17 Heavy electrons

Although the single-impurity Kondo problem was essentially solved by the early 1970s, it took a further decade before the physics community was ready to accept the notion that the same phenomenon could occur in a dense Kondo lattice of local moments, forming quasiparticles with greatly enhanced masses that we now call *heavy electrons*. The early resistance to change was rooted in a number of misconceptions about spin physics and the Kondo effect. Some of the first heavy-electron systems to be discovered are superconductors, yet it was well known that small concentrations of magnetic ions, typically a few percent, suppress conventional superconductivity, so the appearance of superconductivity in a dense magnetic system appeared at first sight to be impossible. Indeed, the observation of superconductivity in UBe_{13} in 1973 [1] was dismissed as an artifact, and ten more years passed before it was revisited and acclaimed as a heavy-fermion superconductor, in which the Kondo effect quenches the local moments to form a new kind of *heavy-fermion metal* [2, 3]. In this chapter, we will study some of the key physics of Kondo lattices that makes this possible.

17.1 The Kondo lattice and the Doniach phase diagram

Local-moment metals normally develop antiferromagnetic order at low temperatures. A magnetic moment induces a cloud of Friedel oscillations in the spin density of a metal with a magnetization profile given by

$$\langle \vec{M}(\mathbf{x}) \rangle = -J \int d^3x' \, \chi(\mathbf{x}-\mathbf{x}') \langle \vec{S}(\mathbf{x}') \rangle, \tag{17.1}$$

where J is the strength of the Kondo coupling and

$$\chi(\mathbf{x}) = \int_{\vec{\mathbf{q}}} \chi(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{x}},$$
$$\chi(\mathbf{q}) = 2 \int_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}} \tag{17.2}$$

is the the non-local susceptibility of the metal. If a second local moment is introduced at location $\mathbf{x}$, then it couples to $\langle M(\mathbf{x}) \rangle$, shifting the energy by an amount $J\vec{S}(\mathbf{x}) \cdot \langle \vec{M}(\mathbf{x}) \rangle$, giving rise to a long-range magnetic interaction called the *RKKY interaction* (named after Ruderman, Kittel, Kasuya, and Yosida [4]):

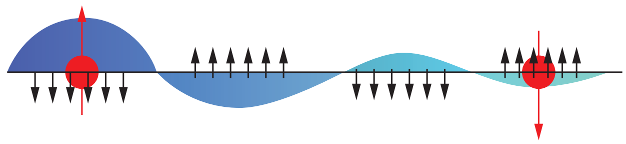


Fig. 17.1 Illustrating how the polarization of spin around a magnetic impurity gives rise to Friedel oscillations, inducing an RKKY interaction between the spins.

$$H_{RKKY} = \frac{1}{2}\sum_{\mathbf{x},\mathbf{x}'} \overbrace{-J^2\chi(\mathbf{x}-\mathbf{x}')}^{J_{RKKY}(\mathbf{x}-\mathbf{x}')}\vec{S}(\mathbf{x})\cdot\vec{S}(\mathbf{x}'), \tag{17.3}$$

where the factor of $\frac{1}{2}$ arises because of the summation over $\mathbf{x}$ and $\mathbf{x}'$. The sharp discontinuity in electron occupancy at the Fermi surface manifests itself as $q = 2k_F$ Friedel oscillations in the RKKY interaction (see Example 17.1),

$$J_{RKKY}(r) \sim J^2\rho\frac{\cos 2k_F r}{|r|^3}, \tag{17.4}$$

where r is the distance from the impurity and ρ is the conduction electron density of states per spin (see Figure 17.1). The oscillatory nature of this magnetic interaction tends to frustrate the interaction between spins, so that, in alloys containing a dilute concentration of magnetic transition metal ions, the RKKY interaction gives rise to a frustrated, glassy magnetic state known as a spin glass, but in dense systems the RKKY interaction typically gives rise to an ordered antiferromagnet with a Néel temperature $T_N \sim J^2\rho$.

The first heavy-electron materials to be discovered are now called *Kondo insulators* [5]. In the late 1960s, Anthony Menth, Ernest Buehler, and Ted Geballe at AT&T Bell Laboratories [6] discovered an unusual metal, SmB_6, containing magnetic Sm^{3+} ions. While apparently a magnetic metal with a Curie–Weiss susceptibility at room temperature, on cooling SmB_6 transforms continuously into a paramagnetic insulator with a tiny 10 meV gap. The subsequent discovery of similar behavior in SmS under pressure led Brian Maple and Dieter Wohlleben [7], working at the University of California, San Diego, to propose that quantum mechanically coherent valence fluctuations in rare-earth ions destabilize magnetism, allowing the f-spin to delocalize into the conduction sea. SmS and SmB_6 are special cases, where the additional heavy f-quasiparticles dope the metal to form a highly correlated insulator. More typically, however, this process gives rise to a heavy-fermion metal.

The first heavy-fermion metal, $CeAl_3$ was discovered by Klaus Andres, John Graebner, and Hans Ott in 1976 [3]. Like many other heavy-fermion metals, this metal displays:

- a Curie–Weiss susceptibility $\chi \sim (T+\theta)^{-1}$ at high temperatures
- a paramagnetic spin susceptibility $\chi \sim$ constant at low temperatures, in this case below 1 K
- a dramatically enhanced linear specific heat $C_V = \gamma T$ at low temperatures, where in $CeAl_3$ $\gamma \sim 1600\,\mathrm{mJ/(mol\,K^2)}$ is about 1600 times larger than in copper
- a quadratic temperature dependence of the low-temperature resistivity $\rho = \rho_0 + AT^2$.

Andres, Graebner, and Ott proposed that the ground-state excitations of $CeAl_3$ were those of a *Landau Fermi-liquid*, in which the effective mass of the quasiparticles is about 1000 bare electron masses. The Landau Fermi-liquid expressions for the magnetic susceptibility χ and the linear specific heat coefficient γ are

$$\chi = (\mu_B)^2 \frac{N^*(0)}{1 + F_0^a}$$
$$\gamma = \frac{\pi^2 k_B^2}{3} N^*(0), \tag{17.5}$$

where $N^*(0) = \frac{m^*}{m} N(0)$ is the renormalized density of states and F_0^a is the spin-dependent part of the s-wave interaction between quasiparticles. What could be the origin of this huge mass renormalization? Like other cerium heavy-fermion materials, the cerium atoms in this metal are in a $Ce^{3+}(4f^1)$ configuration, and because they are spin–orbit coupled, they form huge local moments with a spin of $J = 5/2$. In their paper, Andres, Ott, and Graebner suggested that a lattice version of the Kondo effect is responsible.

