condens. Matter 13, L337(2001).
- [84] N. Andrei, C. Destri, Phys. Rev. Lett. 52, 364 (1984).
- [85] A. M. Tsvelik, P. B. Wiegmann, J. Stat. Phys. 38, 125 (1985).
- [86] I. Affleck, A. W. W. Ludwig Nucl. Phys. B 352, 849 (1991); ibid. 360,641 (1991).
- [87] See D. L. Cox and A. Zawadowski, "Exotic Kondo effects in metals: magnetic ions in a crystalline electric field and tunneling centers", Advances in Physics, 47 599 (1998) and references therein.
- [88] V. J. Emery, S. Kivelson, Phys. Rev. B 46, 10812 (1992).
- [89] D. L. Cox and M. Jarrell, J. Phys.: Condens. Matter 8, 9825-9853 (1996).
- [90] M. Jarrell, H. Pang and D. L. Cox, Phys. Rev. Lett 78, 1996-2000 (1997).
- [91] B.A. Jones and C.M. Varma, Phys. Rev. B 40, 324(1989).
- [92] J. Gan, Phys. Rev. B 51, 8287(1995).
- [93] P. Fazekas, *Lecture Notes on Electron Correlation and Magnetism*(World Scientific, Singapore, 1999).
- [94] D.M. Newns and N. Read, Adv. in Phys. 36, 799 (1987).
- [95] A. Blandin and J. Friedel, J. Phys. Radium 19, 573 (1958).
- [96] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
- [97] A. Georges and G. Kotliar, Phys. Rev. B 45, 6479 (1992).
- [98] J. Hubbard, Proc. Royal Soc. London A 277 237 (1964).
- [99] H. Keiter and J.C. Kimball, Int J. Magn. 1, 233 (1971).
- [100] S. E. Barnes, J. Phys. F 6, 1375 (1976); 7, 2637 (1977).
- [101] P. Coleman, Phys. Rev. B 29, 3035 (1984).
- [102] C. Kittel Introduction to Solid State Physics, Eight Edition, (John Wiley and Sons, 2005).
- [103] J. H. de Boer and E. J. W. Verwey, Proc. Phys. Soc. London 49, 59 (1937)
- [104] J. L. Smith and E. A. Kmetko, J. Less-Common Metals 90 83-88 (1983).
- [105] J. Hubbard, Proc. Royal Soc. London A 276, 238-257 (1963).
- [106] J.G. Bednorz and K. A. Müller, Z. Phys. B Condensed Matter 64, 189 (1986).
- [107] C.W. Chu *et al*, Nature **365**, 323 (1993).

- [108] K. Ishida, Y. Nakai and H. Hosono, J. Phys. Soc. Jpn. 78, 062001 (2009).
- [109] I.I. Mazin and J. Schamlian, arxiv:0901.4790 (2009).
- [110] Q. Si and E. Abrahams, Phys. Rev. Lett. 101, 076401(2008).
- [111] P. Morel and P.W. Anderson, Phys. Rev. 125, 1263 (1962).
- [112] J. Spalek, Physica B, 86-88, 375 (1977).
- [113] C. Cohen-Tannoudji, B. Diu and F. Laloë, Quantum Mechanics, Volumme II, Hermann (Paris) (1977)
- [114] H. Georgi, Lie Algebras in Particle Physics, pp61, Westview Press (1999).
- [115] P. Chandra and P. Coleman, Phys. Rev. Lett. 66, 100 (1991).
- [116] X. G. Wen, Frank Wilczek, and A. Zee, Phys. Rev. B 39, 11413 (1989).
- [117] J. J. Sakurai, Modern Quantum Mechanics Revised Edition, pp 277, (Addison Wesley), (1994).
- [118] G.D. Mahan, Many Particle Physics, Third Edition (Klewer Academic/Plenum Publishers, New York, 2000).
- [119] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 1113 (1940).
- [120] C. Wu and S. Zhang, Phys. Rev. B 71, 155115(2005).
- [121] H.A. Ceccatto, C.J. Gazza and A.E. Trumper, Phys. Rev. B 47, 12329 (1993).
- [122] P. Coleman, A. M. Tsvelik, N. Andrei and H. Y. Kee, Phys. Rev. B 60, 3608 3628 (1999).
- [123] D.P. Arovas and A. Auerbach, Phys. Rev. B 38, 316 (1988).
- [124] N. Read, and D. M. Newns, J. Phys. C 16, L1055, (1983).
- [125] N. Read and D.M. Newns, J. Phys. C 16, 3273 (1983).
- [126] A. Auerbach, and K. Levin, Phys. Rev. Lett. 57, 877 (1986).
- [127] N. Read and D.M. Newns, J. Phys. C 18 2651 (1985).
- [128] Note that  $\lambda_i \rightarrow \lambda_i + \partial_\tau \theta_i$  if the gauge transformation is time dependent.
- [129] X.G. Wen and P.A. Lee, Phys. Rev. Lett. 76, 503 (1996).
- [130] S. Sachdev, Phys. Rev. B 45, 12377(1992).
- [131] S.-H. Lee et al., Nature Materials 6, 853 857 (2007).
- [132] O. Tchenyshyov, R. Moessner and S. L. Sondhi, Europhysics Letters 73, 278 (2006).
- [133] Y. Okamoto, M. Nohara, H. Aruga-Katori and H. Takagi, Phys. Rev. Lett. 99, 137207 (2007).
- [134] J. M. Hopkinson, S. V. Isakov, H.-Y. Kee, and Y. B. Kim, Phys. Rev. Lett. 99, 037201 (2007).

