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# HEAVY FERMIONS: ELECTRONS AT THE EDGE OF MAGNETISM II

Lecture Notes III.

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1. Doniach's Kondo Lattice Hypothesis
2. The Large N Kondo Lattice
3. The Charge of the f-electron.
4. Optical Conductivity.
5. Heavy fermion Superconductivity using large N.

details about the local Fermi liquid that forms, we refer the reader to the accompanying chapter on the Kondo effect by Jones (2007).

### 2.2.4 Doniach's Kondo lattice concept

The discovery of heavy-electron metals prompted Doniach (1977) to make the radical proposal that heavy-electron materials derive from a dense lattice version of the Kondo effect, described by the **Kondo Lattice model** (Kasuya, 1956)

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_j \vec{S}_j \cdot c^{\dagger}_{\mathbf{k}\alpha} \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}'\beta} \mathrm{e}^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_j} \tag{58}$$

In effect, Doniach was implicitly proposing that the key physics of heavy-electron materials resides in the interaction of neutral local moments with a charged conduction electron sea.

Most local moment systems develop an antiferromagnetic order at low temperatures. A magnetic moment at location $\mathbf{x}_0$ induces a wave of 'Friedel' oscillations in the electron spin density (Figure 14)

$$\langle \vec{\sigma}(\mathbf{x}) \rangle = -J\chi(\mathbf{x}-\mathbf{x}_0)\langle \vec{S}(\mathbf{x}_0) \rangle \tag{59}$$

where

$$\chi(\mathbf{x}) = 2\sum_{\mathbf{k},\mathbf{k}'} \left( \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}'})}{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}}} \right) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \tag{60}$$

is the nonlocal susceptibility of the metal. The sharp discontinuity in the occupancies $f(\epsilon_k)$ at the Fermi surface is responsible for Friedel oscillations in induced spin density that decay with a power law

$$\langle \vec{\sigma}(r) \rangle \sim -J\rho \frac{\cos 2k_{\mathrm{F}} r}{|k_{\mathrm{F}} r|^3} \tag{61}$$

where $\rho$ is the conduction electron density of states and $r$ is the distance from the impurity. If a second local moment is introduced at location $\mathbf{x}$, it couples to this Friedel oscillation with energy $J\langle \vec{S}(\mathbf{x}) \cdot \vec{\sigma}(x) \rangle$, giving rise to the 'RKKY' (Ruderman and Kittel, 1954; Kasuya, 1956; Yosida, 1957) magnetic interaction,

$$H_{\mathrm{RKKY}} = \overbrace{-J^2\chi(\mathbf{x}-\mathbf{x}')}^{J_{\mathrm{RKKY}}(\mathbf{x}-\mathbf{x}')} \vec{S}(\mathbf{x}) \cdot \vec{S}(\mathbf{x}') \tag{62}$$

where

$$J_{\mathrm{RKKY}}(r) \sim -J^2\rho \frac{\cos 2k_{\mathrm{F}} r}{k_{\mathrm{F}} r} \tag{63}$$

In alloys containing a dilute concentration of magnetic transition-metal ions, the oscillatory RKKY interaction gives rise to a frustrated, glassy magnetic state known as a *spin glass*. In dense systems, the RKKY interaction typically gives rise to an ordered antiferromagnetic state with a Néel temperature $T_{\mathrm{N}}$ of the order $J^2\rho$. Heavy-electron metals narrowly escape this fate.

Doniach argued that there are two scales in the Kondo lattice, the single-ion Kondo temperature $T_{\mathrm{K}}$ and $T_{\mathrm{RKKY}}$, given by

$$\begin{aligned} T_{\mathrm{K}} &= D\mathrm{e}^{-1/(2J\rho)} \\ T_{\mathrm{RKKY}} &= J^2\rho \end{aligned} \tag{64}$$

When $J\rho$ is small, then $T_{\mathrm{RKKY}}$ is the largest scale and an antiferromagnetic state is formed, but, when the $J\rho$ is large, the Kondo temperature is the largest scale so a dense Kondo lattice ground state becomes stable. In this paramagnetic state, each site resonantly scatters electrons with a phase shift $\sim\pi/2$. Bloch's theorem then insures that the resonant elastic scattering at each site acts coherently, forming a renormalized band of width $\sim T_{\mathrm{K}}$ (Figure 15).

As in the impurity model, one can identify the Kondo lattice ground state with the large $U$ limit of the Anderson lattice model. By appealing to adiabaticity, one can then link the excitations to the small $U$ Anderson lattice model. According to this line of argument, the quasiparticle Fermi surface volume must count the number of conduction and f electrons (Martin, 1982), even in the large $U$ limit, where it corresponds to the number of electrons *plus* the number of spins

$$2\frac{\mathcal{V}_{\mathrm{FS}}}{(2\pi)^3} = n_e + n_{\mathrm{spins}} \tag{65}$$

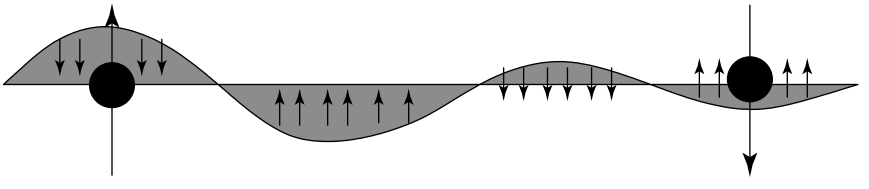


**Figure 14.** Spin polarization around magnetic impurity contains Friedel oscillations and induces an RKKY interaction between the spins.

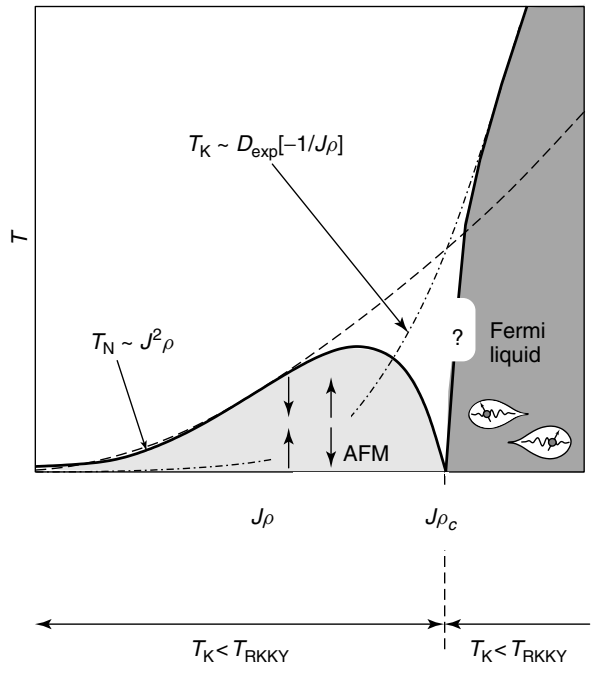



**Figure 15.** Doniach diagram, illustrating the antiferromagnetic regime, where $T_K < T_{RKKY}$ and the heavy-fermion regime, where $T_K > T_{RKKY}$. Experiment has told us in recent times that the transition between these two regimes is a quantum critical point. The effective Fermi temperature of the heavy Fermi liquid is indicated as a solid line. Circumstantial experimental evidence suggests that this scale drops to zero at the antiferromagnetic quantum critical point, but this is still a matter of controversy.

Using topology, and certain basic assumptions about the response of a Fermi liquid to a flux, Oshikawa (2000) was able to short circuit this tortuous path of reasoning, proving that the Luttinger relationship holds for the Kondo lattice model without reference to its finite $U$ origins.