Three years later, in 1979, Frank Steglich and collaborators, working at the Technical Hochshule in Darmstadt, Germany [2], discovered that the heavy-fermion metal $CeCu_2Si_2$ becomes superconducting at 0.5 K. This pioneering result was initially treated with great scepticism, but today we recognize it as the discovery of electronically mediated superconductivity, establishing not only that heavy fermions form within a Kondo lattice, but that they can also pair to form heavy-fermion superconductors.

These discoveries prompted Neville Mott [8] and Sebastian Doniach [9] 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. The simplest Kondo lattice Hamiltonian [10] is

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_j \vec{S}_j \cdot c^{\dagger}_{j\alpha} \vec{\sigma}_{\alpha\beta} c_{j\beta}, \tag{17.6}$$

where

$$c^{\dagger}_{j\alpha} = \frac{1}{\sqrt{\mathcal{N}_s}} \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{R}_j} \tag{17.7}$$

creates an electron at site j. Mott and Doniach pointed out that there are two energy scales in the Kondo lattice: the Kondo temperature T_K and the RKKY scale E_{RKKY}:

$$T_K = De^{-1/(2J\rho)}$$
$$E_{RKKY} = J^2\rho. \tag{17.8}$$

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. Working at Stanford, Remi Jullien, John Fields, and Sebastian Doniach were later able to confirm the correctness of this argument in a simplified one-dimensional "Kondo necklace" model [11], finding that the transition between the two regimes is a continuous quantum phase transition in which the characteristic scale of the antiferromagnet and paramagnet drops to zero at the transition (see Figure 17.2). This led Doniach to conjecture [9] that the general transition between the antiferromagnet and the dense Kondo state is a continuous quantum phase transition. In the Kondo lattice ground state which ensues, Bloch's theorem ensures that the resonant elastic scattering at each site will generate a renormalized f-band, of width $\sim T_K$. In contrast with the impurity

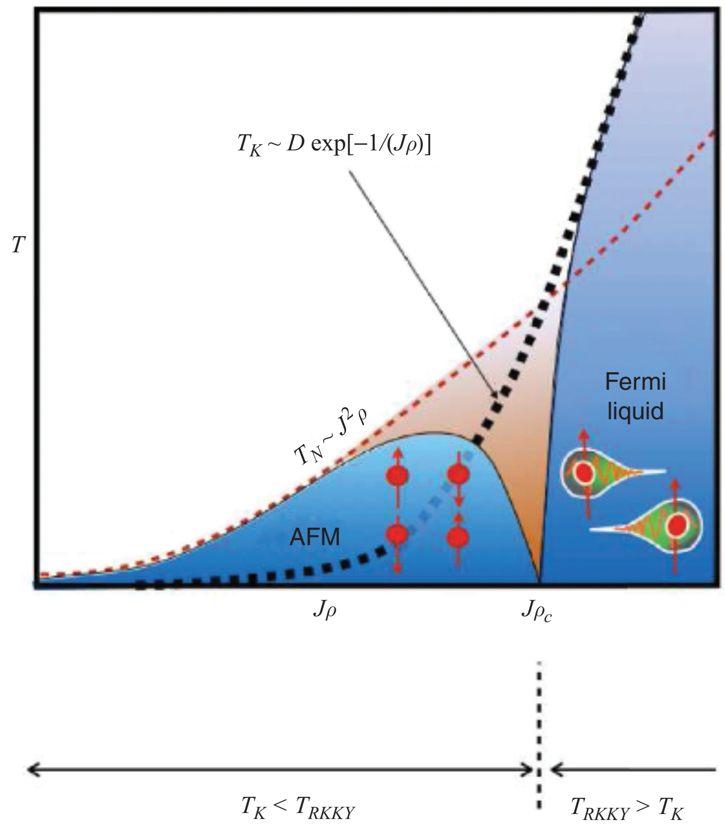


Fig. 17.2 Doniach phase diagram for the Kondo lattice, illustrating the antiferromagnetic regime and the heavy-fermion regime for $T_K < T_{RKKY}$ and $T_K > T_{RKKY}$, respectively. The effective Fermi temperature of the heavy Fermi liquid is indicated by a solid line. Experimental evidence suggests that in many heavy-fermion materials this scale drops to zero at the antiferromagnetic quantum critical point.

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 Figure 17.3(a)).

One of the fascinating aspects of the Kondo lattice concerns the Luttinger sum rule. Richard Martin [14], working at the Xerox Palo Alto Research Center, pointed out that the Kondo impurity and lattice models can both be regarded as the result of adiabatically increasing the interaction strength U in a corresponding Anderson model, while preserving the valence of the magnetic ion. During this process, the conservation of charge gives rise to “node-counting” sum rules. In the previous chapter we saw that, for an impurity, the scattering phase shift at the Fermi energy counts the number of localized electrons, according to the Friedel sum rule,

$$\sum_{\sigma} \frac{\delta_\sigma}{\pi} = n_f = 1.$$

This sum rule survives to large U, and reappears as the constraint on the scattering phase shift created by the Kondo. In the lattice, the corresponding sum rule is the ‘Luttinger sum rule’, which states that the Fermi surface volume counts the number of electrons, which at small U is just the number of localized ($4f$, $5f$, or $3d$) and conduction electrons. When U becomes large, the number of localized electrons is now the number of spins, so that