- [135] M. J. Lawler, H.Y. Kee, Y. B. Kim, and A. Vishwanath, Phys. Rev. Lett. 100, 227201 (2008)
- [136] N. Read and S. Sachdev, Phys. Rev. Lett. 62, 1694 (1989).
- [137] (Technical note on representations: SU(N) naturally has N-1 fundamental representations, labeled by the index m. The representations can be extended to treat larger spins by increasing n = 2S. Each of these (m, n) representations can be treated with either fermions or bosons - the physics lies in the matrices chosen to represent the spins, not the fermionic or bosonic operators. However, for bosonic representations, taking m > 1 requires an additional flavor index  $a = 1, \ldots, m$  (since bosons must be symmetrized), while larger n can be treated by modifying the constraint to  $n_b = n$ . Fermions have the opposite problem - they can represent any m by fixing  $n_f = m$ , but because they must be antisymmetrized, they require an additional flavor index to treat n > 1. We will generally take only one flavor index and use bosons to describe S > 1/2 (in fact to represent physical S = 1/2, we wish to keep S/N = 1/2 fixed. Fermions with one flavor index can only treat the extreme quantum limit,  $S \ll N$ , but have the advantage of being able to choose the self-conjugate fundamental representation, m = N/2, which only exists for even N. This allows antiferromagnetism to be treated on any lattice with SU(N) spins.)
- [138] A. Auerbach, Interacting electrons and quantum magnetism (Springer-Verlag, New York, 1994).
- [139] H. Bethe, Z. Phys. 71, 205 (1931); L. Hultén, Ark. Mat. Astron. Fys. 26A, 1(1938).
- [140] I. Affleck, Z. Zou, T. Hsu and P. W. Anderson, Phys. Rev. B 38, 745, (1988).
- [141] J.E. Hirsch and S. Tang, Phys. Rev. B 39, 2850 (1989).
- [142] S. Sachdev and N. Read, Int. J. Mod. Phys. B 5, 219(1991).
- [143] S. Sachdev and J. Ye, Phys. Rev. Lett. 70, 3339(1993); A. Georges and O. Parcollet and S. Sachdev, Phys. Rev. Lett. 85, 840(2000)
- [144] T.N. De Silva, M. Ma, and F.C. Zhang, Phys. Rev. B 66, 104417 (2002).
- [145] C. Weber, F. Becca and F. Mila. Phys. Rev. B 72, 024449 (2005).
- [146] P. Chandra and B. Doucot, Phys. Rev. B38, 9335, 1988.
- [147] J.H. Xu and C.S. Ting, Phys. Rev. B 42, 6861-6864(1990).
- [148] A.E. Trumper, L.O. Manuel, C.J. Gazza and H.A. Ceccatto, Phys. Rev. Lett. 78, 2216(1997).
- [149] L. Capriotti, Int. J. Mod. Phys. B 15, 1799 (2001) and references therein.
- [150] F. Krüger and S. Scheidl, Europhys. Lett. 74, 896(2006).
- [151] We could still treat the other case(after all it's just a gauge symmetry) by using staggered bond values instead of uniform., but this would require doubling the unit cell.
- [152] K. Haule, J. H. Shim, G. Kotliar, Phys. Rev. Lett. 100, 226402 (2008).
- [153] T. Yildirim, Phys. Rev. Lett **101**, 057010 (2008).
- [154] C. Xu, M. Muller, S. Sachdev, Phys. Rev. B 78, 020501(R)(2008).

