5 Heavy Fermions and the Kondo Lattice: a 21st Century Perspective

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1 Heavy Electrons

1.1 Introduction

In a world where it is possible to hold a levitated high temperature superconductor in the palm of one’s hand, it is easy to forget the ongoing importance of low temperature research. Heavy electron materials are a class of strongly correlated electron material containing localized magnetic moments which, by entangling with the surrounding electrons, profoundly transform the metallic properties. A heavy fermion metal can develop electron masses 1000 times that of copper, it can also develop unconventional superconductivity, transform into new forms of quantum order, exhibit quantum critical and topological behavior. Although most of these properties develop well below the boiling point of nitrogen, the diversity and highly tunable nature of their ground-states make them an invaluable vital work-horse for exploring and researching the emergent properties of correlated quantum matter.

This lecture will give an introduction to heavy fermion materials, trying to emphasize a 21st century perspective. More extensive discussion and development of the ideas in these notes can be found in an earlier review article [1] and the latter chapters of my book “Introduction to Many Body Physics” [2].

![Kmetko-Smith diagram](image)

**Fig. 1:** The Kmetko-Smith diagram [3], showing the broad trends towards increasing electron localization in the d- and f-electron compounds.

In the periodic table, the most strongly interacting electrons reside in orbitals that are well-localized. In order of increasing localization, partially filled orbitals are ordered as follows:

\[ 5d < 4d < 3d < 5f < 4f. \]  

(1)

In addition, when moving along a row of the periodic table, the increasing nuclear charge pulls the orbitals towards the nucleus. These trends are summarized in the “Kmetko-Smith
diagram”[3] in Fig 1. The d-orbital metals at the bottom left of this diagram are highly itinerant and exhibit conventional superconductivity. By contrast, in rare earth and actinide metals towards the top right-hand corner, the f-shell electrons are localized, forming magnets or antiferromagnets. It is the materials that lie in the cross-over between these two regions that are particularly interesting, for these materials are “on the brink of magnetism”. It is in this cross-over region that many strongly correlated materials reside: it is here for instance, that we find cerium and uranium, which are key atoms for a wide range of 4f and 5f heavy electron materials.

1.2 Local moments and the Kondo effect

Heavy electron materials contain a lattice of localized electrons immersed in a sea of mobile conduction electrons. To understand their physics, we need to first step back and discuss individual localized moments, and the mechanism by which they interact with the surrounding conduction sea.

The key feature of a localized moment, is that the Coulomb interaction has eliminated the high frequency charge fluctuations, leaving behind a low energy manifold of degenerate spin states. In rare earth and actinide ions, the orbital and spin angular momentum combine into a single entity with angular momentum \( \vec{j} = \vec{l} + \vec{s} \). For example, a Ce\(^{3+} \) ion contains a single unpaired 4f-electron in the state \( 4f^1 \), with \( l = 3 \) and \( s = 1/2 \). Spin-orbit coupling gives rise to low-lying multiplet with \( j = 3 - \frac{1}{2} = \frac{5}{2} \), consisting of \( 2j + 1 = 6 \) degenerate orbitals \(|4f^1 : Jm\rangle\), \((m_j \in [-\frac{5}{2}, \frac{5}{2}]\)) with an associated magnetic moment \( M = 2.64 \mu_B \). In a crystal, the \( 2j + 1 \) fold degeneracy of such a magnetic ion is split, and provided there are an odd number of electrons in the ion, Kramer’s theorem guarantees that the lowest lying state has at least, a two fold degeneracy. (Fig. 2 a and b.)

One of the classic signatures of localized moments, is a high temperature Curie Weiss susceptibility, given by

\[
\chi \approx n_i \frac{M^2}{3(T + \theta)} \quad M^2 = g^2 \mu_B^2 j(j + 1),
\]

where, \( n_i \) is the concentration of magnetic moments while \( M \) is the magnetic moment with total angular momentum quantum number \( j \) and gyro-magnetic ratio (“g-factor”) \( g \). \( \theta \) is the “Curie Weiss” temperature, a phenomenological scale which takes account of interactions between spins.

The presence of such local moments inside a metal profoundly alters its properties. The physics of an isolated magnetic ion is described by the Kondo model

\[
H = \sum_{k,r} \epsilon_k c^\dagger_{k,r} c_{k,r} + \sum_{\mathbf{r}} J \psi^\dagger(0) \partial_r \psi(0) \cdot \vec{S}_f.
\]

where \( c^\dagger_{k,r} \) creates a conduction electron of energy \( \epsilon_k \), momentum \( k \) and \( \psi^\dagger(0) = \mathcal{N}_s^{-1/2} \sum_k c^\dagger_{k,r} \) creates a conduction at the origin, where \( \mathcal{N}_s \) is the number of sites in the lattice. The conduction sea interacts with local moment via an antiferromagnetic contact interaction of strength \( J \). The antiferromagnetic sign \( (J > 0) \) of this interaction is an example of “super-exchange”, first
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Fig. 2: (a) In isolation, the localized atomic states of an atom form a stable, sharp excitation lying below the continuum. (b) In a crystal, the $2j+1$ fold degenerate state splits into multiplets, typically forming a low lying Kramers doublet. (c) The inverse of the Curie-Weiss susceptibility of local moments $\chi^{-1}$ is a linear function of temperature, intersecting zero at $T = -\theta$.

predicted by Philip W. Anderson [4, 5], which results from high energy valence fluctuations. Jun Kondo [6] first analyzed the effect of this scattering, showing that as the temperature is lowered, the effective strength of the interaction grows logarithmically, according to

$$J \rightarrow J(T) = J + 2J^2 \rho \ln \left( \frac{D}{T} \right)$$  \hspace{1cm} (4)$$

where $\rho$ is the density of states of the conduction sea (per spin) and $D$ is the band-width. The growth of this interaction enabled Kondo to understand why in many metals at low temperatures, the resistance starts to rise as the temperature is lowered, giving rise to resistance minimum.

Fig. 3: (a) Schematic temperature-field phase diagram of the Kondo effect. At fields and temperatures large compared with the Kondo temperature $T_K$, the local moment is unscreened with a Curie susceptibility. At temperatures and fields small compared with $T_K$, the local moment is screened, forming an elastic scattering center within a Landau Fermi liquid with a Pauli susceptibility $\chi \sim \frac{1}{T_K}$. (b) Schematic susceptibility curve for the Kondo effect, showing cross-over from Curie susceptibility at high temperatures to Pauli susceptibility at temperatures below the Kondo temperature $T_K$. (c) Specific heat curve for the Kondo effect. Since the total area is the full spin entropy $R \ln 2$ and the width is of order $T_K$, the height must be of order $\gamma \sim \frac{R \ln 2}{T_K}$. This sets the scale for the zero temperature specific heat coefficient.

Today, we understand this logarithmic correction as a renormalization of the Kondo coupling constant, resulting from fact that as the temperature is lowered, more and more high frequency
quantum spin fluctuations become coherent, and these strengthen the Kondo interaction. The effect is closely analogous to the growth of the strong-interaction between quarks, and like quarks, the local moment in the Kondo effect is asymptotically free at high energies. However, as you can see from the above equation, once the temperature becomes of order

\[ T_K \sim D \exp \left( -\frac{1}{2J\rho} \right) \]

the correction becomes as large as the original perturbation, and at lower temperatures, the Kondo interaction can no longer be treated perturbatively. In fact, non-perturbative methods tell us that this interaction scales to strong coupling at low energies, causing electrons in the conduction sea to magnetically screen the local moment to form an inert Kondo singlet denoted by

\[ |GS\rangle = \frac{1}{\sqrt{2}} (|⇑\downarrow\rangle - |\downarrow⇑\rangle), \] (5)

where the thick arrow refers to the spin state of the local moment and the thin arrow refers to the spin state of a bound-electron at the site of the local moment. The key features of the impurity Kondo effect are:

- The electron fluid surrounding the Kondo singlet forms a Fermi liquid, with a Pauli susceptibility \( \chi \sim 1/T_K \).

- The local moment is a kind of qubit which entangles with the conduction sea to form a singlet. As the temperature \( T \) is raised, the entanglement entropy converts to thermal entropy, given by the integral of the specific heat coefficient,

\[ S(T) = \int_0^T dT' \frac{C_v(T')}{T'}. \]

Since the total area under the curve, \( S(T \to \infty) = R \ln 2 \) per mole is the high temperature spin entropy, and since the characteristic width is the Kondo temperature, it follows that the characteristic zero temperature specific heat coefficient must be of order the inverse Kondo temperature: \( \gamma = \frac{C_v}{T}(T \to 0) \sim \frac{R \ln 2}{T_K} \). (See Fig. 3 b)

- The only scale in the physics is \( T_K \). For example, the resistivity created by magnetic scattering off the impurity has a universal temperature dependence

\[ \frac{R(T)}{R_U} = n_i \Phi \left( \frac{T}{T_K} \right) \] (6)

where \( n_i \) is the concentration of magnetic impurities, \( \Phi(x) \) is a universal function and \( R_U \) is the unit of unitary resistance (basically resistance with a scattering rate of order the Fermi energy),

\[ R_U = \frac{2ne^2}{\pi\hbar\rho} \] (7)

Experiment confirms that the resistivity in the Kondo effect can indeed be scaled onto a single curve that fits forms derived from the Kondo model (see Fig. 4).
• The scattering off the Kondo singlet is resonantly confined to a narrow region of order $T_K$, called the Kondo or Abriksov-Suhl resonance.