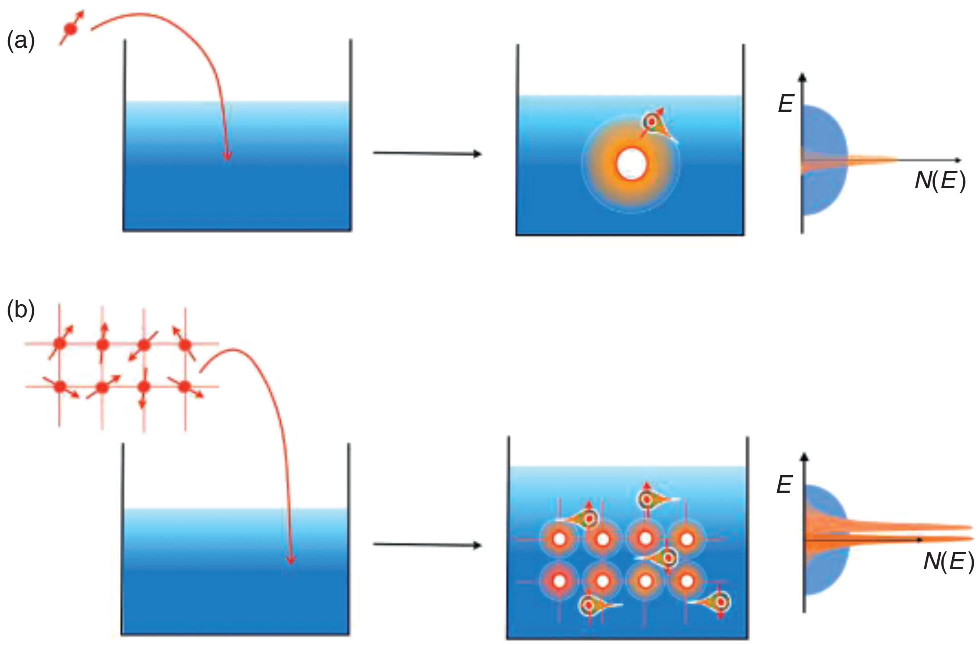


Fig. 17.4

Schematic illustration of the Kondo effect. (a) Single spin in a conduction sea "ionizes" into a Kondo singlet and a heavy fermion orbiting in the vicinity of the Kondo singlet, forming a Kondo resonance at the Fermi surface. (b) Immersion of a lattice of spins in a conduction sea injects a resonance at each site in the lattice, giving rise to a new band of delocalized heavy fermions with a hybridization gap. The density of carriers is increased in the Kondo lattice.

dramatic drop in the resistivity. The thermodynamics of the dense and dilute systems are essentially identical, but the transport properties display the effects of coherence.

The most direct evidence that the Fermi surface of f-electron systems counts the f-electrons derives from quantum oscillation (de Haas–van Alphen and Shubnikov–de Haas oscillation) measurements of the Fermi surface [16, 17]. Typically, in the heavy Fermi liquid, the measured de Haas–van Alphen orbits are consistent with band-structure calculations in which the f-electrons are assumed to be delocalized. By contrast, the measured masses of the heavy electrons often exceed the band-structure calculated masses of the narrow f-band by an order of magnitude or more. Perhaps the most remarkable discovery of recent years is the observation that the volume of the f-electron Fermi surface appears to "jump" to a much smaller value when the f-electrons antiferromagnetically order, indicating that, once the Kondo effect is interrupted by magnetism, the heavy f-electrons relocalize [18].

Example 17.1 The RKKY interaction between two moments in a Fermi liquid is given by

$$J_{RKKY}(\mathbf{x}) = -J^2 \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{x}} \chi(\mathbf{q}), \tag{17.10}$$

where, as shown in Chapter 7, $\chi(\mathbf{q}) = 2\rho F[q/2k_F]$ is the static magnetic susceptibility and

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| \tag{17.11}$$

is the Lindhard function. Use the Fourier transform

$$\int_0^\infty dy \sin(\alpha y) \ln\left|\frac{1+y}{1-y}\right| = \pi \frac{\sin\alpha}{\alpha} \tag{17.12}$$

to show that the real-space RKKY interaction between local moments is given by

$$J_{RKKY}(r) = J^2\rho \frac{1}{2\pi^2 r^3}\left[\cos 2k_F r - \frac{\sin 2k_F r}{2k_F r}\right], \tag{17.13}$$

where r is measured in lattice units.

Solution

We begin by using the isotropy of $\chi(\mathbf{q}) = \chi(q)$ to carry out the angular integral in the Fourier transform:

$$\begin{aligned}\chi(\mathbf{x}) &= \int_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}\chi(\mathbf{q}) = \int_0^\infty \frac{4\pi q^2 dq}{(2\pi)^3} \overbrace{\int \frac{d\Omega}{4\pi} e^{i\mathbf{q}\cdot\mathbf{x}}}^{\frac{\sin qr}{qr}} \chi(q) = \frac{1}{2\pi^2 r}\int_0^\infty dq\, q \sin(qr)\chi(q) \\ &= \frac{2\rho}{2\pi^2 r}\int_0^\infty dq\, q\sin(qr) F\left[\frac{q}{2k_F}\right].\end{aligned} \tag{17.14}$$

If we change variable to $y = q/(2k_F)$, so that $dq\, q = (2k_F)^2 y\, dy$, we obtain

$$\chi(r) = \frac{\rho}{\pi^2 r}(2k_F)^2 \int_0^\infty dy\, y \sin(2k_F r y) F[y] = \frac{\rho}{\pi^2 r}(2k_F)^2 G[2k_F r], \tag{17.15}$$

where

$$G[\alpha] = \int_0^\infty dy \sin(\alpha y)\left(\frac{y}{2} + \frac{(1-y^2)}{4}\ln\left|\frac{1+y}{1-y}\right|\right). \tag{17.16}$$

Notice that near $y \sim 1$ the singular part of the integrand goes as $dy(y-1)\ln(y-1)$, and since the singular part of the integral has dimension $[y^2] \equiv [\alpha^{-2}]$, we expect this integral to have a $1/\alpha^2 \sim 1/(k_F r)^2$ dependence. To Fourier transform the last two terms in (17.16), we use the result

$$\int_0^\infty dy \sin(\alpha y) \ln\left|\frac{1+y}{1-y}\right| = \pi \frac{\sin\alpha}{\alpha}. \tag{17.17}$$