- [155] Clarina de la Cruz et al., Nature(London) 453, 899-902(2008).
- [156] C. Weber *et al.*, Phys. Rev. Lett. **91**, 177202(2003).
- [157] L. Capriotti, A. Fubini, T. Roscilde, and V. Tognetti, Phys. Rev. Lett. 92, 157202(2004).
- [158] R. Melzi et al., Phys. Rev. Lett. 85, 1318-1321(2000).
- [159] S.E. Sebastian *et al.*, Nature **441**, 617 (2006).
- [160] O. Rösch and M. Vojta, Phys. Rev. B 76, 180401(R)(2007).
- [161] U. Hizi, P. Sharma and C. L. Henley, Phys. Rev. Lett. 95, 167203(2005).
- [162] S. Liang, B. Doucot, and P.W. Anderson Phys. Rev. Lett. 61, 365(1988).
- [163] P. Chandra, P. Coleman, and A.I. Larkin, J. Phys.: Condens. Matter2, 7933(1990).
- [164] G. Baskaran, Z. Zou and P.W. Anderson, Solid State Comm. 63, 973 (1987).
- [165] G. Kotliar and J. Liu, Phys. Rev. B 38, 5142(1988).
- [166] K. Tanaka, H. Ikeda and K. Yamada, J. Phys. Soc. Japan 73, 1285-1289 (2004).
- [167] P. Coleman, Phys. Rev. B 28, 5255 (1983).
- [168] P. W. Anderson in *Valence Fluctuations in Solids*, edited by L.M. Falicov, W. Hanke and M.P. Maple p. 451 (North Holland, Amsterdam, 1981).
- [169] C. Lacroix and M. Cyrot, Phys. Rev. B 20, 1969(1979).
- [170] N. Read, D.M. Newns and S. Doniach, Phys. Rev. B 30, 3841 (1984).
- [171] P. Coleman, Phys. Rev. B 35, 5072 (1987).
- [172] R. M. Martin, Phys. Rev. Lett. 48, 362 (1982).
- [173] M. Oshikawa, Phys. Rev. Lett. 84, 3370 (2000).
- [174] N. E. Bickers, Rev. Mod. Phys. 59, 845 (1987).
- [175] P. Coleman, Lectures on the Physics of Highly Correlated Electron Systems VI, Editor F. Mancini, American Institute of Physics, New York, p 79 - 160(2002).
- [176] E. Abrahams, A. Balatsky, D.J. Scalapino, and J. R. Schrieffer, Phys. Rev. B 52, 1271(1995).
- [177] N. J. Curro *et al.*, Nature (London) **434**, 622-625 (2005).
- [178] G. E. Blonder, M. Tinkham and T. M. Klapwijk, Phys. Rev. B 25, 4515-4532 (1982).
- [179] A. Kaminski, Yu. V. Nazarov, and L. I. Glazman, Phys. Rev. Lett. 83, 384 387 (1999).
- [180] C. Petrovic *et al.*, Europhysics Letters **53**, 354(2001).
- [181] W.K. Park, J.L. Sarrao, J.D. Thompson, & L.H. Greene PRL 100, 177001(2008).
- [182] D. R. Hamann, Phys. Rev. 158, 570 (1967).

- [183] Bauer, E.D., et al., Phys. Rev. Lett. 93, 147005 (2004).
- [184] G. Knebel, D. Aoki & J. Flouquet, arXiv:0911.5223 (2009).
- [185] T. Muramatsu *et al*, J. Phys. Soc. Jap. **70**, 3362(2001).
- [186] M. Nicklas et al., Phys Rev B 70, 020505(R) (2004).
- [187] S. Kawasaki et al., Phys. Rev. Lett. 94, 037007 (2005); PRL 96, 147001 (2006).
- [188] N.J. Curro et al, Phys. Rev. B 64, 180514(R)(2001).
- [189] J.L. Sarrao and J. D. Thompson, J. Phys. Soc. Jap. 76, 051013(2007).
- [190] R. Flint, M. Dzero and P. Coleman, Nat. Phys. 4, 643 (2008).
- [191] A.J. Millis & P.A. Lee, Phys. Rev. B 35, 3394(1987).
- [192] A. D. Christianson *et al.*, PRB **70**, 134505(2004).
- [193] S. Nakatsuji et al, Phys. Rev. Lett. 89, 106402(2002).
- [194] P. Ghaemi and T. Senthil, Phys. Rev. B 75, 144412 (2007).
- [195] H. Weber and M. Vojta, Phys. Rev. B 77, 125118 (2008).
- [196] N. Andrei and P. Coleman, Phys. Rev. Lett. 62, 595 598 (1989).
- [197] V.P. Mineev & M.E.Zhitomirsky, Phys. Rev. B 72, 014432(2005).
- [198] T. Willers *et al*,arXiv:1003.0300 (2010).
- [199] O. Gunnarsson & K. Schonhammer, Phys. Rev. B 28, 4315(1983).
- [200] K. Haule and G. Kotliar, Nat. Phys. 5, 796 799 (2009).
- [201] P. W. Anderson, Phys. Rev. Lett. 34, 953 (1975).
- [202] R. Urbano (private communication).
- [203] A. Bringer, Solid State Comm. 46, 591(1983).
- [204] R.M. White and T. H. Geballe, "Long Range Order in Solids" p.193-194 (Academic Press, New York, 1979).
- [205] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J.Am. Chem. Soc. 130, 3296(2008).
- [206] C. Wang et al, Europhys. Lett. 83, 67006 (2008).
- [207] M.Rotter et al., Phys. Rev. B 78, 020503 (2008).
- [208] A. S. Sefat *et al.*, Phys. Rev. Lett. **101**,117004 (2008).
- [209] F.-C. Hsu et al., Proc. Nat. Acad. Sci. 105,14262 (2008).
- [210] Y. Nie, D. Telesca, J. I. Budnick, B. Sinkovic, B. O. Wells, arXiv:0912.4539 (2009).
- [211] D. J. Singh and M.-H. Du, Phys. Rev. Lett. 100, 237003(2008).