Fig. 4: Temperature dependence of resistivity associated with scattering from an impurity spin from [7,8]. The resistivity saturates at the unitarity limit at low temperatures, due to the formation of the Kondo resonance. Adapted from [7].

1.3 The Kondo lattice

In heavy fermion material, containing a lattice of local moments, the Kondo effect develops coherence. In a single impurity, a Kondo singlet scatters electrons without conserving momentum, giving rise to a huge build-up of resistivity at low temperatures. However, in a lattice, with translational symmetry, this same elastic scattering now conserves momentum, and this leads to coherent scattering off the Kondo singlets. In the simplest heavy fermion metals, this leads to a dramatic reduction in the resistivity at temperatures below the Kondo temperature.

As a simple example, consider CeCu$_6$ a classic heavy fermion metal. Naively, CeCu$_6$ is just a copper alloy, in which 14% of the copper atoms are replaced by cerium, yet this modest replacement radically alters the metal. In this material, it actually proves possible to follow the development of coherence from the dilute single ion Kondo limit, to the dense Kondo lattice, by forming the alloy La$_{1-x}$Ce$_x$Cu$_6$. Lanthanum is iso-electronic to cerium, but has an empty f-shell, so the limit $x \to 0$ corresponds to the dilute Kondo limit, and in this limit the resistivity follows the classic Kondo curve. However, as the concentration of cerium increases, the resistivity curve starts to develop a coherence maximum, an in the concentrated limit drops to zero with a characteristic $T^2$ dependence of a Landau Fermi liquid (see Fig. 5).

CeCu$_6$ displays the following classic features of a heavy fermion metal:

- A Curie-Weiss susceptibility $\chi \sim (T + \theta)^{-1}$ at high temperatures.
- A paramagnetic spin susceptibility $\chi \sim \text{cons}$ at low temperatures.
A dramatically enhanced linear specific heat $C_V = \gamma T$ at low temperatures, where in CeCu$_6$ $\gamma \sim 1000\text{mJ/mol/K}^2$ is about 1000 times larger than in copper.

A quadratic temperature dependence of the low temperature resistivity $\rho = \rho_o + AT^2$

In a Landau Fermi liquid [9], the magnetic susceptibility $\chi$ and the linear specific heat coefficient $\gamma = C_V/T|_{T\to0}$ are given by

$$\chi = (\mu_B)^2 \frac{N^*(0)}{1 + F_o^2}$$

$$\gamma = \frac{\pi^2 k_B^2}{3} N^*(0)$$

where $N^*(0) = \frac{n^*}{m} N(0)$ is the renormalized density of states and $F_o^2$ is the spin-dependent part of the s-wave interaction between quasiparticles. One of the consequences of Fermi liquid theory, is that the density of states factors out of the Sommerfeld or Wilson ratio between the susceptibility and linear specific heat coefficient,

$$W = \frac{\chi}{\gamma} = \left(\frac{\mu_B}{2\pi k_B}\right)^2 \frac{1}{1 + F_o^2}$$

In heavy fermion metals, this ratio remains approximately fixed across several decades of variation in $\chi$ and $\gamma$. This allows us to understand heavy fermion metals as a lattice version of the Kondo effect gives rise to a renormalized density of states $N^*(0) \sim \frac{1}{T_K}$.

The discovery of heavy electron compounds in the 1970s led Mott [10] and Doniach [11] to propose that heavy electron systems should be modeled as a “Kondo-lattice”, where a dense array of local moments interact with the conduction sea via an antiferromagnetic interaction $J$. In such a lattice, the local moments polarize the conduction sea, and the resulting Friedel oscillations in the magnetization give rise to an antiferromagnetic RKKY (Rudermann Kittel Kasuya Yosida) magnetic interaction [12–14] that tends to order the local moments. Mott and Doniach realized that this interaction must compete with the Kondo effect.

The simplest Kondo lattice Hamiltonian [15] is

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_j (\hat{S}_j \cdot \mathbf{\sigma}) \sum_{\alpha\beta} c^\dagger_{j\alpha} \mathbf{\sigma}_{\alpha\beta} c_{j\beta},$$

where

$$c^\dagger_{j\sigma} = \frac{1}{\sqrt{N_s}} \sum_k c^\dagger_{k\sigma} e^{-i k \mathbf{R}_j}$$

creates an electron at site $j$. Mott and Doniach [10,11] pointed out that there are two energy scales in the Kondo lattice: the Kondo temperature $T_K = D e^{-1/(2J\rho)}$ and the RKKY scale $E_{RKKY} = J^2 \rho$. For small $J\rho$, $E_{RKKY} >> T_K$ leading to an antiferromagnetic ground-state, but when $J\rho$ is large, $T_K >> E_{RKKY}$, stabilizing a ground-state in which every site in the lattice resonantly scatters electrons. Based on a simplified one-dimensional “Kondo necklace” model [16], Doniach conjectured [11] that the transition between the antiferromagnet and the dense Kondo ground state is a continuous quantum phase transition. Experiment confirms
Fig. 5: Doniach phase diagram for the Kondo lattice, illustrating the antiferromagnetic regime and the heavy fermion regime, for $T_K < T_{RKKY}$ and $T_K > T_{RKKY}$ respectively. The effective Fermi temperature of the heavy Fermi liquid is indicated as a solid line. Experimental evidence suggests that in many heavy fermion materials this scale drops to zero at the antiferromagnetic quantum critical point.

this conjecture, and today we have several examples of such quantum critical points, including CeCu$_6$ doped with gold to form CeCu$_{6-x}$Au$_x$ and CeRhIn$_5$ under pressure [17–19]. In the fully developed Kondo lattice ground state Bloch’s theorem insures that the resonant elastic scattering at each site will generate a renormalized f- band, of width $\sim T_K$. In contrast with the impurity Kondo effect, here elastic scattering at each site acts coherently. For this reason, as the heavy electron metal develops at low temperatures, its resistivity drops towards zero (see Fig. 6).

In a Kondo lattice, spin entanglement is occurring on a truly macroscopic scale, but this entanglement need not necessarily lead to a Fermi liquid. Experimentally, many other possibilities are possible. Here are some examples,

- Ce$_3$Bi$_4$Pt$_3$, a Kondo insulator in which the formation of Kondo singlets with the Ce moments drives the development of a small insulating gap at low temperatures and

- CeRhIn$_5$, an antiferromagnet on the brink of forming a Kondo lattice, which under pressure becomes a heavy fermion superconductor with $T_c=2K$.

- UBe$_{13}$ a heavy fermion superconductor which transitions directly from an incoherent
metal with resistivity 200$\mu$Ωcm, into a superconducting state.

Each of these materials has qualitatively the same high temperature Curie Weiss magnetism and the same Kondo resistivity at high temperatures, due to incoherent scattering off the local moments. However at low temperatures the scattering off the magnetic Ce ions becomes coherent and new properties develop.

**Fig. 6:** (a) Resistivity of Ce$_x$La$_{1-x}$Cu$_6$. Dilute Ce atoms in LaCu$_6$ exhibit a classic “Kondo” resistivity, but as the Ce concentration becomes dense, elastic scattering off each Ce atom leads to the development of a coherent heavy fermion metal. (b) Resistivities of four heavy fermion materials showing the development of coherence. A variety of antiferromagnetic magnetic, Fermi liquid, superconducting and insulating states are formed (see text).

## 2 Kondo insulators: the simplest heavy fermions

In many ways, the Kondo insulator is the simplest ground-state of the Kondo lattice. The first Kondo insulator (KI), SmB$_6$ was discovered almost fifty years ago [20] and today there are several known examples including Ce$_3$Bi$_4$Pt$_3$. At room temperature, these KIs are metals containing a dense array of magnetic moments, yet on cooling they develop a narrow gap due the formation of Kondo singlets which screen the local moments [21][24]. We can gain a lot of insight by examining the strong coupling limit in which the dispersion of the conduction sea is much smaller than the Kondo coupling $J$. Consider a simple tight-binding Kondo lattice

$$H = -t \sum_{\langle i,j \rangle \sigma} (c_i^{\dagger} \sigma_j c_{j\sigma} + \text{H.c.}) + J \sum_{j} \vec{\sigma}_j \cdot \vec{S}_j, \quad \vec{\sigma}_j \equiv (c_j^{\dagger} \sigma \sigma_j c_j)$$  \hspace{1cm} (12)

in which $t/J << 1$ is a small parameter. In this limit, the inter-site hopping is a perturbation to the on-site Kondo interaction,

$$H \xrightarrow{t/J \rightarrow 0} J \sum_{j} \vec{\sigma}_j \cdot \vec{S}_j + O(t),$$ \hspace{1cm} (13)
and the corresponding ground-state corresponds to the formation of a spin singlet at each site, denoted by the wavefunction

$$|KI⟩ = \prod_j \frac{1}{\sqrt{2}} \big(\uparrow_j \downarrow_j - \downarrow_j \uparrow_j\big)$$  \hspace{1cm} (14)$$

where the double and single arrows denote the localized moment and conduction electron respectively.