(This result is obtained as the inverse Fourier transform of $\sin\alpha/\alpha$.) By differentiating both sides twice with respect to α, we then obtain

$$\begin{aligned}\int_0^\infty dy \sin(\alpha y)(1-y^2)\ln\left|\frac{1+y}{1-y}\right| &= \pi\left(1 + \frac{d^2}{d\alpha^2}\right)\frac{\sin\alpha}{\alpha} \\ &= -2\pi\left(\frac{\cos\alpha}{\alpha^2} - \frac{\sin\alpha}{\alpha^3}\right),\end{aligned} \tag{17.18}$$

with the expected $1/\alpha^2$ dependence. To complete the job we need to Fourier transform the first term in (17.16). If we differentiate $\int_{-\infty}^{\infty} dx \cos\alpha y = 2\pi\delta(\alpha)$ with respect to α, we obtain

$$\int_0^\infty dy\, y \sin\alpha y = -\pi\delta'(\alpha). \tag{17.19}$$

Combining (17.18) and (17.19), we obtain

$$G[\alpha] = \frac{\pi}{2}\left[\frac{\sin\alpha}{\alpha^3} - \frac{\cos\alpha}{\alpha^2} - \delta'(\alpha)\right]. \tag{17.20}$$

When inserted into (17.15) we finally obtain

$$J_{RKKY}(r) = -J^2\chi(r) = \frac{J^2\rho}{2\pi r^3}\left[\cos 2k_F r - \frac{\sin 2k_F r}{2k_F r}\right], \tag{17.21}$$

where we have dropped the $\delta'(2k_F r)$ term. Notice that at small distances $J_{RKKY}(r) < 0$ is a ferromagnetic interaction.

17.2 The Coqblin–Schrieffer model

17.2.1 Construction of the model

The stabilization of the heavy-fermion state in f-electron materials owes its origins to the strong spin–orbit coupling, which locks the spin and orbital angular momentum into a large half-integer moment that is unquenched by crystal fields. For example, in Ce^{3+} ions, the $4f^1$ electron is spin–orbit coupled into a state with $j = 3 - \frac{1}{2} = \frac{5}{2}$, giving a spin degeneracy of $N = 2j + 1 = 6$. Ytterbium heavy-fermion materials involve the Yb:$4f^{13}$ configuration, which is most readily understood as a single hole in the filled $4f^{14}$ f-shell, with one hole in the upper spin–orbit multiplet with angular momentum $j = 3 + \frac{1}{2} = \frac{7}{2}$, or $N = 8$. The large spin degeneracy $N = 2j + 1$ of the local moments has the effect of enhancing the Kondo temperature to a point where the zero-point spin fluctuations destroy magnetism.

The presence of large spin–orbit coupling requires a generalization of the Kondo model developed by Coqblin and Schrieffer [19]: they considered a spin–orbit coupled version of the infinite U Anderson model in which the z component of the electron angular momentum, $M \in [-j, j]$, runs from $-j$ to j:

$$H = \sum_{k,M} \epsilon_k c^\dagger_{\mathbf{k}M} c_{\mathbf{k}M} + E_f \sum_M |f^1 : M\rangle\langle f^1 : M| + \sum_{k,M} V\left[c^\dagger_{kM}|f^0\rangle\langle f^1 : M| + \text{H.c.}\right]. \tag{17.22}$$

In this model, both the f- *and* the conduction electrons carry spin indices M that run from $-j$ to j. This strange feature is a consequence of rotational invariance, which causes total angular momentum $\vec{J}$ to be conserved by hybridization process: this means that the hybridization is diagonal in a basis where partial-wave states of the conduction sea are written in states of definite j. In this basis, spin–orbit coupled f-states hybridize diagonally with partial wave-states of the conduction electrons in the same spin–orbit coupled j states as the f-electron. Suppose $|\mathbf{k}\sigma\rangle$ represents a plane wave of momentum $\mathbf{k}$; then one can construct a state of definite orbital angular momentum l by integrating the plane wave with a spherical harmonic, as follows:

$$|klm\sigma\rangle = \int \frac{d\Omega}{4\pi} |\mathbf{k}\sigma\rangle Y_{lm}(\hat{\mathbf{k}}). \tag{17.23}$$

When spin–orbit interactions are strong, one must work with a partial wave of definite j, obtained by combining these states in the following linear combinations:

$$|kM\rangle = \sum_{\sigma=\pm\frac{1}{2}} |klM-\sigma,\ \sigma\rangle \left(lM-\sigma, \frac{1}{2}\sigma \middle| jM \right), \tag{17.24}$$

where $(lm, \frac{1}{2}\sigma \,|\, jM)$ is the Clebsch–Gordan coefficient between the spin–orbit coupled state $|jM\rangle$ and the l–s coupled state $|lm,\sigma\rangle$. These coefficients can be explicitly evaluated as

$$\left(lM-\sigma, \frac{1}{2}\,\sigma \middle| jM \right) = \begin{cases} \sqrt{\frac{1}{2} + \frac{2M\sigma}{(2l+1)}}, & j = l+\frac{1}{2} \\ \operatorname{sgn}\sigma\sqrt{\frac{1}{2} - \frac{2M\sigma}{2l+1}}, & j = l-\frac{1}{2} \end{cases} \qquad \left(M \in [-j,j],\ \sigma = \pm\frac{1}{2} \right). \tag{17.25}$$

Putting this all together, a partial-wave state of definite j, M can then be written as

$$c^{\dagger}_{kM} = \sum_{\sigma=\pm\frac{1}{2}} \int \frac{d\Omega}{4\pi}\, c^{\dagger}_{\mathbf{k},\sigma}\, \mathcal{Y}_{\sigma,M}(\hat{\mathbf{k}}), \tag{17.26}$$

where

$$\mathcal{Y}_{\sigma,M}(\mathbf{k}) = \big(l, M-\sigma\ ; \frac{1}{2}\sigma \,|\, jM\big) Y_{l,M-\sigma}(\hat{\mathbf{k}}) \tag{17.27}$$

is a spin–orbit coupled spherical harmonic. Note that the spin–orbit coupled partial-wave states form a complete basis for an impurity model involving a single spherically symmetric magnetic site. This is no longer the case in a lattice, where the set of partial waves at different sites is overcomplete, and an electron which sets off in one partial-wave state at one site can arrive in another partial-wave state at another site.