- [212] M. D. Johannes, Igor Mazin, Phys. Rev. B 79, 220510R (2009)
- [213] A. Kutepov, K. Haule, S.Y. Savrasov, G. Kotliar, arXiv:1005.0885 (2010).
- [214] Andriy H. Nevidomskyy and P. Coleman, Phys. Rev. Lett. 103, 147205 (2009).
- [215] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. 101, 057003 (2008).
- [216] V. I. Anisimov, E. Z. Kurmaev, A. Moewes, I. A. Izyumov, Physica C 469, 442 (2009).
- [217] S.L. Skornyakov et al., Phys. Rev. B 80, 092501 (2009).
- [218] F. Ning et al., J. Phys. Soc. Jap. 77, 103705 (2008).
- [219] X. Zhang et al., Phys. Rev. Lett. 102, 147002 (2009).
- [220] L. Wray et al., Phys. Rev. B 78, 184508 (2008); H. Ding et al., Eur. Phys. Lett. 83, 47001 (2008).
- [221] K. Hashimoto et al., Phys. Rev. Lett. 102, 207001 (2009).
- [222] K. Seo, B. A. Bernevig, and J. Hu, Phys. Rev. Lett. 101, 206404 (2008).
- [223] M. M. Parish, J. Hu, and B. A. Bernevig, Phys. Rev. B 78, 144514 (2008).
- [224] A.V. Chubukov, D.V. Efremov, and I. Eremin, Phys. Rev. B 78, 134512(2008).
- [225] T.A. Maier, S. Graser, D.J. Scalapino, P.J. Hirschfeld, Phys. Rev. B 79, 224510 (2009).
- [226] F. Wang, H. Zhai, Y. Ran, A. Vishwanath, and D.-H. Lee, Phys. Rev. Lett. 102, 1047005 (2009).
- [227] R. Sknepnek, G. Samolyuk, Y. Lee, J. Schmalian, Phys. Rev. B 79, 054511 (2009).
- [228] Z.-J. Yao, J.-X. Li, and Z. D. Wang, New J. Phys. 11, 025009 (2009).
- [229] A. F. Ruckenstein, P. Hirschfeld, J. Appel, Phys. Rev. B 36, 857 (1987).
- [230] M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. B 62, 6721(2000).
- [231] For an extensive review, see P. A. Lee, N. Nagaosa, and X.G. Wen, Rev. Mod. Phys. 78, 17 (2006).

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## Publications

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- 2. Rebecca Flint, Andriy Nevidomskyy and Piers Coleman, "Composite pairing in a mixed valent two channel Anderson model", in preparation.
- 3. Rebecca Flint and Piers Coleman, "Tandem Pairing in Heavy Fermion Superconductors", arXiv:0912.2339, submitted to Phys. Rev. Lett. (2010).
- 4. R. Flint, H.-T. Yi, P. Chandra, S.-W. Cheong, and V. Kiryukhin, "Spin State Crossover in the Multiferroic Ca<sub>3</sub>Co<sub>2-x</sub>Mn<sub>x</sub>O<sub>6</sub>", Phys. Rev. B **81**, 092402 (2010).
- 5. Rebecca Flint and P. Coleman, "Symplectic N and time reversal in frustrated magnetism", Phys. Rev. B **79**, 014424 (2009).
- 6. Rebecca Flint, M. Dzero and P. Coleman, "Heavy electrons and the symplectic symmetry of spin", Nat. Phys. 4, 643 (2008).