Each singlet has a ground-state energy $E = -\frac{3}{2}J$ per site and a singlet-triplet spin gap of magnitude $\Delta E = 2J$. Moreover, if we either remove an electron from site $i$, we break a Kondo singlet and create an unpaired spin with excited energy $\frac{3}{2}J$,

$$|qp^+, i \uparrow⟩ = \prod_{j \neq i} \frac{1}{\sqrt{2}} \big(\uparrow_j \downarrow_j - \downarrow_j \uparrow_j\big) = \sqrt{2}c^\dagger_i|KI⟩,$$  \hspace{1cm} (15)$$
as illustrated in Fig[7](a). Similarly, if we add an electron, we create an electron quasiparticle, corresponding to an unpaired local moment and a doubly occupied conduction electron orbital

$$|qp^-, i \uparrow⟩ = \prod_{j \neq i} \big(\uparrow_j \downarrow_j\big) \frac{1}{\sqrt{2}} \big(\uparrow_j \downarrow_j - \downarrow_j \uparrow_j\big) = \sqrt{2}c^\dagger_j|KL⟩,$$  \hspace{1cm} (16)$$
as illustrated in Fig[7](b).

![Fig. 7: Showing (a) hole and (b) electron doping of strong coupling Kondo insulator. (c) Dispersion of strong coupling Kondo insulator. A small amount of hold doping $δ$ gives rise to a “large” Fermi surface containing $2 - δ$ heavy electrons.](image)

If we now reintroduce the hopping $-t$ between sites, then these quasiparticle excitations become mobile, as illustrated in Fig.[7](a) and (b). From the explicit form of the states, we find that the nearest neighbor hopping matrix elements are $⟨qp^+, iσ|H|qp^+, jσ⟩ = ±\frac{t}{2}$, giving quasiparticle energies

$$E_{qp^\pm}(k) = ±t(c_x + c_y + c_z) + \frac{3}{2}J.$$  \hspace{1cm} (17)$$
To transform from the quasiparticle, to the electron basis, we need to reverse the sign of the hole \((q\text{p}^\dagger)\) dispersion to obtain the valence band dispersion, so that the band energies predicted by the strong coupling limit of the Kondo lattice are

\[
E_k^\pm = -t(c_x + c_y + c_z) \pm \frac{3}{2}J,
\]

separated by an energy \(3J\) as shown in Fig. 7(c). Note that these are “hard core” fermions that cannot occupy the same lattice site simultaneously.

In this way, the half-filled strong coupling Kondo lattice forms an insulator with a charge gap of size \(3J\) and a spin gap of size \(2J\). Notice finally that if we dope the insulator with an amount \(\delta\) of holes, we form a band of heavy fermions. In this way, Kondo insulators can be considered the parent states of heavy electron materials. However, we’d like to examine the physics of a Kondo lattice at weak coupling, and to do this requires a different approach.

3 Large \(N\) Expansion for the Kondo Lattice

3.1 Philosophy and Formulation

One of the great difficulties with the Kondo lattice, is that there is no natural small parameter to carry out an approximate treatment. One way around this difficulty, is to use a large \(N\) expansion, in which we extend the number of spin components of the electrons from 2 to \(N\). Historically, Anderson [25] pointed out that the large spin-orbit coupling in heavy fermion compounds generates (if we ignore crystal fields) a large spin degeneracy \(N = 2j + 1\), furnishing a small parameter \(1/N\) for a controlled expansion about the limit \(N \to \infty\). One of the observations arising from Anderson’s idea [26, 27] is that the RKKY interaction becomes negligible (of order \(O(1/N^2)\)) in this limit and the Kondo lattice ground-state becomes stable. This observation opened the way to path integral mean-field treatments of the Kondo lattice [27–32].

The basic idea of the large \(N\) limit is to examine a limit where every term in the Hamiltonian grows extensively with \(N\). In the path integral for the partition function, the corresponding action then grows extensively with \(N\), so that

\[
Z = \int \mathcal{D}[\psi] e^{-NS} = \int \mathcal{D}\psi \exp \left[ -\frac{S}{N} \right] \equiv \int \mathcal{D}[\psi] \exp \left[ -\frac{S}{\hbar_{\text{eff}}} \right].
\]

(19)

Here \(\hbar_{\text{eff}} \sim \hbar_{\text{eff}}\) behaves as an effective Planck’s constant for the theory, focusing the path integral into a non-trivial “semi-classical” or “mean field” solution as \(\hbar_{\text{eff}} \to 0\). As \(N \to \infty\), the quantum fluctuations of intensive variables \(\hat{a}\), such as the electron density per spin, become smaller and smaller, scaling as \(\langle \delta a^2 \rangle / \langle a^2 \rangle \sim 1/N\), causing the path integral to focus around a non-trivial mean-field trajectory. In this way, one can obtain new results by expanding around the solvable large \(N\) limit in powers of \(\frac{1}{N}\). (Fig. 8).

We will use a simplified Kondo lattice model introduced by Read and Newns [27], in which all electrons have a spin degeneracy \(N = 2j + 1\),

\[
H = \sum_{k\alpha} \epsilon_k c_{k\alpha}^\dagger c_{k\alpha} + \frac{J}{N} \sum_{\alpha\beta} c_{j\beta}^\dagger c_{j\alpha} S_{\alpha\beta}(j).
\]

(20)
where \( c^\dagger_{jr} = \frac{1}{\sqrt{N}} \sum_k c^\dagger_{kr} e^{-ik\cdot \vec{R}_j} \) creates an electron localized at site \( j \) and the spin of the local moment at position \( \vec{R}_j \) is represented by pseudo-fermions

\[
S_{\alpha\beta}(j) = f_{jr}^\dagger f_{jr} - \frac{n_f(j)}{N} \delta_{\alpha\beta}.
\]  

(21)

This representation requires that we set a value for the conserved \( f \) occupancy \( n_f(j) = Q \) at each site. This interaction can be rewritten in a factorized form

\[
H = \sum_{kr} \epsilon_k c^\dagger_{kr} c_{kr} - \frac{J}{N} \sum_{j\alpha\beta} \left( f^{\dagger}_{jr\beta} f_{jr\beta} \right) \left( f^{\dagger}_{jr\alpha} c_{jr} \right):
\]  

(22)

Read Newns model for the Kondo lattice

where the potential scattering terms resulting from the rearrangement of the f-operators have been absorbed into a shift of the chemical potential. Note that:

- the model has a global \( SU(N) \) symmetry associated with the conserved magnetization.

- the Read Newns (RN) model is a lattice version of the Coqblin-Schrieffer Hamiltonian \([33]\) introduced to describe the Kondo interaction in strongly spin-orbit coupled rare-earth ions. While the Coqblin-Schrieffer interaction is correct at each site, the assumption that the \( SU(N) \) spin is conserved by electron hopping is an oversimplification. (This is a price one pays for a solvable model.)

- in this factorized form, the antiferromagnetic Kondo interaction is “attractive”. 

Fig. 8: Illustration of the convergence of a quantum path integral about a semi-classical trajectory in the large \( N \) limit.
the coupling constant has been scaled to vary as $J/N$, to ensure that the interaction grows extensively with $N$. The interaction involves a product of two terms that scale as $O(N)$, so that $J/N \times O(N^2) \sim O(N)$.

- the RN model also has a local gauge invariance: the absence of f-charge fluctuations allows us to change the phase of the f-electrons independently at each site

$$f_{j\sigma} \rightarrow e^{i\phi_j} f_{j\sigma}. \quad (23)$$

A tricky issue concerns the value we give to the conserved charge $n_f = Q$. In the physical models of interest, $n_f = 1$ at each site, so one might be inclined to explicitly maintain this condition. However, the large $N$ expansion requires that the action is extensive in $N$, and this forces us to consider more general classes of solution where $Q$ scales with $N$ so that the filling factor $q = Q/N$ is finite as $N \rightarrow \infty$. Thus if we’re interested in a Kramer’s doublet Kondo model, we take the half-filled case $q = 1/2, Q = N/2$, but if we want to understand a $j = 7/2$ Yb$^{3+}$ atom without crystal fields, then in the physical system $N = 2j + 1 = 8$, and we should fix $q = Q/N = 1/8$.