When $E_f << 0$, the valence of the ion approaches unity ($n_f \to 1$) and one can integrate out the virtual fluctuations $f^1 \rightleftharpoons f^0 + e^-$ via a Schrieffer–Wolff transformation, to obtain the Coqblin–Schrieffer model,

$$H_{CS} = \sum_{kM} \epsilon_k c^{\dagger}_{kM} c_{kM} - J \sum_{k,k',M,M'} (f^{\dagger}_{M} c_{k'M})(c^{\dagger}_{kM'} f_{M'}) \qquad (M, M' \in [-j,j]), \tag{17.28}$$

where $J = V^2/|E_f|$ is the amplitude for the virtual process. The second term describes a virtual fluctuation in which an f-electron with $j_z = M'$ jumps out into the conduction sea, creating a state with excitation energy of order $|E_f|$, only to be subsequently replaced by an electron with $j_z = M$. Notice how the f-charge $Q = n_f$ of the impurity is *conserved*, by the spin-exchange interaction, $[H, n_f] = 0$, so that the interaction in the Coqblin–Schrieffer model only involves the spin degrees of freedom. It is sometimes useful to rewrite the Coqblin–Schrieffer model in the form

$$H_{CS} = \sum_{kM} \epsilon_k c^{\dagger}_{kM} c_{kM} + J \sum_{k,k',M,M'} c^{\dagger}_{kM} c_{k'M'} \overbrace{\left(f^{\dagger}_{M'} f_M - \frac{1}{N} n_f \delta_{M,M'} \right)}^{S_{M'M}} + \hat{V} \qquad (M, M' \in [-j,j]), \tag{17.29}$$

where $S_{M'M}$ is the $SU(N)$ generalization of a traceless Pauli spin operator. This form of the model emphasizes that the interaction is a pure spin-exchange process. In writing this expression, we have omitted the elastic scattering term $\hat{V} = J\left(\frac{n_f}{N}\right)\sum_{k,k',M}(c^{\dagger}_{kM}c_{k'M} - \delta_{k,k'})$ which results from the rearrangement of the operators. This term does not renormalize, and may be absorbed into a potential scattering phase shift of the conduction electrons off the impurity, or a shift of the chemical potential (in the Kondo lattice).

Example 17.2 In a certain tetragonal crystalline environment, the low-lying ground state of a Ce^{3+} ion is a $|j = 5/2, M_J = \pm\frac{3}{2}\rangle$ state. The hybridization of this state with Bloch waves of momentum $|\mathbf{k}| = k$ is described by the Hamiltonian

$$H_{mv} = V \sum_{M=\pm\frac{3}{2}} \int \frac{k^2 dk}{2\pi^2} \left[c^{\dagger}_{kM} f_M + \text{H.c.}\right], \tag{17.30}$$

where V is the strength of hybridization near the Fermi energy and $c^{\dagger}_{kM}$ creates a conduction electron in an $l = 3, j = 5/2, M_J = \pm\frac{3}{2}$ partial-wave state of wavevector k.

(a) Recast H_{mv} using a plane-wave basis for the conduction electrons.
(b) Show that the hybridization vanishes along the z-axis of momentum space. Why does this happen?

Solution

(a) We begin by rewriting the partial-wave states as plane waves. Using (17.26), we have

$$c^{\dagger}_{kM} = \sum_{\sigma=\pm\frac{1}{2}} \int \frac{d\Omega}{4\pi}\, c^{\dagger}_{\mathbf{k},\sigma} \mathcal{Y}_{\sigma M}(\mathbf{k}), \tag{17.31}$$

where

$$\begin{aligned} \mathcal{Y}_{\sigma M}(\mathbf{k}) &= \left(3, M-\sigma\, ; \frac{1}{2}\sigma \middle| \frac{5}{2} M\right) Y_{3,M-\sigma}(\hat{\mathbf{k}}) \\ &= \operatorname{sgn}\sigma \sqrt{\frac{1}{2} - \frac{\operatorname{sgn}(M\sigma)}{14}}\, Y_{3,M-\sigma}(\hat{\mathbf{k}}) \qquad \left(\sigma = \pm\frac{1}{2}, M = \pm\frac{3}{2}\right). \end{aligned} \tag{17.32}$$

The hybridization Hamiltonian is then written

$$H_{mv} = V \sum_{\mathbf{k}\sigma, M} \left[c^{\dagger}_{\mathbf{k}\sigma} \mathcal{Y}_{\sigma M}(\hat{\mathbf{k}}) f_M + \text{H.c.}\right]. \tag{17.33}$$

(b) Now the Clebsch–Gordan coefficients are either $\pm\sqrt{3/7}$ or $\pm\sqrt{4/7}$, so that

$$\mathcal{Y}_{\sigma M}(\mathbf{k}) = \begin{pmatrix} \mathcal{Y}_{\frac{1}{2}\,\frac{3}{2}}(\hat{\mathbf{k}}) & \mathcal{Y}_{\frac{1}{2}\,-\frac{3}{2}}(\hat{\mathbf{k}}) \\ \mathcal{Y}_{-\frac{1}{2}\,\frac{3}{2}}(\hat{\mathbf{k}}) & \mathcal{Y}_{-\frac{1}{2}\,-\frac{3}{2}}(\hat{\mathbf{k}}) \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{3}{7}} Y_{3,1}(\hat{\mathbf{k}}) & \sqrt{\frac{4}{7}} Y_{3,-2}(\hat{\mathbf{k}}) \\ -\sqrt{\frac{4}{7}} Y_{3,2}(\hat{\mathbf{k}}) & -\sqrt{\frac{3}{7}} Y_{3,-1}(\hat{\mathbf{k}}) \end{pmatrix}. \tag{17.34}$$

The spherical harmonics are given by (Mathematica: SphericalHarmonicY)

$$\begin{aligned} Y_{3,\pm1}(\hat{\mathbf{k}}) &= \mp\sqrt{\frac{21}{64\pi}}(\hat{k}_x \pm i\hat{k}_y)(4\hat{k}_z^2 - 1) \propto \mp(\hat{k}_x \pm i\hat{k}_y) \\ Y_{3,\pm2}(\hat{\mathbf{k}}) &= \sqrt{\frac{105}{32\pi}}(\hat{k}_x \pm i\hat{k}_y)^2 \hat{k}_z \propto \mp(\hat{k}_x \pm i\hat{k}_y)^2. \end{aligned} \tag{17.35}$$