There are, however, aspects to the Doniach argument that leave cause for concern:

- It is purely a comparison of energy scales and does not provide a detailed mechanism connecting the heavy-fermion phase to the local moment AFM.
- Simple estimates of the value of $J\rho$ required for heavy-electron behavior give an artificially large value of the coupling constant $J\rho \sim 1$. This issue was later resolved by the observation that large spin degeneracy $2j+1$ of the spin-orbit coupled moments, which can be as large as $N = 8$ in Yb materials, enhances the rate of scaling to strong coupling, leading to a Kondo temperature (Coleman, 1983)

$$T_K = D(NJ\rho)^{\frac{1}{N}} \exp\left[-\frac{1}{NJ\rho}\right] \qquad (66)$$

  Since the scaling enhancement effect stretches out across decades of energy, it is largely robust against crystal fields (Mekata *et al*., 1986).
- Nozières' exhaustion paradox (Nozières, 1985). If one considers each local moment to be magnetically screened by a cloud of low-energy electrons within an energy $T_K$ of the Fermi energy, one arrives at an 'exhaustion paradox'. In this interpretation, the number of electrons available to screen each local moment is of the order $T_K/D \ll 1$ per unit cell. Once the concentration of magnetic impurities exceeds $\frac{T_K}{D} \sim 0.1\%$ for ($T_K = 10\,\mathrm{K}$, $D = 10^4\,\mathrm{K}$), the supply of screening electrons would be exhausted, logically excluding any sort of dense Kondo effect. Experimentally, features of single-ion Kondo behavior persist to much higher densities. The resolution to the exhaustion paradox lies in the more modern perception that spin screening of local moments extends *up* in energy, from the Kondo scale $T_K$ out to the bandwidth. In this respect, Kondo screening is reminiscent of Cooper pair formation, which involves electron states that extend upward from the gap energy to the Debye cutoff. From this perspective, the Kondo length scale $\xi \sim v_F/T_K$ is analogous to the coherence length of a superconductor (Burdin, Georges and Grempel, 2000), defining the length scale over which the conduction spin and local moment magnetization are coherent without setting any limit on the degree to which the correlation clouds can overlap (Figure 16).

## 2.3 The large $N$ Kondo lattice

### *2.3.1 Gauge theories, large N, and strong correlation*

The 'standard model' for metals is built upon the expansion to high orders in the strength of the interaction. This approach, pioneered by Landau, and later formulated in the language of finite temperature perturbation theory by Landau (1957), Pitaevskii (1960), Luttinger and Ward (1960), and Nozières and Luttinger (1962), provides the foundation for our understanding of metallic behavior in most conventional metals.

The development of a parallel formalism and approach for strongly correlated electron systems is still in its infancy, and there is no universally accepted approach. At the heart of the problem are the large interactions, which effectively remove large tracts of Hilbert space and impose strong constraints on the low-energy electronic dynamics. One way to describe these highly constrained Hilbert spaces is through the use of gauge theories. When written as a field theory, local constraints manifest themselves as locally conserved quantities. General principles link these conserved quantities

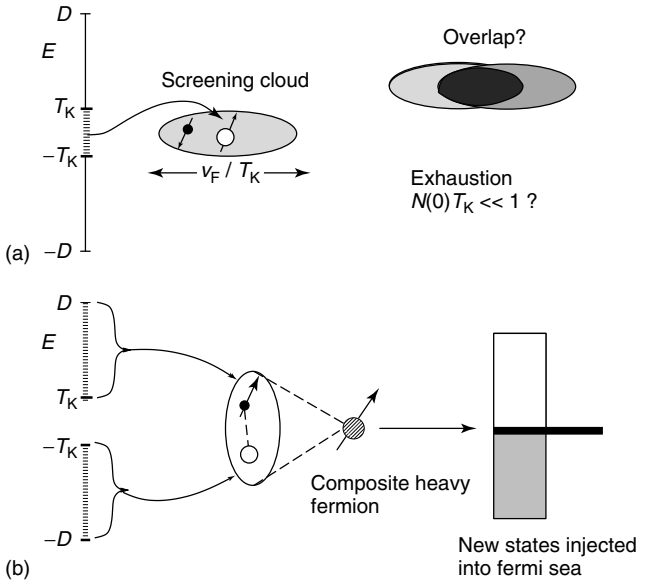



**Figure 16.** Contrasting (a) the 'screening cloud' picture of the Kondo effect with (b) the composite fermion picture. In (a), low-energy electrons form the Kondo singlet, leading to the exhaustion problem. In (b), the composite heavy electron is a highly localized bound-state between local moments and high-energy electrons, which injects new electronic states into the conduction sea at the chemical potential. Hybridization of these states with conduction electrons produces a singlet ground state, forming a Kondo resonance in the single impurity, and a coherent heavy electron band in the Kondo lattice.

with a set of gauge symmetries. For example, in the Kondo lattice, if a spin $S = 1/2$ operator is represented by fermions,

$$\vec{S}_j = f^\dagger_{j\alpha} \left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta} f_{j\beta} \tag{67}$$

then the representation must be supplemented by the constraint $n_f(j) = 1$ on the conserved f number at each site. This constraint means one can change the phase of each f fermion at each site arbitrarily

$$f_j \to \mathrm{e}^{i\phi_j} f_j \tag{68}$$

without changing the spin operator $\vec{S}_j$ or the Hamiltonian. This is the local gauge symmetry.

Similar issues also arise in the infinite $U$ Anderson or Hubbard models where the 'no double occupancy' constraint can be established by using a slave boson representation (Barnes, 1976; Coleman, 1984) of Hubbard operators:

$$X_{\sigma 0}(j) = f^\dagger_{j\sigma} b_j, \qquad X_{0\sigma}(j) = b^\dagger_j f_{j\sigma} \tag{69}$$

where $f^\dagger_{j\sigma}$ creates a singly occupied f state, $f^\dagger_{j\sigma}|0\rangle \equiv |f^1, j\sigma\rangle$, while $b^\dagger$ creates an empty $f^0$ state, $b^\dagger_j|0\rangle = |f^0, j\rangle$. In the slave boson, the gauge charges

$$Q_j = \sum_\sigma f^\dagger_{j\sigma} f_{j\sigma} + b^\dagger_j b_j \tag{70}$$

are conserved and the physical Hilbert space corresponds to $Q_j = 1$ at each site. The gauge symmetry is now $f_{j\sigma} \to e^{i\theta_j} f_{j\sigma}$, $b_j \to e^{i\theta_j} b_j$. These two examples illustrate the link between strong correlation and gauge theories.

$$\begin{aligned} \text{Strong correlation} &\leftrightarrow \text{Constrained Hilbert space} \\ &\leftrightarrow \text{Gauge theories} \end{aligned} \tag{71}$$

A key feature of these gauge theories is the appearance of 'fractionalized fields', which carry either spin or charge, but not both. How, then, can a Landau–Fermi liquid emerge within a Gauge theory with fractional excitations?

Some have suggested that Fermi liquids cannot reconstitute themselves in such strongly constrained gauge theories. Others have advocated against gauge theories, arguing that the only reliable way forward is to return to 'real-world' models with a full fermionic Hilbert space and a finite interaction strength. A third possibility is that the gauge theory approach is valid, but that heavy quasiparticles emerge as bound-states of gauge particles. Quite independently of one's position on the importance of gauge theory approaches, the Kondo lattice poses a severe computational challenge, in no small part, because of the absence of any small parameter for resumed perturbation theory. Perturbation theory in the Kondo coupling constant $J$ always fails below the Kondo temperature. How, then, can one develop a controlled computational tool to explore the transition from local moment magnetism to the heavy Fermi liquid?

One route forward is to seek a family of models that interpolates between the models of physical interest, and a limit where the physics can be solved exactly. One approach, as we shall discuss later, is to consider Kondo lattices in variable dimensions $d$, and expand in powers of $1/d$ about the limit of infinite dimensionality (Georges, Kotliar, Krauth and Rozenberg, 1996; Jarrell, 1995). In this limit, electron self-energies become momentum independent, the basis of the DMFT. Another approach, with the advantage that it can be married with gauge theory, is the use of large $N$ expansions. The idea here is to generalize the problem to a family of models in which the f-spin degeneracy $N = 2j + 1$ is artificially driven to infinity. In this extreme limit, the key physics is captured as a mean-field theory, and finite $N$ properties are obtained through an expansion in the small parameter $1/N$. Such large $N$ expansions have played an important role in the context of the spherical model of statistical mechanics (Berlin and Kac, 1952) and in field theory (Witten, 1978). The next section discusses how the

gauge theory of the Kondo lattice model can be treated in a large $N$ expansion.