The partition function for the Kondo lattice is then

$$Z = \text{Tr} \left[ e^{-\beta H} \prod_j \delta(\hat{n}_f(j) - Q) \right] \quad (24)$$

where $\delta(\hat{n}_f(j) - Q)$ projects out the states with $n_f(j) = Q$ at site $j$. By re-writing the delta function as a Fourier transform, the partition function can be can be rewritten as a path-integral,

$$Z = \int \mathcal{D}[\psi^\dagger, \psi, \lambda] \exp \left[ -\int_0^\beta d\tau \left( \psi^\dagger \partial_\tau \psi + H[\bar{\psi}, \psi, \lambda] \right) + \text{boundary terms} \right] \quad (25)$$

where $\psi^\dagger \equiv (\{c^\dagger\}, \{f^\dagger\})$ schematically represent the conduction and f-electron fields,

$$H[\lambda] = \sum_{k\alpha} \epsilon_k c_{k\alpha}^\dagger c_{k\alpha} - \frac{J}{N} \sum_{j,\alpha\beta} \left( c_{j\beta}^\dagger f_{j\beta} (f_{j\alpha}^\dagger c_{j\alpha}) + \sum_j \lambda_j (n_{fj} - Q) \right). \quad (26)$$

The field $\lambda_j$ is a fluctuating Lagrange multiplier that enforces the constraint $n_j = Q$ at each site. Next we carry out a Hubbard Stratonovich transformation on the interaction,

$$-\frac{J}{N} \sum_{\alpha\beta} (c_{j\beta}^\dagger f_{j\beta}) (f_{j\alpha}^\dagger c_{j\alpha}) \rightarrow \sum_\alpha \left[ \bar{V}_j (c_{j\alpha}^\dagger f_{j\alpha}) + (f_{j\alpha}^\dagger c_{j\alpha}) V_j \right] + N \frac{\bar{V}_j V_j}{J}. \quad (27)$$

In the original Kondo model, we started out with an interaction between electrons and spins. Now, by carrying out the Hubbard Stratonovich transformation, we have formulated the interaction as the exchange of a charged boson

$$\frac{J}{N} \delta(\tau - \tau') \equiv c_{\beta}^\dagger f_{\beta} \quad \Rightarrow \quad \frac{J}{N} \delta(\tau - \tau') \cdot f_{\alpha}^\dagger c_{\alpha}$$
\[-\frac{J}{N} \sum_{k,k',\alpha, \beta} (c_{\beta}^\dagger f_{\beta}^\dagger)(f_{\alpha}^\dagger c_{\alpha})\]  \hspace{1cm} (28)

where the solid lines represent the conduction electron propagators, and the dashed lines represent the f-electron operators. Notice how the bare amplitude associated with the exchange boson is frequency independent, i.e. the interaction is instantaneous. Physically, we may interpret this exchange process as due an intermediate valence fluctuation.

The path integral now involves an additional integration over the hybridization fields \(V\) and \(\bar{V}\),

\[
Z = \int \mathcal{D}[\bar{V}, V, \lambda] \int \mathcal{D}[\psi^\dagger, \psi] \exp\left[ -\int_0^\beta (\bar{\psi}^\dagger \partial_\tau \psi + H[\bar{V}, V, \lambda]) \right]
\]

\[
H[\bar{V}, V, \lambda] = \sum_k \epsilon_k c_{-k\sigma}^\dagger c_{k\sigma} + \sum_j \left[ \bar{V}_j (c_{j\sigma}^\dagger f_{j\sigma}) + (f_{j\sigma}^\dagger c_{j\sigma}) V_j + \lambda_j (n_{f_j} - Q) + N \frac{\bar{V}_j V_j}{J} \right]
\]

Read Newns path integral for the Kondo lattice.

where we have suppressed summation signs for repeated spin indices (summation convention).

The RN path integral allows us to develop a mean-field description of the many body Kondo scattering processes that captures the physics and is asymptotically exact as \(N \to \infty\). In this approach, the condensation of the hybridization field describes the formation of bound-states between spins and electrons that can not be dealt with in perturbation theory. Bound-states induce long range temporal correlations in scattering: once the hybridization condenses, the interaction lines break-up into independent anomalous scattering events, denoted by

\[
\langle \delta \bar{V}(1) \delta V(2) \rangle \rightarrow \bar{V}(1) \bar{V}(2)
\]

The hybridization \(V\) in the RN action carries the local \(U(1)\) gauge charge of the f-electrons, giving rise to an important local gauge invariance:

\[
f_{j\sigma} \rightarrow e^{i\phi_j} f_{j\sigma}, \hspace{1cm} V_j \rightarrow e^{i\phi_j} V_j, \hspace{1cm} \lambda_j \rightarrow \lambda_j - i\dot{\phi}_j(\tau).
\]

Read Newns gauge transformation.

This invariance can be used to choose a gauge in which \(V_j\) is real, by absorbing the phase of the hybridization \(V_j = |V_j| e^{i\phi_j}\) into the f-electron. In the radial gauge,
Heavy Fermions and the Kondo Lattice

5.15

\[
Z = \int \mathcal{D}[|V|, \lambda] \int \mathcal{D}[\psi^\dagger, \psi] \exp \left[ - \int_0^\beta (\psi^\dagger \partial_\tau \psi + H(|V|, \lambda)) \right]
\]

\[
H(|V|, \lambda) = \sum_k \epsilon_k c_k^\dagger c_k + \sum_j |V_j| (c_j^\dagger f_j f_j^\dagger + f_j^\dagger f_j c_j) + \lambda_j (n_f - Q) + N \left| \frac{|V_j|^2}{J} \right|
\]

(31)

Read Newns path integral: “radial gauge”.

Subsequently, when we use the radial gauge, we will drop the modulii sign. The interesting feature about this Hamiltonian, is that with the real hybridization, the conduction and f-electrons now transform under a single global $U(1)$ gauge transformation, i.e the f-electrons have become charged.

### 3.2 Mean-Field Theory

The interior fermion integral in the path integral (31) defines an effective action $S_E[V, \lambda]$ by the relation

\[
Z_E = \exp \left[ -NS_E[V, \lambda] \right] \equiv \int \mathcal{D}[\psi^\dagger, \psi] \exp \left[ -S[V, \lambda, \psi^\dagger, \psi] \right],
\]

(32)

The extensive growth of the effective action with $N$ means that at large $N$, the integration in (29) is dominated by its stationary points, allowing us to dispense with the integrals over $V$ and $\lambda$.

\[
Z = \int \mathcal{D}[\lambda, V] \exp \left[ -NS_E[V, \lambda] \right] \approx \exp \left[ -NS_E[V, \lambda] \right]_{\text{Saddle Point}}
\]

(33)

In practice, we seek uniform, static solutions, $V_j(\tau) = V, \lambda_j(\tau) = \lambda$. In this case the saddle point partition function $Z_E = \text{Tr} e^{-\beta H_{MFT}}$ is simply the partition function of the static mean-field Hamiltonian

\[
H_{MFT} = \sum_{k\sigma} \left( c_{k\sigma}^\dagger f_{k\sigma}^\dagger \right) \left( \frac{\epsilon_k}{\overline{V}} \right) \left( \frac{V}{\lambda} \right) + N N_s \left( \frac{|V|^2}{J} - \lambda q \right)
\]

(34)

Here, $f_{k\sigma}^\dagger = \frac{1}{\sqrt{N_s}} \sum_j f_{j\sigma}^\dagger e^{ik \cdot R_j}$ is the Fourier transform of the $f$-electron field and we have introduced the two component notation

\[
\psi_{k\sigma} = \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix}, \quad \psi_{k\sigma}^\dagger = \begin{pmatrix} c_{k\sigma}^\dagger, f_{k\sigma}^\dagger \end{pmatrix}, \quad h(k) = \begin{pmatrix} \epsilon_k \ \overline{V} \\ \lambda \end{pmatrix}.
\]

(35)

We should think about $H_{MFT}$ as a renormalized Hamiltonian, describing the low energy quasi-particles, moving through a self-consistently determined array of resonant scattering centers.
Later, we will see that the f-electron operators are composite objects, formed as bound-states between spins and conduction electrons.

The mean-field Hamiltonian can be diagonalized in the form

$$H_{MFT} = \sum_{k\sigma} \begin{pmatrix} a_{k\sigma} & b_{k\sigma}^* \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & E_k \end{pmatrix} \begin{pmatrix} a_{k\sigma}^\dagger \\ b_{k\sigma}^\dagger \end{pmatrix} + N N_s \left( \frac{\bar{V} V}{J} - \lambda q \right). \quad (36)$$

Here $a_{k\sigma} = u_k c_{k\sigma} + v_k f_{k\sigma}^\dagger$ and $b_{k\sigma} = -v_k c_{k\sigma} + u_k f_{k\sigma}^\dagger$ are linear combinations of $c_{k\sigma}$ and $f_{k\sigma}^\dagger$, playing the role of “quasiparticle operators” with corresponding energy eigenvalues

$$\text{Det} \begin{pmatrix} E_k^\pm - \left( \frac{\epsilon_k}{\bar{V}} \lambda \right) \end{pmatrix} = (E_{k\pm} - \epsilon_k)(E_{k\pm} - \lambda) - |V|^2 = 0, \quad (37)$$

or

$$E_{k\pm} = \frac{\epsilon_k + \lambda}{2} \pm \left[ \left( \frac{\epsilon_k - \lambda}{2} \right)^2 + |V|^2 \right]^{1/2}, \quad (38)$$

and eigenvectors taking the BCS form

$$\begin{cases} u_k \\ v_k \end{cases} = \frac{1}{2} \pm \frac{(\epsilon_k - \lambda)/2}{2 \sqrt{\left( \frac{\epsilon_k - \lambda}{2} \right)^2 + |V|^2}} \right]^{1/2}. \quad (39)$$

The hybridized dispersion described by these energies is shown in Fig. 9.

Note that:

- The Kondo effect injects an f-band into the conduction sea, hybridizing with the conduction band to create two bands separated by a direct “hybridization gap” of size $2V$ and a much smaller indirect gap. If we put $\epsilon_k = \pm D$, we see that the upper and lower edges of the gap are given by

$$E^\pm = \frac{\pm D + \lambda}{2} \pm \sqrt{\left( \frac{\pm D - \lambda}{2} \right)^2 + V^2} \approx \lambda \pm \frac{V^2}{D}, \quad (D >> \lambda) \quad (40)$$
so the indirect gap has a size $\Delta_g \sim 2V^2/D$, where $D$ is the half-bandwidth. We will see shortly that $V^2/D \sim T_K$ is basically the single-ion Kondo temperature, so that $V \sim \sqrt{T_KD}$ is the geometric mean of the band-width and Kondo temperature.