We see that, near the z-axis of momentum space, the off-diagonal components of $\mathcal{Y}$ vanish quadratically with k, whereas the diagonal components vanish linearly, so that

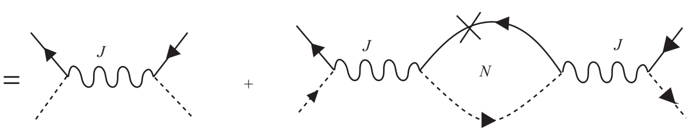
$$\mathcal{Y}(\hat{\mathbf{k}}) \sim \begin{pmatrix} \hat{k}_x + i\hat{k}_y & 0 \\ 0 & (\hat{k}_x - i\hat{k}_y) \end{pmatrix}, \tag{17.36}$$

which vanishes linearly with $(\hat{k}_x, \hat{k}_y)$ along the z-axis. This mismatch occurs because plane waves traveling along the z-axis carry $\pm\frac{1}{2}$ units of angular momentum in their direction of motion, and therefore cannot hybridize with the high-spin $M_J = \pm\frac{3}{2}$ f-states, giving rise to a vorticity in the hybridization. This phenomenon is believed to be important for the semi-metallic behavior in the compounds CeNiSn and CeRhSb [20], sometimes called *failed Kondo insulators*.

17.2.2 Enhancement of the Kondo temperature

To get an idea of how the Kondo effect is modified by the large degeneracy, consider the first-order renormalization of the interaction, which is given by the diagrams

$$J_{eff}(D') =$$



$$= J + NJ^2\rho \ln\left(\frac{D}{D'}\right), \tag{17.37}$$

where the cross on the intermediate conduction electron state indicates that all states in the energy window $|\epsilon_k| \in [D', D]$ are integrated out. The important point to notice here is that the rate of renormalization has been enhanced by a factor of N, due to the multiplicity of intermediate hole states. We can immediately see that the second term is comparable with the first at a scale $D' \equiv T_K = D \exp\left[-\frac{1}{NJ\rho}\right]$, with an N-fold enhancement of the coupling constant. More precisely, we see that the beta function $\beta(g) = \partial g(D')/\partial \ln D' = -g^2$, where $g(D') = N\rho J_{eff}(D')$. A more extensive calculation shows that the beta function to third order takes the form

$$\beta(g) = \frac{dg}{d \ln D'} = -g^2 + \frac{g^3}{N}. \tag{17.38}$$

The beta function describes a family of Kondo models with different cut-offs D' but the same low-energy physics. We can determine T_K as the temperature where the coupling constant becomes of order unity, $g \sim 1$. If we integrate out the conduction electrons with energy greater than T_K, we find

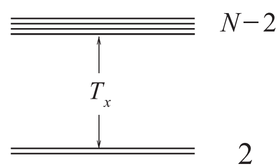
$$\int_{T_K}^{D} d\ln D' = \ln\left(\frac{D}{T_K}\right) = \int_1^{NJ\rho} \frac{dg}{-g^2 + g^3/N} \approx \int_1^{NJ\rho} dg\left[-\frac{1}{g^2} - \frac{1}{Ng}\right]$$
$$= \frac{1}{NJ\rho} - 1 - \frac{1}{N}\ln(NJ\rho), \tag{17.39}$$

which leads to the Kondo temperature

$$T_K = De(NJ\rho)^{\frac{1}{N}} \exp\left[-\frac{1}{NJ\rho}\right], \tag{17.40}$$

so that large degeneracy enhances the Kondo temperature in the exponential factor. By contrast, the RKKY interaction strength is given by $T_{RKKY} \sim J^2\rho$, and it does not involve any N-fold enhancement factors. Thus, in systems with large spin degeneracy, the enhancement of the Kondo temperature favors the formation of the heavy-fermion ground state.

In practice, rare-earth ions are exposed to the crystal fields of their host, which splits the $(N = 2j+1)$-fold degeneracy into many multiplets. Even in this case, the large degeneracy is helpful, because the crystal field splitting is small compared with the bandwidth. At energies D' large compared with the crystal field splitting T_x, $D' >> T_x$, the physics is that of an N-fold degenerate ion, whereas at energies D' small compared with the crystal field splitting, the physics is typically that of a Kramers doublet, i.e.



$$\frac{\partial g}{\partial \ln D} = \begin{cases} -g^2 & (D >> T_x) \\ -\frac{2}{N}g^2 & (D << T_x), \end{cases} \tag{17.41}$$

from which we see that, at low-energy scales, the leading-order renormalization of g is given by

$$\frac{1}{g(D')} = \frac{1}{NJ\rho} - \ln\left(\frac{D}{T_x}\right) - \frac{2}{N}\ln\left(\frac{T_x}{D'}\right),$$

where the first logarithm describes the high-energy screening with spin degeneracy N, and the second logarithm describes the low-energy screening with spin degeneracy 2. This expression is ~ 0 when $D' \sim T_K^*$, the Kondo temperature, so that

$$0 = \frac{1}{NJ\rho} - \ln\left(\frac{D}{T_x}\right) - \frac{2}{N}\ln\left(\frac{T_x}{T_K^*}\right),$$

from which we deduce that the renormalized Kondo temperature has the form [21]

$$T_K^* = D\exp\left(-\frac{1}{2J_0\rho}\right)\left(\frac{D}{T_X}\right)^{\frac{N}{2}-1}.$$

Here the first factor is the expression for the Kondo temperature of a spin factor $\frac{1}{2}$ Kondo model. The second captures the enhancement of the Kondo temperature derived from the renormalization on scales larger than the crystal field splitting. For $T_x \sim 100\,\mathrm{K}$, $D \sim 1000\,\mathrm{K}$ and $N = 6$, the enhancement factor is of order $10^{6/2-1} = 100$. In short, spin–orbit coupling substantially enhances the Kondo temperature even in the presence of crystal fields, and this is an important source of stabilization for the Kondo lattice in local-moment rare-earth and actinide materials. The absence of this effect in transition metal systems means that they are much more prone to the formation of spin glasses rather than heavy-fermion metals.[1]

[1] To obtain heavy-fermion behavior in transition metal systems, one needs magnetic frustration. A good example of such behavior is provided by the pyrochlore transition metal heavy-fermion system LiV_2O_3; see [22].