### 2.3.2 *Mean-field theory of the Kondo lattice*

Quantum large $N$ expansions are a kind of semiclassical limit, where $1/N \sim \hbar$ plays the role of a synthetic Planck's constant. In a Feynman path integral

$$\langle x_f(t)|x_i, 0\rangle = \int \mathcal{D}[x] \exp\left[\frac{i}{\hbar} S[x, \dot{x}]\right] \tag{72}$$

where $S$ is the classical action and the quantum action $A = \frac{1}{\hbar}S$ is 'extensive' in the variable $\frac{1}{\hbar}$. When $\frac{1}{\hbar} \to \infty$, fluctuations around the classical trajectory vanish and the transition amplitude is entirely determined by the classical action to go from $i$ to $f$. A large $N$ expansion for the partition function $Z$ of a quantum system involves a path integral in imaginary time over the fields $\phi$

$$Z = \int \mathcal{D}[\phi] \mathrm{e}^{-NS[\phi,\dot{\phi}]} \tag{73}$$

where $NS$ is the action (or free energy) associated with the field configuration in space and time. By comparison, we see that the large $N$ limit of quantum systems corresponds to an alternative classical mechanics, where $1/N \sim \hbar$ emulates Planck's constant and new types of collective behavior not pertinent to strongly interacting electron systems start to appear.

Our model for a Kondo lattice of spins localized at sites $j$ is

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_j H_I(j) \tag{74}$$

where

$$H_I(j) = \frac{J}{N} S_{\alpha\beta}(j) c^\dagger_{j\beta} c_{j\alpha} \tag{75}$$

is the Coqblin Schrieffer form of the Kondo interaction Hamiltonian (Coqblin and Schrieffer, 1969) between an f spin with $N = 2j + 1$ spin components and the conduction sea. The spin of the local moment at site $j$ is represented as a bilinear of Abrikosov pseudofermions

$$S_{\alpha\beta}(j) = f^\dagger_{j\alpha} f_{j\beta} - \frac{n_f}{N}\delta_{\alpha\beta} \tag{76}$$

and

$$c^\dagger_{j\sigma} = \frac{1}{\sqrt{\mathcal{N}}} \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} \mathrm{e}^{-i\mathbf{k}\cdot\vec{R}_j} \tag{77}$$

creates an electron localized at site $j$, where $\mathcal{N}$ is the number of sites.

Although this is a theorists' idealization – a 'spherical cow approximation', it nevertheless captures key aspects of the physics. This model ascribes a spin degeneracy of $N = 2j + 1$ to both the f electrons *and* the conduction electrons. While this is justified for a single impurity, a more realistic lattice model requires the introduction of Clebsch–Gordon coefficients to link the spin-1/2 conduction electrons with the spin-$j$ conduction electrons.

To obtain a mean-field theory, each term in the Hamiltonian must scale as $N$. Since the interaction contains two sums over the spin variables, this criterion is met by rescaling the coupling constant replacing $J \to \frac{\tilde{J}}{N}$. Another important aspect to this model is the constraint on charge fluctuations, which in the Kondo limit imposes the constraint $n_f = 1$. Such a constraint can be imposed in a path integral with a Lagrange multiplier term $\lambda(n_f - 1)$. However, with $n_f = 1$, this is not extensive in $N$, and cannot be treated using a mean-field value for $\lambda$. The resolution is to generalize the constraint to $n_f = Q$, where $Q$ is an integer chosen so that as $N$ grows, $q = Q/N$ remains fixed. Thus, for instance, if we are interested in $N = 2$, this corresponds to $q = n_f/N = \frac{1}{2}$. In the large $N$ limit, it is then sufficient to apply the constraint on the average $\langle n_f\rangle = Q$ through a static Lagrange multiplier coupled to the difference $(n_f - Q)$.

The next step is to carry out a 'Hubbard–Stratonovich' transformation on the interaction

$$H_I(j) = -\frac{J}{N}\left(c^\dagger_{j\beta} f_{j\beta}\right)\left(f^\dagger_{j\alpha} c_{j\alpha}\right) \tag{78}$$

Here, we have absorbed the term $-\frac{J}{N} n_f c^\dagger_{j\alpha} c_{j\alpha}$ derived from the spin-diagonal part of (equation (76)) by a shift $\mu \to \mu - \frac{Jn_f}{N^2}$ in the chemical potential. This interaction has the form $-gA^\dagger A$, with $g = \frac{J}{N}$ and $A = f^\dagger_{j\alpha} c_{j\alpha}$, which we factorize using a Hubbard–Stratonovich transformation,

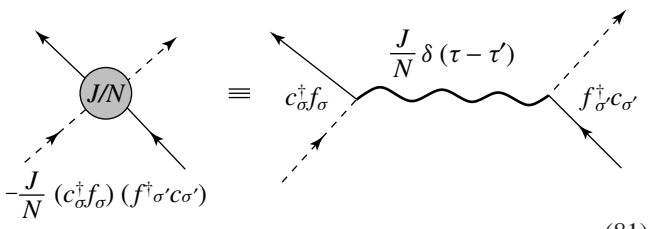
$$-gA^\dagger A \to A^\dagger V + \overline{V} A + \frac{\overline{V} V}{g} \tag{79}$$

so that (Lacroix and Cyrot, 1979; Read and Newns, 1983a)

$$H_I(j) \to H_I[V, j] = \overline{V}_j \left(c^\dagger_{j\sigma} f_{j\sigma}\right) + \left(f^\dagger_{j\sigma} c_{j\sigma}\right) V_j + N\frac{\overline{V}_j V_j}{J} \tag{80}$$

This is an exact transformation, provided the $V_j(\tau)$ are treated as fluctuating variables inside a path integral. The $V_j$ can be regarded as a spinless exchange boson for the Kondo effect. In the parallel treatment of the infinite Anderson model (Coleman, 1987a), $V_j = Vb_j$ is the 'slave boson' field associated with valence fluctuations.

In diagrams:




(81)

The path integral for the Kondo lattice is then

$$Z = \int \mathcal{D}[V,\lambda] \overbrace{\int \mathcal{D}[c,f] \exp\left[-\int_0^\beta \left(\sum_{k\sigma} c^\dagger_{\mathbf{k}\sigma}\partial_\tau c_{\mathbf{k}\sigma} + \sum_{j\sigma} f^\dagger_{j\sigma}\partial_\tau f_{j\sigma} + H[V,\lambda]\right)\right]}^{=\mathrm{Tr}\left[Texp\left(-\int_0^\beta H[V,\lambda]d\tau\right)\right]} \tag{82}$$

where

$$H[V,\lambda] = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_j \left(H_I[V_j, j] + \lambda_j[n_f(j) - Q]\right) \tag{83}$$

This is the 'Read–Newns' path integral formulation (Read and Newns, 1983a; Auerbach and Levin, 1986) of the Kondo lattice model. The path integral contains an outer integral $\int \mathcal{D}[V,\lambda]$ over the gauge fields $V_j$ and $\lambda_j(\tau)$, and an inner integral $\int \mathcal{D}[c,f]$ over the fermion fields moving in the environment of the gauge fields. The inner path integral is equal to a trace over the time-ordered exponential of $H[V,\lambda]$.

Since the action in this path integral grows extensively with $N$, the large $N$ limit is saturated by the saddle point configurations of $V$ and $\lambda$, eliminating the the outer integral in equation (83). We seek a translationally invariant, static, saddle point, where $\lambda_j(\tau) = \lambda$ and $V_j(\tau) = V$. Since the Hamiltonian is static, the interior path integral can be written as the trace over the Hamiltonian evaluated at the saddle point,

$$Z = \mathrm{Tr} e^{-\beta H_{\mathrm{MFT}}} \qquad (N \to \infty) \tag{84}$$

where

$$H_{\mathrm{MFT}} = H[V,\lambda] = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{j,\sigma}\left(\overline{V} c^\dagger_{j\sigma} f_{j\sigma} + V f^\dagger_{j\sigma} c_{j\sigma} + \lambda f^\dagger_{j\sigma} f_{j\sigma}\right) + Nn\left(\frac{\overline{V}V}{J} - \lambda_o q\right) \tag{85}$$