- In the case when the chemical potential lies in the gap, a Kondo insulator is formed.
- A conduction sea of electrons has been transformed into a heavy Fermi sea of holes.
- The Fermi surface volume expands in response to the formation of heavy electrons (see Fig. 10) to count the total number of occupied quasiparticle states

$$N_{\text{tot}} = \langle \sum_{k,\lambda} n_{k,\lambda\sigma} \rangle = \langle \hat{n}_f + \hat{n}_c \rangle$$

where $n_{k,\lambda\sigma} = a_{k,\lambda\sigma}^\dagger a_{k,\lambda\sigma}$ is the number operator for the quasiparticles and $n_c$ is the total number of conduction electrons. This means

$$N_{\text{tot}} = N V_{\text{FS}} a_3^3 \left( \frac{2\pi}{3} \right) = Q + n_c,$$

where $a_3$ is the volume of the unit cell. This is rather remarkable, for the expansion of the Fermi surface implies an increased negative charge density in the Fermi sea. Since charge is conserved, we are forced to conclude there is a compensating $+Q|e|$ charge density per unit cell provided by the Kondo singlets formed at each site, as illustrated in Fig. 10.

![Fig. 10:](image)

(a) High temperature state: small Fermi surface with a background of spins; (b) Low temperature state where large Fermi surface develops against a background of positive charge. Each spin “ionizes” into $Q$ heavy electrons, leaving behind a background of Kondo singlets, each with charge $+Q|e|$.

### 3.3 Free energy and Saddle Point

Let us now use the results of the last section to calculate the mean-field free energy $F_{\text{MFT}}$ and determine, self-consistently the parameters $\lambda$ and $V$ which set the scales of the Kondo lattice. By diagonalizing the mean field Hamiltonian, we obtain

$$\frac{F}{N} = -T \sum_{k,\pm} \ln \left[ 1 + e^{-\beta E_k} \right] + N_s \left( \frac{V^2}{J} - \lambda q \right).$$
Let us discuss the ground-state, in which only the lower-band contributes to the Free energy. As $T \to 0$, we can replace $-T \ln(1+e^{-\beta E_k}) \to \theta(-E_k)E_k$, so the ground-state energy $E_0 = F(T = 0)$ involves an integral over the occupied states of the lower band:

$$\frac{E_o}{NN_s} = \int_{-\infty}^{0} dE \rho^*(E)E + \left(\frac{V^2}{J} - \lambda q\right)$$

(44)

where we have introduced the density of heavy electron states $\rho^*(E) = \sum_{k,\pm} \delta(E - E_k^{(\pm)})$. Now by (37) the relationship between the energy $E$ of the heavy electrons and the energy $\epsilon$ of the conduction electrons is

$$E = \epsilon + \frac{V^2}{E - \lambda}.$$

As we sum over momenta $\mathbf{k}$ within a given energy shell, there is a one-to-one correspondence between each conduction electron state and each quasiparticle state, so we can write $\rho^*(E)dE = \rho(\epsilon)d\epsilon$, where the density of heavy electron states

$$\rho^*(E) = \rho \frac{d\epsilon}{dE} = \rho \left(1 + \frac{V^2}{(E - \lambda)^2}\right).$$

(45)

Here we have approximated the underlying conduction electron density of states by a constant $\rho = 1/(2D)$. The originally flat conduction electron density of states is now replaced by a “hybridization gap”, flanked by two sharp peaks of width approximately $\pi \rho V^2 \sim T_K$ (Fig. 9). Note that the lower band-width is lowered by an amount $-V^2/D$. With this information, we can carry out the integral over the energies, to obtain

$$\frac{E_o}{NN_s} = \rho \int_{-\infty}^{0} dE \left(1 + \frac{V^2}{(E - \lambda)^2}\right) + \left(\frac{V^2}{J} - \lambda q\right)$$

(46)

where we have assumed that the upper band is empty, and the lower band is partially filled. Carrying out the integral we obtain

$$\frac{E_o}{NN_s} = \frac{-\rho}{2} \left(D + \frac{V^2}{D}\right)^2 + \frac{A}{\pi} \ln \left(\frac{\lambda}{D}\right) + \left(\frac{V^2}{J} - \lambda q\right)$$

$$= \frac{-D^2 \rho}{2} + \frac{A}{\pi} \ln \left(\frac{\lambda}{D}\right) + \left(\frac{V^2}{J} - \lambda q\right)$$

(47)

where we have replaced $\Delta = \pi \rho V^2$, which is the width of an isolated f-resonance, and have dropped terms of order $O(\Delta^2/D)$. We can rearrange this expression, absorbing the band-width $D$ and Kondo coupling constant into a single Kondo temperature $T_K = De^{-\frac{\lambda}{\rho V^2}}$ as follows

$$\frac{E_o}{NN_s} = \frac{-D^2 \rho}{2} + \frac{A}{\pi} \ln \left(\frac{\lambda}{D}\right) + \left(\frac{\pi \rho V^2}{\pi \rho J} - \lambda q\right)$$

$$= \frac{-D^2 \rho}{2} + \frac{A}{\pi} \ln \left(\frac{\lambda}{D}\right) + \left(\frac{\Delta}{\pi \rho J} - \lambda q\right)$$

$$= \frac{-D^2 \rho}{2} + \frac{A}{\pi} \ln \left(\frac{\lambda}{De^{-\frac{\lambda}{\rho V^2}}}\right) - \lambda q$$
\[
 E_0(V) = \frac{\Delta}{\pi} \ln \left( \frac{\Delta}{\pi q e T_K} \right) - \frac{D^2 \rho}{2}, \quad (A = \pi |V|^2) \tag{49}
\]

Let us pause for a moment to consider this energy functional qualitatively. There are two points to be made

- **The energy surface** \( E_0(V) \) **is actually independent of the phase of** \( V = |V|e^{i\phi} \) (see Fig. 11), and has the form of “Mexican Hat” at low temperatures. The minimum of this functional will then determine a family of saddle point values \( V = |V_o|e^{i\phi} \), where \( \phi \) can have any value. If we differentiate the ground-state energy with respect to \( A \), we obtain

\[
 0 = \frac{1}{\pi} \ln \left( \frac{\Delta}{\pi q e T_K} \right)
\]

**or**

\[
 A = \pi q T_K
\]

confirming that \( A \sim T_K \).

- **The mean-field value of the constraint field** \( \lambda \) is determined relative to the Fermi energy \( \mu \). Were we to introduce a slowly varying external potential field to the conduction electron sea, then the chemical potential becomes locally shifted so that \( \mu \rightarrow \mu + e\phi(t) \). So long as the field \( \phi(t) \) is varied at a rate slowly compared with the Kondo temperature, the constraint field will always track with the chemical potential, and since the constraint field is pinned to the chemical potential, \( \lambda \rightarrow \lambda + e\phi(t) \). In the process, the constraint term will become

\[
 \lambda(\hat{n}_f(j) - Q) \rightarrow \lambda(\hat{n}_f(j) - Q) + e\phi(t)(\hat{n}_f(j) - Q). \tag{50}
\]
Since the f-electrons now couple to the external potential $e\phi$ we have to ascribe a physical charge $e = -|e|$ to them. By contrast, the $-Q$ term in the constraint must be interpreted as a “background positive charge” $|e|Q \equiv |e|$ per site. These lines of reasoning indicate that we should think of the Kondo effect as an **many-body ionization phenomenon** in which the neutral local moment splits up into a negatively charged heavy electron and a stationary positive background charge we can associate with the formation of a Kondo singlet.

### 3.4 The Composite nature of the f-electron

The matrix Green’s function of the Kondo lattice reminds us of the Nambu Green’s function in superconductivity. It is given by

$$G_k(\tau) = -\langle \psi_{k\sigma}(\tau)\psi_{k\sigma}^\dagger(0) \rangle \equiv \begin{bmatrix} G_c(k,\tau) & G_{cf}(k,\tau) \\ G_{fc}(k,\tau) & G_f(k,\tau) \end{bmatrix}$$

where $G_c(k,\tau) = -\langle c_k(\tau)c_{k\sigma}^\dagger(0) \rangle$, $G_{cf}(k,\tau) = -\langle c_k(\tau)f_{k\sigma}^\dagger(\tau) \rangle$ and so on. The anomalous off-diagonal members of this Green’s function remind us of the Gor’kov functions in BCS theory, and develop with the coherent hybridization. Using the two component notation (35), this Green’s function can be written

$$G_k(\tau) = -(\partial_\tau + \hbar_k)^{-1} \lim_{\omega_n \to -i} G_k(i\omega_n) = (i\omega_n - \hbar_k)^{-1},$$

where F.T denotes a Fourier transform in imaginary time $(\partial_\tau \to -i\omega_n)$, or more explicitly,

$$G_k(z) = (z - \hbar_k)^{-1} = \begin{pmatrix} z - \epsilon_k & -V \\ -V & z - \lambda \end{pmatrix}^{-1} = \begin{pmatrix} G_c(k,z) & G_{cf}(k,z) \\ G_{fc}(k,z) & G_f(k,z) \end{pmatrix}$$

$$= \frac{1}{(z - \epsilon_k)(z - \lambda) - V^2} \begin{pmatrix} z - \lambda & V \\ V & z - \epsilon_k \end{pmatrix},$$

where we have taken the liberty of analytically extending $i\omega_n \to z$ into the complex plane. Now we can read off the Green’s functions. In particular, the “hybridized” conduction electron Green’s function is

$$G_c(k,z) = \frac{z - \lambda}{(z - \epsilon_k)(z - \lambda) - V^2}$$

$$= \frac{1}{z - \epsilon_k - \Sigma_c(z)} \equiv \frac{1}{z - \epsilon_k - \Sigma_c(z)}$$

which we can interpret physically as conduction electrons scattering off resonant f-states at each site, giving rise to a momentum-conserving self energy

$$\Sigma_c(z) = \frac{V}{z - \epsilon_k - \lambda} \equiv \frac{V^2}{z - \lambda}.$$