17.3 Large-N expansion for the Kondo lattice

17.3.1 Preliminaries

In the early 1980s, Anderson [23] pointed out that the large spin degeneracy $N = 2j + 1$ furnishes a small parameter $1/N$ which could be used to develop a controlled expansion about the limit $N \to \infty$. Anderson's observation opened up a new approach to the heavy-fermion problem: the *large-N expansion* [24, 25].

In 1983, two groups, Dennis Newns and Nicholas Read at Imperial College, London, working with Sebastian Doniach at Stanford University [26], and Piers Coleman, the author, working with Philip W. Anderson at Princeton [27], realized that, in the large-N limit, the *RKKY* interaction in the Kondo model could be ignored relative to the Kondo effect. The basic idea is simple: since the Kondo temperature in the N-fold degenerate Coqblin–Schrieffer model is given by (17.40),

$$T_K = De(NJ\rho)^{\frac{1}{N}} \exp\left[-\frac{1}{NJ\rho}\right], \tag{17.42}$$

then to take the large-N limit at fixed Kondo temperature, one must keep $\tilde{J} = NJ$ fixed. However, if one takes $N \to \infty$, the rescaled RKKY interaction $J^2\rho = \frac{1}{N^2}\tilde{J}^2\rho \sim O(1/N^2)$ is of order $1/N^2$, and hence vanishes in the large-N limit (Figure 17.5(b)), so the Kondo lattice is stable against magnetism in the large-N limit.

Building on this idea, and taking advantage of Edward Witten's large-N approach to the Gross–Neveu problem [24] and earlier path-integral formulations of the Kondo problem [28, 29], Nicholas Read and Dennis Newns formulated a large-N path integral approach for the Kondo lattice [26, 30, 31], work later extended by Assa Auerbach and Kathryn Levin at the University of Chicago [32]. We shall later examine how this method can be extended to include valence fluctuations in the infinite Anderson model using *slave bosons* [30, 31, 33–35].

The basic idea is to take 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

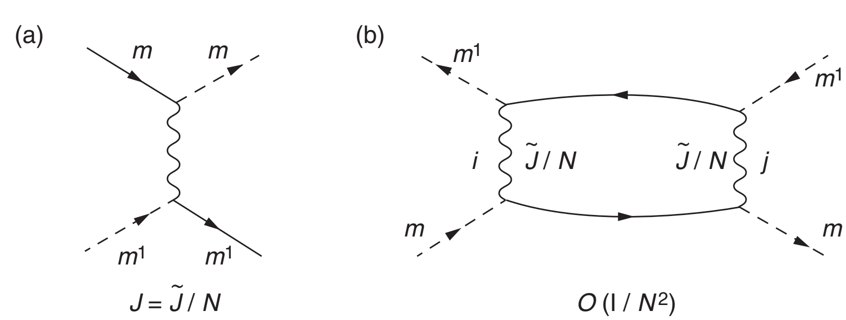


Fig. 17.5 Diagrams from [27]: (a) The Kondo exchange process is of order $O(1/N)$ so that (b) the RKKY interaction, which exchanges spin between two sites, is of order $O(1/N^2)$ and may be neglected in the large-N limit.

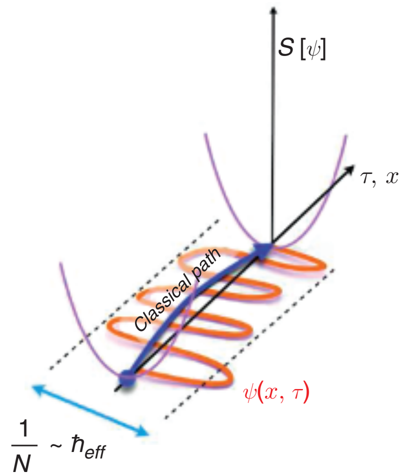


Fig. 17.6 Schematic diagram illustrating the convergence of a quantum path integral about a semiclassical trajectory in the large-N limit.

$$Z = \int \mathcal{D}[\psi] e^{-NS} = \int \mathcal{D}\psi \exp\left[-\frac{S}{1/N}\right] \equiv \int \mathcal{D}[\psi] \exp\left[-\frac{S}{\hbar_{eff}}\right]. \tag{17.43}$$

Here

$$\frac{1}{N} \sim \hbar_{eff}$$

behaves as an effective Planck's constant for the theory, focusing the path integral into a non-trivial "semiclassical" or mean-field solution as $\hbar_{eff} \to 0$. 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 $\frac{1}{N}$. For the Kondo model, we are lucky, because much of the important physics of is already captured by the large-N limit (Figure 17.6).

For simplicity, we shall consider a *toy Kondo lattice*, in which all electrons have a spin degeneracy $N = 2j + 1$, interacting with the local moment at each site via a Coqblin–Schrieffer interaction,

$$H = \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \frac{J}{N} \sum_{j,\alpha\beta} c^{\dagger}_{j\beta} c_{j\alpha} S_{\alpha\beta}(j), \tag{17.44}$$

where $c^{\dagger}_{j\alpha} = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} e^{-i\mathbf{k}\cdot\vec{R}_j}$ creates an electron localized at site j, and the spin of the local moment at position $\mathbf{R}_j$ is represented by pseudo-fermions:

$$S_{\alpha\beta}(j) = f^{\dagger}_{j\alpha} f_{j\beta} - \frac{n_f(j)}{N} \delta_{\alpha\beta}. \tag{17.45}$$

This representation requires that we set a value for the conserved f-occupancy $n_f(j)$ at each site. In preparation for a path integral approach, we rewrite the interaction in the factorized form encountered in (17.28), so that now

$$H = \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \frac{J}{N} \sum_{j,\alpha\beta} : \left(c^{\dagger}_{j\beta} f_{j\beta}\right) \left(f^{\dagger}_{j\alpha} c_{j\alpha}\right) :, \tag{17.46}$$

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. Notice the following:

- In this factorized form, the antiferromagnetic Kondo interaction is attractive.
- The coupling constant has been scaled to vary as J/N, to ensure that the interaction grows extensively with N. The interaction involves the product of two terms that scale as $O(N)$, scaling as $J/N \times O(N^2) \sim O(N)$.
- The model has a global $SU(N)$ symmetry associated with the conservation of the total magnetization.
- This model neglects the effects of spin–orbit coupling and the non-conservation of spin that is present in a typical rare-earth or actinide Kondo lattice material.
- The Coqblin–Schrieffer 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:

  $$f_{j\sigma} \rightarrow e^{i\phi_j} f_{j\sigma}. \tag{17.47}$$

  The appearance of local gauge symmetries in a strongly correlated electron problem is actually a general phenomenon. Here, the incompressible nature of the f-electrons gives rise to a constraint on the Hilbert space, which manifests itself as a gauge field.