The saddle point is determined by the condition that the Free energy $F = -T\ln Z$ is stationary with respect to variations in $V$ and $\lambda$. To impose this condition, we need to diagonalize $H_{MFT}$ and compute the Free energy. First we rewrite the mean-field Hamiltonian in momentum space,

$$H_{\mathrm{MFT}} = \sum_{\mathbf{k}\sigma} \left(c^\dagger_{\mathbf{k}\sigma}, f^\dagger_{\mathbf{k}\sigma}\right) \begin{bmatrix} \epsilon_{\mathbf{k}} & \overline{V} \\ V & \lambda \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} + Nn\left(\frac{\overline{V}V}{J} - \lambda q\right) \tag{86}$$

where

$$f^\dagger_{\vec{k}\sigma} = \frac{1}{\sqrt{N}} \sum_j f^\dagger_{j\sigma} e^{i\vec{k}\cdot\vec{R}_j} \tag{87}$$

is the Fourier transform of the f-electron field. This Hamiltonian can then be diagonalized in the form

$$H_{\mathrm{MFT}} = \sum_{\mathbf{k}\sigma} \left(a^\dagger_{\mathbf{k}\sigma}, b^\dagger_{\mathbf{k}\sigma}\right) \begin{bmatrix} E_{\mathbf{k}+} & 0 \\ 0 & E_{\mathbf{k}-} \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}\sigma} \\ b_{\mathbf{k}\sigma} \end{pmatrix} + N\mathcal{N}_s\left(\frac{|V|^2}{J} - \lambda q\right) \tag{88}$$

where $a^\dagger_{\mathbf{k}\sigma}$ and $b^\dagger_{\mathbf{k}\sigma}$ are linear combinations of $c^\dagger_{\mathbf{k}\sigma}$ and $f^\dagger_{\vec{k}\sigma}$, which describe the quasiparticles of the theory. The momentum state eigenvalues $E = E_{k\pm}$ are the roots of the equation

$$\mathrm{Det}\left[E\underline{1} - \begin{pmatrix} \epsilon_{\mathbf{k}} & \overline{V} \\ V & \lambda \end{pmatrix}\right] = (E - \epsilon_{\mathbf{k}})(E - \lambda) - |V|^2 = 0 \tag{89}$$

so

$$E_{\mathbf{k}\pm} = \frac{\epsilon_{\mathbf{k}} + \lambda}{2} \pm \left[\left(\frac{\epsilon_{\mathbf{k}} - \lambda}{2}\right)^2 + |V|^2\right]^{\frac{1}{2}} \tag{90}$$

are the energies of the upper and lower bands. The dispersion described by these energies is shown in Figure 17. Notice that:

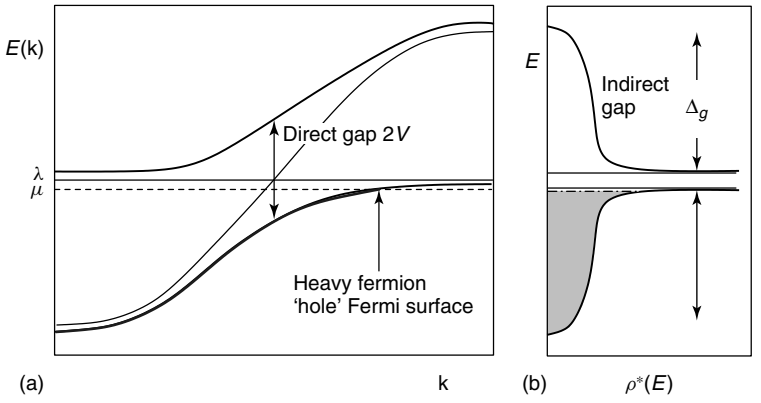



**Figure 17.** (a) Dispersion produced by the injection of a composite fermion into the conduction sea. (b) Renormalized density of states, showing 'hybridization gap' ($\Delta_g$).

- hybridization between the f-electron states and the conduction electrons builds an upper and lower Fermi band, separated by an indirect 'hybridization gap' of width $\Delta_g = E_g(+) - E_g(-) \sim T_{\rm K}$, where

$$E_g(\pm) = \lambda \pm \frac{V^2}{D_\mp} \tag{91}$$

  and $\pm D_\pm$ are the top and bottom of the conduction band. The 'direct' gap between the upper and lower bands is $2|V|$.
- From (89), the relationship between the energy of the heavy electrons ($E$) and the energy of the conduction electrons ($\epsilon$) is given by $\epsilon = E - |V|^2/(E-\lambda)$, so that the density of heavy-electron states $\rho^*(E) = \sum_{\mathbf{k},\pm}\delta(E - E^{(\pm)}_{\mathbf{k}})$ is related to the conduction electron density of states $\rho(\epsilon)$ by

$$\rho^*(E) = \rho\frac{{\rm d}\epsilon}{{\rm d}E} = \rho(\epsilon)\left(1 + \frac{|V|^2}{(E-\lambda)^2}\right) \sim \begin{cases} \rho\left(1+\frac{|V|^2}{(E-\lambda)^2}\right) & \text{outside hybridization gap,} \\ 0 & \text{inside hybridization gap,} \end{cases} \tag{92}$$

  so the 'hybridization gap' is flanked by two sharp peaks of approximate width $T_{\rm K}$.
- The Fermi surface volume **expands** in response to the injection of heavy electrons into the conduction sea,

$$Na^D\frac{V_{\rm FS}}{(2\pi)^3} = \left\langle \frac{1}{\mathcal{N}_s}\sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}\right\rangle = Q + n_c \tag{93}$$

  where $a^D$ is the unit cell volume, $n_{\mathbf{k}\sigma} = a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} + b^\dagger_{\mathbf{k}\sigma}b_{\mathbf{k}\sigma}$ is the quasiparticle number operator and $n_c$ is the number of conduction electrons per unit cell. More instructively, if $n_e = n_c/a^D$ is the electron density,

$$\underbrace{e^-\text{ density}}_{n_e} \quad = \quad \overbrace{N\frac{V_{\rm FS}}{(2\pi)^3}}^{\text{quasi particle density}} \quad - \quad \underbrace{\frac{Q}{a^D}}_{\text{positive background}} \tag{94}$$

  so the electron density $n_c$ divides into a contribution carried by the enlarged Fermi sea, whose enlargement is compensated by the development of a positively charged background. Loosely speaking, each neutral spin in the Kondo lattice has 'ionized' to produce $Q$ negatively charged heavy fermions, leaving behind a Kondo singlet of charge $+Qe$ (Figure 18).

To obtain $V$ and $\lambda$, we must compute the free energy

$$\frac{F}{N} = -T\sum_{\mathbf{k},\pm}\ln\left[1 + {\rm e}^{-\beta E_{\mathbf{k}\pm}}\right] + \mathcal{N}_s\left(\frac{|V|^2}{J} - \lambda q\right) \tag{95}$$

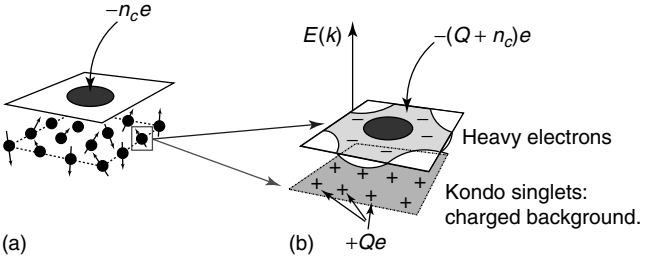



**Figure 18.** Schematic diagram from Coleman, Paul and Rech (2005a). (a) High-temperature state: small Fermi surface with a background of spins; (b) Low-temperature state, where large Fermi surface develops against a background of positive charge. Each spin 'ionizes' into $Q$ heavy electrons, leaving behind a a Kondo singlet with charge $+Qe$. (Reproduced from P. Coleman, I. Paul, and J. Rech, *Phys. Rev. B* **72**, 2005, 094430, copyright © 2005 by the American Physical Society, with permission of the APS.)