We see that the Kondo effect has injected a resonant scattering pole at energy $z = \lambda$ in the conduction electron self-energy. This resonant scattering lies at the heart of the Kondo effect.
3.4.1 An absurd digression: the nuclear Kondo effect

The appearance of this pole in the scattering raises a vexing question in the Kondo effect: what is the meaning of the f-electron? This might seem like a dumb question, for in electronic materials the Kondo effect certainly involves localized f electrons, and surely, we can interpret this pole as as the adiabatic renormalization of a hybridized band-structure. This is certainly true. Yet as purists, we do have to confess that our starting model, was a pure Kondo lattice model with only spin degrees of freedom: they could even have been nuclear spins! This might seem absurd, yet nuclear spins do couple antiferromagnetically with conduction electrons to produce nuclear antiferromagnetism. Leaving aside practical issues of magnitude, we can learn something from the thought experiment in which the the nuclear spin coupling to electrons is strong enough to overcome the nuclear magnetism. In this case, resonant bound-states would form with the nuclear spin lattice giving rise to charged heavy electrons, presumably with an expanded Fermi surface. From this line of argument we see that while it’s tempting to associate the heavy fermion with a physical f- or d- electron localized inside the local moment, from a renormalization group perspective, the heavy electron is an emergent excitation: a fermionic bound-state formed between the conduction sea and the neutral localized moments. This alternate point-of-view is useful, because it allows us to contemplate the possibility of new kinds of Kondo effect into states that are not adiabatically accessible from a band insulator or metal.

3.5 Cooper pair analogy

There is a nice analogy with superconductivity which helps to understand the composite nature of the heavy electron. In a superconductor, electron pairs behave as loose composite bosons described by the relation

$$\psi_\uparrow(x)\psi_\downarrow(x') = -F(x - x'). \quad (56)$$

Here $F(x - x') = -(\langle \psi_\uparrow(1)\psi_\downarrow(2) \rangle)$ is the anomalous Gor’kov Greens function which determines the Cooper pair wavefunction, extended over the coherence length $\xi \sim v_F / T_c$. A similar phenomenon takes place in the Kondo effect, but here the bound-state develops between spins and electrons, forming a fermion, rather than a boson. For the Kondo lattice, it’s perhaps more useful to think in terms of a screening time $\tau_K \sim h / T_K$, rather than a length. Both the Cooper pair and heavy electron involve electrons that span decades of energy up to a cutoff, beit the Debye energy $\omega_D$ in superconductivity or the (much larger) bandwidth $\Delta$ in the Kondo effect. To follow this analogy in greater depth, recall that in the path integral the Kondo interaction factorizes as

$$\frac{J}{N} c_\beta^\dagger S_{\alpha\beta}c_\alpha \rightarrow \bar{V} \left( c_\alpha^\dagger f_\alpha \right) + \left( f_\alpha c_\alpha \right) V + N \frac{\bar{V}V}{J}, \quad (57)$$

so by comparing the right and left hand side, we see that the composite operators $S_{\beta\alpha}c_\beta$ and $c_\beta^\dagger S_{\alpha\beta}$ behave as a single fermion denoted by the contractions:
\[
\frac{1}{N} \sum_{\beta} S_{\beta\alpha} c_\beta = (\bar{V} \gamma f_{\alpha}, \quad \frac{1}{N} \sum_{\beta} c_\beta^\dagger S_{\alpha\beta} = (\bar{V} \gamma f_{\alpha}), \quad \text{(58)}
\]

Composite Fermion

Physically, this means that the spins bind high energy electrons, transforming themselves into composites which then hybridize with the conduction electrons. The resulting “heavy fermions” can be thought of as moments ionized in the magnetically polar electron fluid to form mobile, negatively charged heavy electrons while leaving behind a positively charged “Kondo singlet”. Microscopically, the many body amplitude to scatter an electron off a local moment develops a bound-state pole, which for large \( N \) we can denote by the diagrams:

\[
\Gamma \equiv O(1) \quad V \quad \bar{V} \quad O(1/N) + \ldots
\]

The leading diagram describes a kind of “condensation” of the hybridization field; the second and higher terms describe the smaller \( O(1/N) \) fluctuations around the mean-field theory. By analogy with superconductivity, we can associate a wavefunction associated with the temporal correlations between spin-flips and conduction electrons, as follows

\[
\frac{1}{N} \sum_{\beta} c_\beta(\tau) S_{\beta\alpha}(\tau') = g(\tau - \tau') \hat{f}_{\alpha}(\tau'). \quad \text{(59)}
\]

where the spin-flip correlation function \( g(\tau - \tau') \) is an analogue of the Gor’kov function, extending over a coherence time \( \tau_K \sim \hbar/T_K \). Notice that in contrast to the Cooper pair, this composite object is a fermion and thus requires a distinct operator \( \hat{f}_{\alpha} \) for its expression.

4 Heavy Fermion Superconductivity

We now take a brief look at heavy fermion superconductivity. There are a wide variety of heavy electron superconductors, almost all of which are nodal superconductors, in which the pairing force derives from the interplay of magnetism and electron motion. In the heavy fermion compounds, as in many other strongly correlated electron systems superconductivity frequently develops at the border of magnetism, near the quantum critical point where the magnetic transition temperature has been suppressed to zero. In some of them, such as UPt₃ \( (T_c=0.5K) \) [36], the superconductivity develops out of a well-developed heavy Fermi liquid, and in these cases, we can consider the superconductor to be paired by magnetic fluctuations within a well-formed heavy Fermi liquid. However, in many other superconductors, such as UBe₁₃ \( (T_c=1K) \) [37, 38], the 115 superconductors CeCoIn₅ \( (T_c=2.3K) \) [39], CeRhIn₅ under pressure \( (T_c=2K) \) [17], NpAl₂Pd₃ \( (T_c=4.5K) \) [40] and PuCoGa₅ \( (T_c=18.5K) \) [41, 42], the superconducting transition temperature is comparable with the Kondo temperature. In many of
these materials, the entropy of condensation

$$S_c = \int_0^T C_V \frac{dT}{T}$$

(60)

can be as large as \((1/3)R \ln 2\) per rare earth ion, indicating that the spin is, in some-way entangling with the conduction electrons to build the condensate. In this situation, we need to be able to consider the Kondo effect and superconductivity on an equal footing.

Fig. 12: (a) Phase diagram of 115 compounds CeMIn\(_5\), adapted from [43], showing magnetic and superconducting phases as a function of alloy concentration. (b) Sketch of specific heat coefficient of CeCoIn\(_5\), (with nuclear Schottky contribution subtracted), showing the large entropy of condensation associated with the superconducting state. (After Petrovic et al 2001 [39]).

4.1 Symplectic spins and SP (N).

Although the SU(N) large \(N\) expansion provides a very useful description of the normal state of heavy fermion metals and Kondo insulators, there is strangely, no superconducting solution. This short-coming lies in the very structure of the SU\((N)\) group. SU\((N)\) is perfectly tailored to particle physics, where the physical excitations - the mesons and baryons appear as color singlets, with the meson a a \(q\bar{q}\) quark-antiquark singlet while the baryon is an \(N\)-quark singlet \(q_1 q_2 \ldots q_N\), (where of course \(N = 3\) in reality). In electronic condensed matter, the meson becomes a particle-hole pair, but there are no two-particle singlets in SU\((N)\) beyond \(N = 2\). The origin of this failure can be traced back to the absence of a consistent definition of time-reversal symmetry in SU\((N)\) for \(N > 2\). This means that singlet Cooper pairs and superconductivity can not develop at the large \(N\) limit.

A solution to this problem which grew out an approach developed by Read and Sachdev [44] for frustrated magnetism, is to use the symplectic group \(SP(N)\), where \(N\) must be an even number
This little-known group is a subgroup of $SU(N)$. In fact for $N = 2$, $SU(2) = SP(2)$ are identical, but they diverge for higher $N$. For example, $SU(4)$ has 15 generators, but its symplectic sub-group $SP(4)$ has only 10. At large $N$, $SP(N)$ has approximately half the number of generators of $SU(N)$. The symplectic property of the group allows it to consistently treat time-reversal symmetry of spins and it also allows the formation of two-particle singlets for any $N$.

One of the interesting aspects of $SP(N)$ spin operators, is their relationship to pair operators. Consider $SP(2) ≡ SU(2)$: the pair operator is $Ψ^\dagger = f^\dagger \uparrow f^\dagger \downarrow$ and since this operator is a singlet, it commutes with the spin operators, $[Ψ, \vec{S}] = [Ψ^\dagger, \vec{S}] = 0$ which, since $Ψ$ and $Ψ^\dagger$ are the generators of particle-hole transformations, implies that the $SU(2)$ spin operator is particle-hole symmetric. It is this feature that is preserved by the $SP(N)$ group, all the way out to $N \to \infty$. In fact, we can use this fact to write down an $SP(N)$ spins as follows: an $SU(N)$ spin is given by $S_{αβ}^{SU(N)} = f^\dagger α fβ$. Under a particle hole transformation $f_α \to \text{Sgn}(α)f_{-α}$. If we take the particle-hole transform of the $SU(N)$ spin and add it to itself we obtain an $SP(N)$ spin,

$$S_{αβ} = f^\dagger α fβ + \text{Sgn}(αβ)f_{-β}f^\dagger_{-α}, \quad (61)$$

**Symplectic Spin operator**

where the values of the spin indices are $α, β \in \{±\frac{1}{2}, \ldots, ±N/2\}$. This spin operator commutes with the three isospin variables

$$τ_3 = n_f - N/2, \quad τ^+ = \sum_{α>0} f^\dagger α f^\dagger_{-α}, \quad τ^- = \sum_{α>0} f_{-α}f_α. \quad (62)$$

With these local symmetries, the spin is continuous invariant under $SU(2)$ particle-hole rotations $f_α \to uf_α + v\text{Sgn}αf^-_{-α}$, where $|u|^2 + |v|^2 = 1$, as you can verify. To define an irreducible representation of the spin, we also have to impose a constraint on the Hilbert space, which in its simplest form is $τ_3 = τ^\pm = 0$, equivalent to $Q = N/2$ in the $SU(N)$ approach. In other-words, the s-wave part of the f-pairing must vanish identically.

![Phase diagram for the two-dimensional Kondo Heisenberg model](image)

**Fig. 13:** Phase diagram for the two-dimensional Kondo Heisenberg model, derived in the $SP(N)$ large $N$ approach, adapted from [47], courtesy Rebecca Flint.
4.2 Superconductivity in the Kondo Heisenberg Model

Let us take a look at the way this works in a nearest neighbor “Kondo Heisenberg model” \[47\].

\[
H = H_c + H_K + H_M. \tag{63}
\]

Here \(H_c = \sum_{k\alpha} \epsilon_k c_{k\alpha}^\dagger c_{k\alpha}\) describes the conduction sea, whereas \(H_K\) and \(H_M\) are the Kondo and Heisenberg (RKKY) interactions, respectively. These take the form

\[
H_K = \frac{J_K}{N} \sum_j c_{j\alpha}^\dagger c_{j\beta} S_{\beta\alpha}(j) \rightarrow -\frac{J_K}{N} \sum_{ij} \left( (c_{j\alpha}^\dagger f_{ja})(f_{j\beta}^\dagger c_{j\beta}) + \tilde{\alpha} \tilde{\beta}(c_{j\alpha}^\dagger f_{j\beta})(f_{j\beta} c_{j\alpha}) \right)
\]

\[
H_M = \frac{J_M}{2N} \sum_{(i,j)} S_{\alpha\beta}(j) S_{\beta\alpha}(j) \rightarrow -\frac{J_H}{N} \sum_j \left[ (f_{i\alpha}^\dagger f_{ja})(f_{j\beta}^\dagger f_{i\beta}) + \tilde{\alpha} \tilde{\beta}(f_{i\alpha}^\dagger f_{j\beta})(f_{j\beta} f_{i\alpha}) \right] \tag{64}
\]

where we’ve introduced the notation \(\tilde{\alpha} = \text{Sgn}(\alpha)\) and have shown how the interactions are expanded into particle-hole and particle-particle channels. Notice how the interactions are equally divided between particle-hole and particle-particle channels. When we carry out the Hubbard Stratonovich decoupling, in each of these terms, we obtain

\[
H_K \to \sum_j \left[ c_{j\alpha}^\dagger \left( V_j f_{ja} + \tilde{\alpha} \Delta_j^K f_{j\alpha}^\dagger \right) + \text{H.c.} \right] + N \left( \frac{|V_j|^2 + |\Delta_j|^2}{J_K} \right)
\]

\[
H_H \to \sum_{(i,j)} \left[ t_{ij} f_{i\alpha}^\dagger f_{ja} + \Delta_{ij} \tilde{\alpha} f_{i\alpha}^\dagger f_{j\alpha}^\dagger + \text{H.c.} \right] + N \left( \frac{|t_{ij}|^2 + |\Delta_{ij}|^2}{J_H} \right) \tag{65}
\]

At each site, we can always rotate the f-electrons in particle-hole space to remove the “Kondo pairing” component and set \(\Delta_j^K = 0\), but the pairing terms in the Heisenberg component can not be eliminated. This mean-field theory describes a kind of Kondo stabilized spin-liquid \[47\].

The physical picture is as follows: in practice, a spin-liquid is unstable to magnetism, but its happy co-existence with the Kondo effect brings its energy below that of the antiferromagnet. The hybridization of the f with the conduction sea converts the spinons of the spin-liquid into charged fermions. The \(t_{ij}\) terms describe various kind of exotic density waves. The \(\Delta_{ij}\) terms now describe pairing amongst the composite fermions.

To develop a simple theory of the superconducting state, we restrict our attention to uniform, static saddle points, dropping the \(t_{ij}\). Lets look at the resulting mean-field theory. In two dimensions, this becomes

\[
H = \sum_{k\alpha>0} \left( \tilde{c}_{k\alpha}^\dagger , \tilde{f}_{k\alpha}^\dagger \right) \left[ \frac{\epsilon_k \tau_3}{V \tau_1} \tilde{W} \cdot \tilde{\tau} + \Delta_{ik} \tau_1 \right] \left( \tilde{c}_{k\alpha}, \tilde{f}_{k\alpha} \right) + N_i N \left( \frac{|V|^2}{J_K} + 2 \frac{|\Delta_H|^2}{J_H} \right) \tag{66}
\]

where

\[
\tilde{c}_{k\alpha}^\dagger = (c_{k\alpha}^\dagger, \tilde{\alpha} c_{-k,-\alpha}), \quad \tilde{f}_{k\alpha}^\dagger = (f_{k\alpha}^\dagger, \tilde{\alpha} f_{-k,-\alpha}) \tag{67}
\]

are Nambu spinors for the conduction and f-electrons. The vector \(\tilde{W}\) of Lagrange multipliers couples to the isospin of the f-electrons: stationarity of the Free energy with respect to this variable imposes the mean-field constraint that \(\langle \tilde{f}^\dagger \tilde{\tau} \tilde{f} \rangle = 0\). The function \(\Delta_{ik} = A_k (\cos k_x - \)
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\[ \cos k_y \] is the f-electron pair wavefunction. Here we've chosen a d-wave form-factor. For this choice, the local f pair density automatically vanishes and so we need only choose \( \vec{w} = (0, 0, \lambda) \), where \( \lambda \) couples to \( \tau_3 \) (imposing the constraint \( n_f = N/2 \)). We could have also tried an extended extended s-wave pair wavefunction, but in this case, the induced s-wave pair density becomes finite, and the effect of the \( \vec{w} \) constraint is to suppress the transition temperature. By seeking stationary points in the free energy with respect to variations in \( \Delta_H \), \( V \) and \( \lambda \) one can derive the phase diagram for d-wave pairing, shown in Fig. 13. The mean-field theory shows that superconductivity develops at the interface between the Fermi liquid and the spin liquid.

5 Topological Kondo Insulators

One of the areas of fascinating development in the last few years, is the discovery that Kondo insulators can develop topological order to form a Topological Kondo insulator. Topological order refers to the idea that a quantum mechanical ground-state can develop a non-trivial topology. One of the defining features of topological ground-states is the development of protected surface states. The best known example of topological order is the integer quantum Hall effect, where an integer filled Landau level develops topological order that is responsible for the robust quantization of the Quantum Hall effect \[48–50\]. In a remarkable series of discoveries in 2006, \[51–58\] it became clear that strong spin orbit coupling can play the role of a synthetic magnetic field, so that band insulators can also develop a non-trivial topology while preserving time-reversal symmetry. Such \( Z_2 \) topological band insulators are defined by a single topological \( Z_2 = \pm 1 \) index that is positive in conventional insulators, but reverses in topological \( Z_2 \) insulators. This topological feature manifests itself through the formation of robust conducting surface states.

In 2007, Liang Fu and Charles Kane showed that if an insulator has both time reversal and inversion symmetry \[58\], this \( Z_2 \) index is uniquely determined by the parities \( \delta_{in} \) of the Bloch states at the high symmetry points \( \Gamma_i \) of the valence band which determine a “\( Z_2 \) index”

\[
Z_2 = \prod_{\Gamma_i} \delta(\Gamma_i) = \begin{cases} 
+1 & \text{conventional insulator} \\
-1 & \text{topological insulator} 
\end{cases}
\]

**Fu Kane formula for the \( Z_2 \) index of topological insulators**

where \( \delta(\Gamma_i) = \prod_n \delta_{in} \) is the the product of the parities of the of the occupied bands at the high-symmetry points in the Brillouin zone. This formula allows one to determine whether an insulator state is topological, merely by checking whether the index \( Z_2 = -1 \), without a detailed knowledge of the ground-state wavefunction.