At $T = 0$, the free energy converges the ground-state energy $E_0$, given by

$$\frac{E_0}{N\mathcal{N}_s} = \int_{-\infty}^{0} \rho^*(E)E + \left(\frac{|V|^2}{J} - \lambda q\right) \tag{96}$$

Using equation (92), the total energy is

$$\begin{aligned}\frac{E_o}{N\mathcal{N}_s} &= \int_{-D}^{0} \mathrm{d}\epsilon\rho E\mathrm{d}E + \int_{-D}^{0} \mathrm{d}E\rho|V|^2\frac{E}{(E-\lambda)^2} \\ &\quad + \left(\frac{|V|^2}{J} - \lambda q\right) \\ &= \overbrace{-\frac{D^2\rho}{2}}^{E_c/(N\mathcal{N}_s)} + \overbrace{\frac{\Delta}{\pi}\ln\left(\frac{\lambda e}{T_{\mathrm{K}}}\right) - \lambda q}^{E_{\mathrm{K}}/(N\mathcal{N}_s)}\end{aligned} \tag{97}$$

where we have assumed that the upper band is empty and the lower band is partially filled. $T_{\mathrm{K}} = De^{-\frac{1}{J\rho}}$ as before. The first term in (97) is the conduction electron contribution to the energy $E_c/Nn_s$, while the second term is the lattice 'Kondo' energy $E_{\mathrm{K}}/N_{\mathcal{N}_s}$. If now we impose the constraint $\frac{\partial E_o}{\partial\lambda} = \langle n_f\rangle - Q = 0$ then $\lambda = \frac{\Delta}{\pi q}$ so that the ground-state energy can be written

$$\frac{E_{\mathrm{K}}}{N\mathcal{N}_s} = \frac{\Delta}{\pi}\ln\left(\frac{\Delta e}{\pi q T_{\mathrm{K}}}\right) \tag{98}$$

This energy functional has a 'Mexican Hat' form, with a minimum at

$$\Delta = \frac{\pi q}{e^2}T_{\mathrm{K}} \tag{99}$$

confirming that $\Delta \sim T_{\mathrm{K}}$. If we now return to the quasiparticle density of states $\rho^*$, we find it has the value

$$\rho^*(0) = \rho + \frac{q}{T_{\mathrm{K}}} \tag{100}$$

at the Fermi energy so the mass enhancement of the heavy electrons is then

$$\frac{m^*}{m} = 1 + \frac{q}{\rho T_{\mathrm{K}}} \sim \frac{qD}{T_{\mathrm{K}}} \tag{101}$$

### *2.3.3 The charge of the f electron*

How does the f electron acquire its charge? We have emphasized from the beginning that the charge degrees of freedom of the original f electrons are irrelevant, indeed, absent from the physics of the Kondo lattice. So how are charged f electrons constructed out of the states of the Kondo lattice, and how do they end up coupling to the electromagnetic field?

The large $N$ theory provides an intriguing answer. The passage from the original Hamiltonian equation (75) to the mean-field Hamiltonian equation (85) is equivalent to the substitution

$$\frac{J}{N}S_{\alpha\beta}(j)c^\dagger_{j\beta}c_{j\alpha} \longrightarrow \overline{V}f^\dagger_{j\alpha}c_{j\alpha} + Vc^\dagger_{j\alpha}\mathrm{f}_{j\alpha} \tag{102}$$

In other words, the composite combination of spin and conduction electron are contracted into a single Fermi field

$$\frac{J}{N}\overbrace{S_{\alpha\beta}(j)c_{j\beta}}^{\dagger} = \left(\frac{J}{N}f^\dagger_{j\alpha}\overbrace{f_{j\beta}c_{j\beta}}^{\dagger}\right) \to Vf^\dagger_{j\alpha} \tag{103}$$

The amplitude $V = \frac{J}{N}\overbrace{f_{j\beta}c_{j\beta}}^{\dagger} = -\frac{J}{N}\langle c^\dagger_{j\beta}f_{j\beta}\rangle$ involves electron states that extend over decades of energy out to the band edges. In this way, the f electron emerges as a composite bound-state of a spin and an electron. More precisely, in the long-time correlation functions,

$$\begin{aligned}&\langle\left[S_{\gamma\alpha}(i)c_{i\gamma}\right](t)\ \ \left[S_{\alpha\beta}(j)c^\dagger_{j\beta}\right](t')\rangle \\ &\xrightarrow{|t-t'|\gg\hbar/T_K} \frac{N|V^2|}{J^2}\langle f_{i\alpha}(t)f^\dagger_{j\alpha}(t')\rangle\end{aligned} \tag{104}$$

Such 'clustering' of composite operators into a single entity is well-known statistical mechanics as part of the operator product expansion (Cardy, 1996). In many-body physics, we are used to the clustering of fermions pairs into a composite boson, as in the BCS model of superconductivity, $-g\overbrace{\psi_\uparrow(x)\psi_\downarrow(x')} \to \Delta(x-x')$. The unfamiliar aspect of the Kondo effect is the appearance of a composite fermion.

The formation of these composite objects profoundly modifies the conductivity and plasma oscillations of the electron fluid. The Read–Newns path integral has two $U(1)$ gauge invariances – an external electromagnetic gauge invariance associated with the conservation of charge and an internal gauge invariance associated with the local constraints. The f electron couples to the internal gauge fields rather than the external electromagnetic fields, so why is it charged?

The answer lies in the broken symmetry associated with the development of the amplitude $V$. The phase of $V$ transforms under both internal and external gauge groups. When $V$ develops an amplitude, its phase does not actually order, but it does develop a stiffness which is sufficient to lock the internal and external gauge fields together so that, at low frequencies, they become synonymous. Written in a schematic long-wavelength form, the gauge-sensitive part of

the Kondo lattice Lagrangian is

$$\mathcal{L} = \sum_{\sigma} \int \mathrm{d}^D x \Big[ c_\sigma^\dagger(x)(-i\partial_t + e\Phi(x) + \epsilon_{\mathbf{p}-e\vec{A}})c_\sigma(x) + f_\sigma^\dagger(x)(-i\partial_t + \lambda(x))f_\sigma(x) + \Big(\overline{V}(x)c_\sigma^\dagger(x)f_\sigma(x) + \text{ H.c}\Big)\Big] \tag{105}$$

where $\mathbf{p} = -i\vec{\nabla}$. Suppose $V(x) = |V(x)|e^{i\phi(x)}$. There are two independent gauge transformations that increase the phase $\phi$ of the hybridization. In the external, electromagnetic gauge transformation, the change in phase is absorbed onto the conduction electron and electromagnetic field, so if $V \to Ve^{i\alpha}$,

$$\begin{aligned} &\phi \to \phi + \alpha, \qquad c(x) \to c(x)e^{-i\alpha(x)}, \\ &e\Phi(x) \to e\Phi(x) + \dot{\alpha}(x), \quad e\vec{A} \to e\vec{A} - \vec{\nabla}\alpha(x) \end{aligned} \tag{106}$$

where $(\Phi, \vec{A})$ denotes the electromagnetic scalar and vector potential at site $j$ and $\dot{\alpha} = \partial_t\alpha \equiv -i\partial_\tau\alpha$ denotes the derivative with respect to real time $t$. By contrast, in the internal gauge transformation, the phase change of $V$ is absorbed onto the f fermion and the internal gauge field (Read and Newns, 1983a), so if $V \to Ve^{i\beta}$,

$$\begin{aligned} &\phi \to \phi + \beta, \qquad f(x) \to f(x)e^{i\beta(x)}, \\ &\lambda(x) \to \lambda(x) - \dot{\beta}(x) \end{aligned} \tag{107}$$