It used to be thought that Kondo insulators could be regarded as “renormalized silicon”. The discovery of topological insulators forced a re-evaluation of this viewpoint. The large spin orbit coupling, and the odd-parity of the f-states led to the proposal, by Dzero, Sun, Galitski and the author, \[59\] that Kondo insulators can become topologically ordered. The Fu-Kane formula has
a special significance for Kondo insulators, which contain odd parity f-electrons hybridizing with even parity d-electrons. Each time an f-electron crosses through the band-gap, exchanging with a conduction d-state, this changes the $Z_2$ index, making it highly likely that certain Kondo insulators are topological. The oldest known Kondo insulator SmB$_6$, discovered almost 50 years ago was well known to possess a mysterious low temperature conductivity plateau [60,61], and the idea that this system might be a topological Kondo insulator provided an exciting way of explaining this old mystery. The recent observation of robust [62, 63] conducting surface states in the oldest Kondo insulator SmB$_6$ supports one of the key elements of this prediction, prompting a revival of interest in Kondo insulators as a new route for studying the interplay of strong interactions and topological order.

SmB$_6$ is really a mixed valent system, which takes us a little beyond the scope of this lecture. One of the other issues with SmB$_6$, is that its local crystal field configuration is likely to be a $\Gamma_8$ quartet state [64], rather than a Kramers doublet. Nevertheless, key elements of its putative topological Kondo insulating state are nicely illustrated by a spin-orbit coupled Kondo-Heisenberg model, describing the interaction of Kramer’s doublet f-states with a d-band. The model is essentially identical with (Eq. 63)

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \psi_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + J_K \sum_{\mathbf{j}} \psi_{j\alpha}^\dagger \psi_{j\beta} S_{\beta\alpha}(j) + J_H \sum_{i,j} S_{\alpha\beta}(i) S_{\beta\alpha}(j)$$

with an important modification that takes into account the large spin-orbit coupling and the odd-parity of the f-states. This forces the local Wannier states $\psi_{j\alpha}$, that exchange spin with the local moment to be odd parity combinations of nearest neighbour conduction electrons, given by

$$\psi_{j\alpha}^\dagger = \sum_{i\sigma} c_{i\sigma}^\dagger \Phi_{\alpha\sigma}(\mathbf{R}_i - \mathbf{R}_j)$$

We’ll consider a simplified model with the form factor

$$\Phi(\mathbf{R}) = \begin{cases} -i\hat{R} \cdot \hat{\sigma}, & \mathbf{R} \in \text{n.n} \\ 0 & \text{otherwise} \end{cases}$$

This form factor describes the spin-orbit mixing between states with orbital angular momentum $l$ differing by one, such as $f$ and $d$ or $p$ and $s$ orbitals. The odd-parity of the form-factor $\Phi(\mathbf{R}) = -\Phi(-\mathbf{R})$ derives from the odd-parity $f$- orbitals, while the prefactor $-i$ ensures that the hybridization is invariant under time-reversal. The Fourier transform of this Form factor, $\Phi(\mathbf{k}) = \sum_{\mathbf{R}} \Phi(\mathbf{R}) e^{-i\mathbf{k}\cdot\mathbf{R}}$ is then

$$\Phi(\mathbf{k}) = \vec{s}_k \cdot \hat{\sigma}$$

where the s-vector $\vec{s}_k = (\sin k_1, \sin k_2, \sin k_3)$ is the periodic equivalent of the unit momentum vector $\hat{k}$. Notice how $\vec{s}(\Gamma_i) = 0$ vanishes at the high symmetry points.

The resulting mean-field Hamiltonian takes the form

$$H_{TKI} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger h(\mathbf{k}) \psi_{\mathbf{k}} + N_s \left[ \left( \frac{V^2}{J_K} + \frac{3\lambda^2}{J_H} - \lambda Q \right) \right]$$
where $\psi_k^\dagger = (c_k^\dagger, f_k^\dagger)$ and

$$h(k) = \begin{pmatrix}
\epsilon_k & V \sigma \cdot s_k \\
V \sigma \cdot s_k & \epsilon_{f(k)}
\end{pmatrix}$$

(74)

while $\epsilon_{f(k)} = 2t_f(c_x + c_y + c_z) + \lambda (c_l \equiv \cos k_l)$ is the dispersion of the f-state resulting from a mean-field decoupling of the intersite Heisenberg coupling in the particle-hole channel. For small $k$, the hybridization in Hamiltonian $h(k)$ takes the form $V \sigma \cdot k$, a form which closely resembles the topologically non-trivial triplet p-wave gap structure of superfluid He-3B. Like He-3B, the hybridization only develops at low temperatures, making SmB$_6$ an adaptive insulator.

**Fig. 14:** (a) When the d-band is above the filled f-band, a trivial insulator is formed. (b) When the d-band crosses the f-band at the three X-points, the $Z_2$ parity changes sign, giving rise to a topological insulator.

Let us for the moment treat $h(k)$ as a rigid band structure. Suppose the f-band were initially completely filled, with a completely empty d-band above it. (See Fig. 14 a). This situation corresponds to a conventional band insulator with $Z_2 = +1$. Next, let us lower the d-conduction band until the two bands cross at a high symmetry point, causing the gap to close, and then to re-open. We know, from dHvA studies of the iso-electronic material LaB$_6$ [65] (whose band-structure is identical to SmB$_6$ but lacks the magnetic f-electrons), from ARPES studies [66,68], that in SmB$_6$, the d-band crosses through the Fermi surface at at the three X points. Once the d-band is lowered through the f-band around the three X points, the odd-parity f-states at the X point move up into the conduction band, to be replaced by even-parity d-states. This changes the sign of $Z_2 \rightarrow (-1)^3 = -1$, producing a topological ground-state. Moreover, since there are three crossing, we expect there to be three spin-polarized surface Dirac cones.

We end by noting that at the time of writing, our understanding of the physics SmB$_6$ is in rapid flux on both the experimental and theoretical front. Spin resolved ARPES [69] measurements have detected the presence of spin-textures in the surface Fermi surfaces around the surface $\bar{X}$ point, a strong sign of topologically protected surface states. Two recent theoreti-
cal works \cite{70,71} have shown that the spin textures seen in these experiments are consistent with a spin-quartet ground-state in SmB$_6$. Despite this progress, consensus on the topological nature of SmB$_6$ has not yet been achieved, and competing groups have offered alternate interpretations of the data, including the possibility of polarity-driven surface metallicity \cite{72} and Rashba-split surface states, both, of a non-topological origin. \cite{73}. Another area of experimental controversy concerns the possible de-Haas van Alphen oscillations created by surface topological excitations, with one report of the detection of surface de Haas van Alphen signals \cite{74} and a recent, very remarkable report of bulk de Haas van Alphen signals associated with unhybridized, quantum critical d-electrons \cite{75}.

6 Co-existing magnetism and Kondo effect

In this short lecture, I’ve given a quick introduction to the paramagnetic phases of heavy fermion systems. One of the of major open questions in heavy fermion and Kondo lattice physics concerns the physics of magnetism, and the right way to describe the development of magnetism within these materials. There is growing evidence that magnetism and the Kondo effect can co-exist, sometimes homogeneously, and sometimes inhomogeneously. For example, In the 115 superconductor CeRhIn$_5$ there is evidence for a microscopic and homogeneous coexistence of local moment magnetism and heavy fermion superconductivity under pressure \cite{76}; By contrast, in the geometrically frustrated CePdAl \cite{77,78}, two thirds of the Cerium sites spontaneously develop magnetism, leaving the other third to undergo a Kondo effect \cite{79}. What is the right way to describe these co-existent states?

One possibility that I have worked on with Aline Ramires \cite{80,81} is the use of a “supersymmetric” spin representation of the spin

\[ S_{\alpha\beta} = f^{\dagger}_{\alpha} f_{\beta} + b^{\dagger}_{\alpha} b_{\beta} \]  

where the $f^{\dagger}_{\alpha}$ and $b^{\dagger}_{\alpha}$ are fermionic and bosonic creation operators. Such a representation permits in principle, the existence of “two fluid” ground-states, involving a Gutzwiller projection of bosonic and fermionic wavefunctions

\[ |\Psi\rangle = \mathcal{P}_G |\Psi_F\rangle |\Psi_B\rangle, \]  

where $|\Psi_F\rangle$ is the fermionic component of the wavefunction describing the Kondo quenched local moments while $|\Psi_B\rangle$ describes the formation of long-range magnetic correlations within a bosonic RVB wavefunction, while

\[ \mathcal{P}_G = \int \prod_j \frac{d\theta_j}{2\pi} e^{i\theta_j(n_k+n_f-1)} \]  

is a Gutzwiller projection operator onto the state with one spin per site. We have been trying to describe such mixed state wavefunctions in the large-$N$ limit, seeking saddle point solutions where a bosonic and fermionic fluid co-exist \cite{81}. One of the ideas that emerges from this kind
of approach, is the possibility that the soft modes at a Quantum Critical point might develop fermionic character, a kind of emergent supersymmetry [82].

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