If we expand the mean-field free energy to quadratic order in small, slowly varying changes in $\lambda(x)$, then the change in the action is given by

$$\delta S = -\frac{\chi_Q}{2}\int \mathrm{d}^D x \mathrm{d}\tau \delta\lambda(x)^2 \tag{108}$$

where $\chi_Q = -\delta^2 F/\delta\lambda^2$ is the f-electron susceptibility evaluated in the mean-field theory. However, $\delta\lambda(x)$ is not gauge invariant, so there must be additional terms. To guarantee gauge invariance under both the internal and external transformation, we must replace $\delta\lambda$ by the covariant combination $\delta\lambda + \dot{\phi} - e\Phi$. The first two terms are required for invariance under the internal gauge group, while the last two terms are required for gauge invariance under the external gauge group. The expansion of the action to quadratic order in the gauge fields must therefore have the form

$$S \sim -\frac{\chi_Q}{2}\int \mathrm{d}\tau \sum_j (\dot{\phi} + \delta\lambda(x) - e\Phi(x))^2 \tag{109}$$

so the phase $\phi$ acquires a rigidity in time that generates a 'mass' or energy cost associated with *difference* of the external and internal potentials. The minimum energy static configuration is when

$$\delta\lambda(\mathbf{x}) + \dot{\phi}(\mathbf{x}) = e\Phi(\mathbf{x}) \tag{110}$$

so when the external potential changes slowly, the internal potential tracks it. It is this effect that keeps the Kondo resonance pinned at the Fermi surface. We can always choose the gauge where the phase velocity $\dot{\phi}$ is absorbed into the local gauge field $\lambda$. Recent work by Coleman, Marston and Schofield (2005b) has extended this kind of reasoning to the case where RKKY couplings generate a dispersion $j_{\mathbf{p}-\mathcal{A}}$ for the spinons, where $\mathcal{A}$ is an internal vector potential, which suppresses currents of the gauge charge $n_f$. In this case, the long-wavelength action has the form

$$S = \frac{1}{2}\int \mathrm{d}^3 x \mathrm{d}\tau \Big[\rho_s\left(e\vec{A} + \vec{\nabla}\phi - \vec{\mathcal{A}}\right)^2 - \chi_Q(e\Phi - \dot{\phi} - \delta\lambda)^2\Big] \tag{111}$$

In this general form, heavy-electron physics can be seen to involve a kind of 'Meissner effect' that excludes the difference field $e\vec{A} - \vec{\mathcal{A}}$ from within the metal, locking the internal field to the external electromagnetic field, so that the f electrons, which couple to it, now become charged (Figure 19).

### 2.3.4 *Optical conductivity of the heavy-electron fluid*

One of the interesting consequences of the heavy-electron charge is a complete renormalization of the electronic plasma frequency (Millis, Lavagna and Lee, 1987b). The electronic

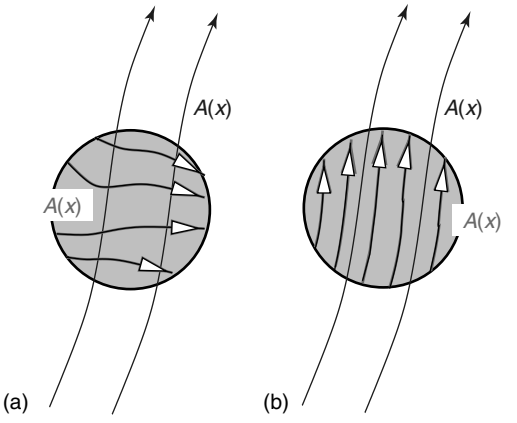



**Figure 19.** (a) Spin liquid, or local moment phase, internal field $\mathcal{A}$ decoupled from electromagnetic field. (b) Heavy-electron phase, internal gauge field 'locked' together with electromagnetic field. Heavy electrons are now charged and difference field $[e\vec{A}(x) - \mathcal{A}(x)]$ is excluded from the material.

plasma frequency is related via a f-sum rule to the integrated optical conductivity

$$\int_0^\infty \frac{\mathrm{d}\omega}{\pi}\sigma(\omega) = f_1 = \frac{\pi}{2}\left(\frac{n_c e^2}{m}\right) \tag{112}$$

where $n_e$ is the density of electrons [2]. In the absence of local moments, this is the total spectral weight inside the Drude peak of the optical conductivity.

When the heavy-electron fluid forms, we need to consider the plasma oscillations of the enlarged Fermi surface. If the original conduction sea was less than half filled, then the renormalized heavy-electron band is more than half filled, forming a partially filled hole band. The density of electrons in a filled band is $N/a^D$, so the effective density of hole carriers is then

$$n_{\mathrm{HF}} = (N - Q - \mathcal{N}_c)/a^D = (N - Q)/a^D - n_c \tag{113}$$

The mass of the excitations is also renormalized, $m \to m^*$. The two effects produce a low-frequency 'quasiparticle' Drude peak in the conductivity, with a small total weight

$$\int_0^{\sim V} \mathrm{d}\omega\sigma(\omega) = f_2 = \frac{\pi}{2}\frac{n_{\mathrm{HF}}e^2}{m^*} \sim f_1 \times \frac{m}{m^*}\left(\frac{n_{\mathrm{HF}}}{n_c}\right) \ll f_1 \tag{114}$$

Optical conductivity probes the plasma excitations of the electron fluid at low momenta. The direct gap between the upper and lower bands of the Kondo lattice are separated by a direct hybridization gap of the order $2V \sim \sqrt{DT_{\mathrm{K}}}$. This scale is substantially larger than the Kondo temperature, and it defines the separation between the thin Drude peak of the heavy electrons and the high-frequency contribution from the conduction sea.

In other words, the total spectral weight is divided up into a small 'heavy fermion' Drude peak, of total weight $f_2$, where

$$\sigma(\omega) = \frac{n_{\mathrm{HF}}e^2}{m^*}\frac{1}{(\tau^*)^{-1} - i\omega} \tag{115}$$

separated off by an energy of the order $V \sim \sqrt{T_{\mathrm{K}}D}$ from an 'interband' component associated with excitations between the lower and upper Kondo bands (Millis and Lee, 1987a; Degiorgi, Anders, Gruner and Society, 2001). This second term carries the bulk $\sim f_1$ of the spectral weight (Figure 20).

Simple calculations, based on the Kubo formula, confirm this basic expectation, (Millis and Lee, 1987a; Degiorgi, Anders, Gruner and Society, 2001) showing that the relationship between the original relaxation rate of the conduction sea and the heavy-electron relaxation rate $\tau^*$ is

$$(\tau^*)^{-1} = \frac{m}{m^*}(\tau)^{-1} \tag{116}$$

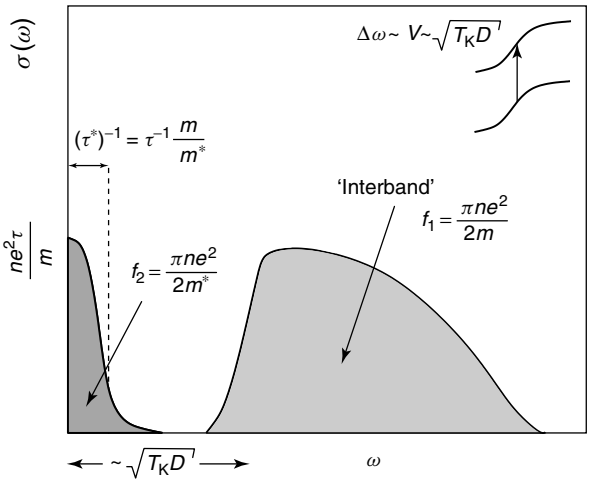



**Figure 20.** Separation of the optical sum rule in a heavy-fermion system into a high-energy 'interband' component of weight $f_2 \sim ne^2/m$ and a low-energy Drude peak of weight $f_1 \sim ne^2/m^*$.

Notice that this means that the residual resistivity

$$\rho_o = \frac{m^*}{ne^2\tau^*} = \frac{m}{ne^2\tau} \tag{117}$$

is unaffected by the effects of mass renormalization. This can be understood by observing that the heavy-electron Fermi velocity is also renormalized by the effective mass, $v_{\mathrm{F}}^* = \frac{m}{m^*}$, so that the mean-free path of the heavy-electron quasiparticles is unaffected by the Kondo effect.

$$l^* = v_{\mathrm{F}}^*\tau^* = v_{\mathrm{F}}\tau \tag{118}$$

The formation of a narrow Drude peak, and the presence of a direct hybridization gap, have been seen in optical measurements on heavy-electron systems (Schlessinger, Fisk, Zhang and Maple, 1997; Beyerman, Gruner, Dlicheouch and Maple, 1988; Dordevic *et al.*, 2001). One of the interesting features about the hybridization gap of size $2V$ is that the mean-field theory predicts that the ratio of the direct to the indirect hybridization gap is given by $\frac{2V}{T_{\mathrm{K}}} \sim \frac{1}{\sqrt{\rho T_{\mathrm{K}}}} \sim \sqrt{\frac{m^*}{m_e}}$, so that the effective mass of the heavy electrons should scale as square of the ratio between the hybridization gap and the characteristic scale $T^*$ of the heavy Fermi liquid

$$\frac{m^*}{m_e} \propto \left(\frac{2V}{T_{\mathrm{K}}}\right)^2 \tag{119}$$

In practical experiments, $T_{\mathrm{K}}$ is replaced by the 'coherence temperature' $T^*$, where the resistivity reaches a maximum. This scaling law is broadly followed (see Figure 21) in measured optical data (Dordevic *et al.*, 2001), and provides further confirmation of the correctness of the Kondo lattice picture.

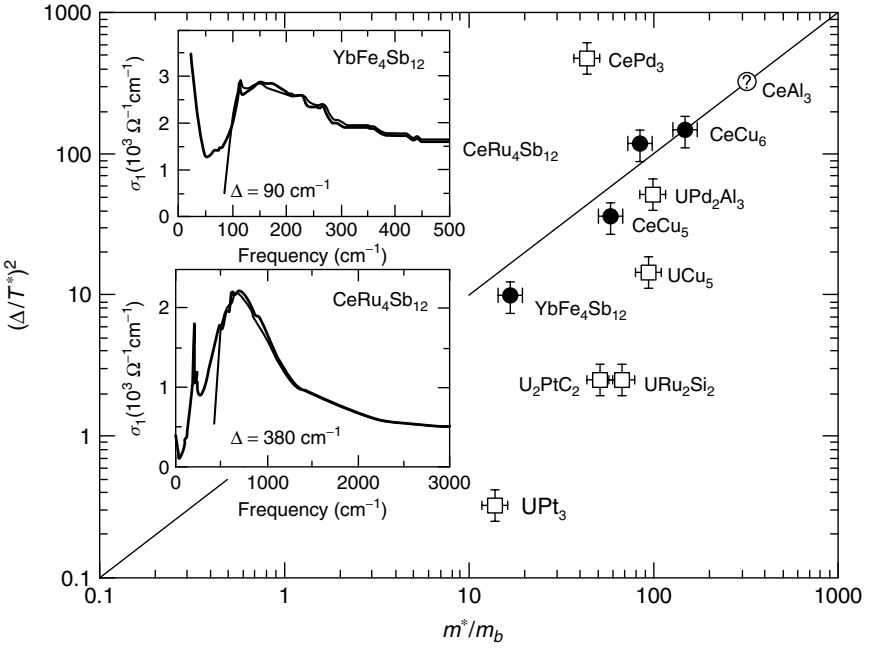



**Figure 21.** Scaling of the effective mass of heavy electrons with the square of the optical hybridization gap. (Reproduced from S.V. Dordevic, D.N. Basov, N.R. Dilley, E.D. Bauer, and M.B. Maple, *Phys. Rev. Lett.* **86**, 2001, 684, copyright © by the American Physical Society, with permission from the APS.)

## 2.4 Dynamical mean-field theory

The fermionic large $N$ approach to the Kondo lattice provides an invaluable description of heavy-fermion physics, one that can be improved upon beyond the mean-field level. For example, the fluctuations around the mean-field theory can be used to compute the interactions, the dynamical correlation functions, and the optical conductivity (Coleman, 1987b; Millis and Lee, 1987a). However, the method does face a number of serious outstanding drawbacks:

- False phase transition: In the large $N$ limit, the crossover between the heavy Fermi liquid and the local moment physics sharpens into a phase transition where the $1/N$ expansion becomes singular. There is no known way of eliminating this feature in the $1/N$ expansion.
- Absence of magnetism and superconductivity: The large $N$ approach, based on the $SU(N)$ group, cannot form a two-particle singlet for $N > 2$. The $SU(N)$ group is fine for particle physics, where baryons are bound-states of $N$ quarks, but, for condensed matter physics, we sacrifice the possibility of forming two-particle or two-spin singlets, such as Cooper pairs and spin-singlets. Antiferromagnetism and superconductivity are consequently absent from the mean-field theory.

Amongst the various alternative approaches currently under consideration, one of particular note is the DMFT. The idea of DMFT is to reduce the lattice problem to the physics of a single magnetic ion embedded within a self-consistently determined effective medium (Georges, Kotliar, Krauth and Rozenberg, 1996; Kotliar *et al*., 2006). The effective medium is determined self-consistently from the self-energies of the electrons that scatter off the single impurity. In its more advanced form, the single impurity is replaced by a cluster of magnetic ions.

Early versions of the DMFT were considered by Kuramoto and Watanabe (1987), and Cox and Grewe (1988), and others, who used diagrammatic means to extract the physics of a single impurity. The modern conceptual framework for DMFT was developed by Metzner and Vollhardt (1989), and Georges and Kotliar (1992). The basic idea behind DMFT is linked to early work of Luttinger and Ward (1960), and Kotliar *et al*. (2006), who found a way of writing the free energy as a variational functional of the full electronic Green's function

$$\mathcal{G}_{ij} = -\langle T\psi_i(\tau)\psi_j^\dagger(0)\rangle \tag{120}$$

Luttinger and Ward showed that the free energy is a variational functional of $F[\mathcal{G}]$ from which Dyson's equation relating the $\mathcal{G}$ to the bare Green's function $\mathcal{G}_0$

$$[\mathcal{G}_0^{-1} - \mathcal{G}^{-1}]_{ij} = \Sigma_{ij}[\mathcal{G}] \tag{121}$$

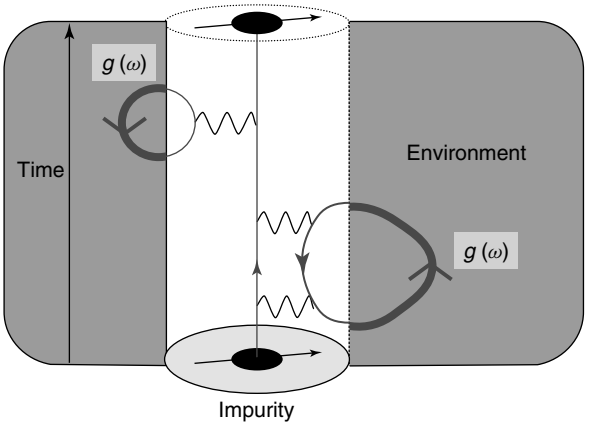



**Figure 22.** In the dynamical mean-field theory, the many-body physics of the lattice is approximated by a single impurity in a self-consistently determined environment. Each time the electron makes a sortie from the impurity, its propagation through the environment is described by a self-consistently determined local propagator $\mathcal{G}(\omega)$, represented by the thick gray line.

The quantity $\Sigma[\mathcal{G}]$ is a functional, a machine which takes the full propagator of the electron and outputs the self-energy of the electron. Formally, this functional is the sum of the one-particle irreducible Feynman diagrams for the self-energy: while its output depends on the input Greens function, the actual the machinery of the functional is determined solely by the interactions. The only problem is that we do not know how to calculate it.

DMFT solves this problem by approximating this functional by that of a single impurity or a cluster of magnetic impurities (Figure 22). This is an ideal approximation for a local Fermi liquid, where the physics is highly retarded in time, but local in space. The local approximation is also asymptotically exact in the limit of infinite dimensions (Metzner and Vollhardt, 1989). If one approximates the input Green function to $\Sigma$ by its on-site component $\mathcal{G}_{ij} \approx \mathcal{G}\delta_{ij}$, then the functional becomes the local self-energy functional of a single magnetic impurity,

$$\Sigma_{ij}[\mathcal{G}_{ls}] \approx \Sigma_{ij}[\mathcal{G}\delta_{ls}] \equiv \Sigma_{\text{impurity}}[\mathcal{G}]\delta_{ij} \tag{122}$$

DMFT extracts the local self-energy by solving an Anderson impurity model embedded in an arbitrary electronic environment. The physics of such a model is described by a path integral with the action

$$S = -\int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' f_\sigma^\dagger(\tau)\mathcal{G}_0^{-1}(\tau-\tau')f_\sigma(\tau') + U\int_0^\beta \mathrm{d}\tau n_\uparrow(\tau)n_\downarrow(\tau) \tag{123}$$

where $G_0(\tau)$ describes the bare Green's function of the f electron, hybridized with its dynamic environment. This quantity is self-consistently updated by the DMFT. There are, by now, a large number of superb numerical methods to solve an Anderson model for an arbitrary environment, including the use of exact diagonalization, diagrammatic techniques, and the use of Wilson's renormalization group (Bulla, 2006). Each of these methods is able to take an input 'environment' Green's function providing as output the impurity self-energy $\Sigma[\mathcal{G}_0] = \Sigma(i\omega_n)$.

Briefly, this is how the DMFT computational cycle works. One starts with an estimate for the environment Green's function $\mathcal{G}_0$ and uses this as input to the 'impurity solver' to compute the first estimate $\Sigma(i\omega_n)$ of the local self-energy. The interaction strength is set within the impurity solver. This local self-energy is used to compute the Green's functions of the electrons in the environment. In an Anderson lattice, the Green's function becomes

$$G(\mathbf{k},\omega) = \left[\omega - E_f - \frac{V^2}{\omega-\epsilon_{\mathbf{k}}} - \Sigma(\omega)\right]^{-1} \tag{124}$$

where $V$ is the hybridization and $\epsilon_{\mathbf{k}}$ the dispersion of the conduction electrons. It is through this relationship that the physics of the lattice is fed into the problem. From $G(\mathbf{k},\omega)$, the local propagator is computed

$$\mathcal{G}(\omega) = \sum_{\mathbf{k}}\left[\omega - E_f - \frac{V^2}{\omega-\epsilon_{\mathbf{k}}} - \Sigma(\omega)\right]^{-1} \tag{125}$$

Finally, the new estimate for the bare environment Green's function $\mathcal{G}_0$ is then obtained by inverting the equation $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$, so that

$$\mathcal{G}_0(\omega) = \left[G^{-1}(\omega) + \Sigma(\omega)\right] \tag{126}$$

This quantity is then reused as the input to an 'impurity solver' to compute the next estimate of $\Sigma(\omega)$. The whole procedure is then reiterated to self-consistency. For the Anderson lattice, Cyzcholl (Schweitzer and Czycholl, 1991) has shown that remarkably good results are obtained using a perturbative expansion for $\Sigma$ to the order of $U^2$ (Figure 23). Although this approach is not sufficient to capture the limiting Kondo behavior much, the qualitative physics of the Kondo lattice, including the development of coherence at low temperatures, is already captured by this approach. However, to go to the strongly correlated regime, where the ratio of the interaction to the impurity hybridization width $U/(\pi\Delta)$ is much larger than unity, one requires a more sophisticated solver.

There are many ongoing developments under way using this powerful new computational tool, including the incorporation of realistic descriptions of complex atoms, and the extension to 'cluster DMFT' involving clusters of magnetic moments embedded in a self-consistent environment. Let me

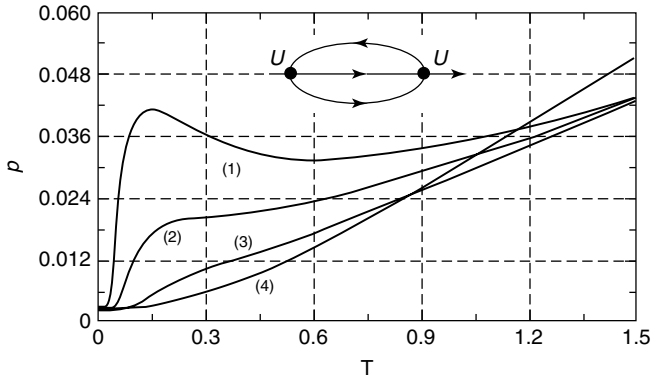



**Figure 23.** Resistivity for the Anderson lattice, calculated using the DMFT, computing the self-energy to order $U^2$. (1), (2), (3), and (4) correspond to a sequence of decreasing electron density corresponding to $n_{\mathrm{TOT}} = (0.8, 0.6, 0.4, 0.2)$ respectively. (Reproduced from H. Schweitzer and G. Czycholl, *Phys. Rev. Lett.* **67**, 1991, 3724 copyright © by the American Physical Society, with permission of the APS.)

end this brief summary with a list of a few unsolved issues with this technique

- There is, at present, no way to relate the thermodynamics of the bulk to the impurity thermodynamics.
- At present, there is no natural extension of these methods to the infinite $U$ Anderson or Kondo models that incorporates the Green's functions of the *localized* f-electron degrees of freedom as an integral part of the DMFT.
- The method is largely a numerical black box, making it difficult to compute microscopic quantities beyond the electron-spectral functions. At the human level, it is difficult for students and researchers to separate themselves from the ardors of coding the impurity solvers, and make time to develop new conceptual and qualitative understanding of the physics.

## 3 KONDO INSULATORS

### 3.1 Renormalized silicon

The ability of a dense lattice of local moments to transform a metal into an insulator, a 'Kondo insulator' is one of the remarkable and striking consequences of the dense Kondo effect (Aeppli and Fisk, 1992; Tsunetsugu, Sigrist and Ueda, 1997; Riseborough, 2000). Kondo insulators are heavy-electron systems in which the the liberation of mobile charge through the Kondo effect gives rise to a filled heavy-electron band in which the chemical potential lies in the middle of the hybridization gap. From a quasiparticle perspective,

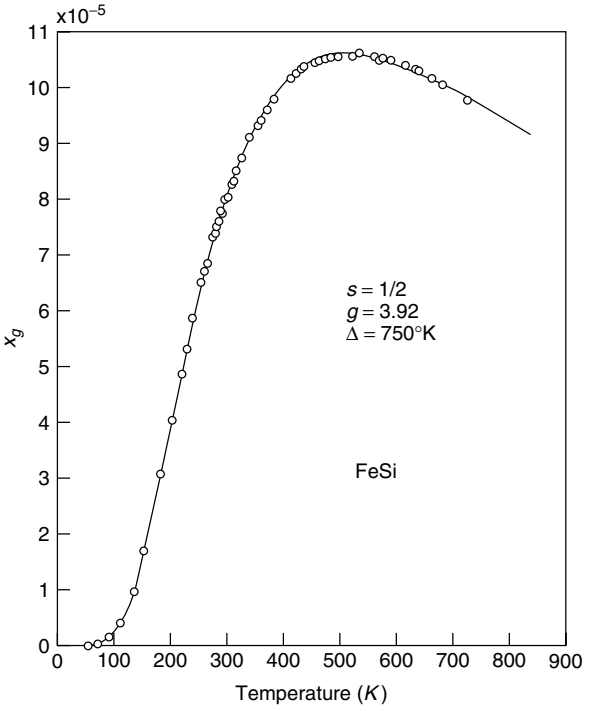



**Figure 24.** Schematic band picture of Kondo insulator, illustrating how a magnetic field drives a metal-insulator transition. Modified from Aeppli and Fisk (1992). (Reproduced from V. Jaccarino, G.K. Wertheim, J.H. Wernick, C.R. Walker and S. Arajs, *Phys. Rev.* **160**, 1967, 476 copyright © 1967 by the American Physical Society, with permission of the APS.)

Kondo insulators are highly renormalized 'band insulators' (Figure 24). The d-electron Kondo insulator FeSi has been referred to as *renormalized silicon*. However, like Mott–Hubbard insulators, the gap in their spectrum is driven by interaction effects, and they display optical and magnetic properties that cannot be understood with band theory.

There are about a dozen known Kondo insulators, including the rare-earth systems $SmB_6$ (Menth, Buehler and Geballe, 1969), $YB_{12}$ (Iga, Kasaya and Kasuya, 1988), $CeFe_4P_{12}$ (Meisner *et al.*, 1985), $Ce_3Bi_4Pt_3$ (Hundley *et al.*, 1990), CeNiSn (Takabatake *et al.*, 1992, 1990; Izawa *et al.*, 1999) and CeRhSb (Takabatake *et al.*, 1994), and the d-electron Kondo insulator FeSi. At high temperatures, Kondo insulators are local moment metals, with classic Curie susceptibilities, but, at low temperatures, as the Kondo effect develops coherence, the conductivity and the magnetic susceptibility drop toward zero. Perfect insulating behavior is, however, rarely observed due to difficulty in eliminating impurity band formation in ultranarrow gap systems. One of the cleanest examples of Kondo-insulating behavior occurs in the d-electron system FeSi (Jaccarino *et al.*, 1967; DiTusa *et al.*, 1997). This 'flyweight' heavy-electron system provides a rather clean realization of the phenomena seen in other

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