Finally, before we continue, we need to decide what value to give the conserved charge $n_f = Q$. Most times, 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 $n_f = Q$ also scales with N so that the f-filling factor $q = Q/N$ is finite as $N \rightarrow \infty$. With this device, even if we only impose the constraint $\langle n_f \rangle = Q$ on the average, the RMS fluctuations $\sqrt{\langle \delta n_f^2 \rangle} \sim O(\sqrt{N})$ can be neglected relative to $Q \sim O(N)$. Thus if we're interested in a Kramers doublet Kondo model, we take the half-filled case $q = \frac{1}{2}$, $Q = N/2$, 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 $q = Q/N = \frac{1}{8}$.

17.4 The Read–Newns path integral

To construct the path integral, we need to first take care of the constraint $n_f = Q$. We want to write the partition function as a trace:

$$Z = \mathrm{Tr}\left[e^{-\beta H} \prod_j P_Q(j) \right], \tag{17.48}$$

where $P_Q(j)$ projects out the states with $n_f(j) = Q$ at site j. The constraints $P_Q(j)$ commute with the Hamiltonian and can be rewritten as a Fourier transform:

$$P_Q(j) = \delta_{n_{fj},Q} = \int_0^{2\pi} \frac{d\alpha_j}{2\pi} \exp\left[-i\alpha_j(n_{fj} - Q)\right] = \int_0^{2\pi iT} \frac{d\lambda_j}{2\pi iT} \exp\left[-\beta\lambda_j(n_{fj} - Q)\right], \tag{17.49}$$

where $\lambda_j = i\alpha_j T$ plays the role of a local chemical potential, integrated between $\lambda_j = 0$ and $\lambda_j = 2\pi iT$ along the imaginary axis. Substituting this expression for $P_Q(j)$ in the partition function, we obtain

$$Z = \int \mathcal{D}[\lambda] \mathrm{Tr}\left[e^{-\beta H[\lambda]}\right], \tag{17.50}$$

where now

$$H[\lambda] = \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \frac{J}{N} \sum_{j,\alpha\beta} : \left(c^\dagger_{j\beta} f_{j\beta}\right) \left(f^\dagger_{j\alpha} c_{j\alpha}\right) : + \sum_j \lambda_j (n_{fj} - Q) \tag{17.51}$$

and formally $\mathcal{D}[\lambda] = \prod_j \frac{d\lambda_j}{2\pi iT}$. Now, following the lines of Chapter 11, we rewrite the trace as a path integral:

$$Z = \int \mathcal{D}[\psi^\dagger, \psi, \lambda] \exp\left[- \int_0^\beta d\tau \overbrace{\left(\psi^\dagger \partial_\tau \psi + H[\bar{\psi}, \psi, \lambda]\right)}^{L[\psi^\dagger, \psi, \lambda]} \right], \tag{17.52}$$

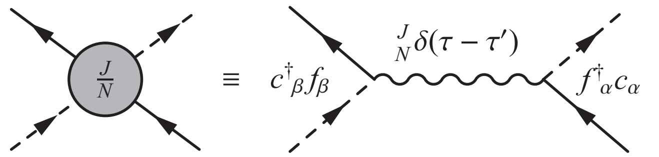
where $\psi^\dagger \equiv (\{c^\dagger\}, \{f^\dagger\})$ schematically represent the conduction and f-electron fields, while ψ is its conjugate. Inside the path integral we shall use $\psi^\dagger$ and ψ to represent the Grassman co-ordinates of the path integral, with the understanding that when used outside the path integral these symbols represents the corresponding field operators. Written in full, the Lagrangian is

$$\begin{aligned} L[\psi^\dagger, \psi, \lambda] = &\sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} + \sum_j f^\dagger_{j\sigma}(\partial_\tau + \lambda_j) f_{j\sigma} \\ &- \frac{J}{N} \sum_{j,\alpha\beta} \left(c^\dagger_{j\beta} f_{j\beta}\right) \left(f^\dagger_{j\alpha} c_{j\alpha}\right) - \sum_j \lambda_j Q. \end{aligned} \tag{17.53}$$

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

$$-\frac{J}{N} \sum_{\alpha\beta} \left(c^\dagger_{j\beta} f_{j\beta}\right) \left(f^\dagger_{j\alpha} c_{j\alpha}\right) \rightarrow \sum_\alpha \left[\bar{V}_j \left(c^\dagger_{j\alpha} f_{j\alpha}\right) + \left(f^\dagger_{j\alpha} c_{j\alpha}\right) V_j\right] + N\frac{\bar{V}_j V_j}{J}. \tag{17.54}$$

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:



$$-\frac{J}{N}\sum_{\mathbf{k},\mathbf{k}',\alpha,\beta}(c^\dagger{}_\beta f_\beta)(f^\dagger{}_\alpha c_\alpha) \tag{17.55}$$

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 to an intermediate valence fluctuation.

The path integral now involves an additional integration over the hybridization fields V and $\bar{V}$:

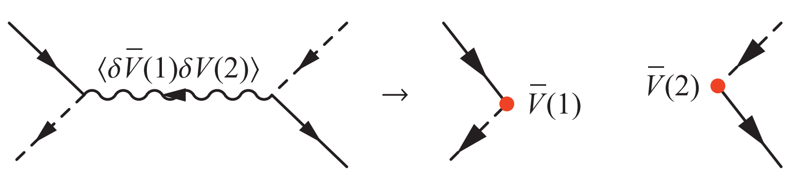
$$Z = \int \mathcal{D}[\bar{V},V,\lambda]\int \mathcal{D}[\psi^\dagger,\psi]\exp\Bigg[-\overbrace{\int_0^\beta (\psi^\dagger\partial_\tau\psi + H[\bar{V},V,\lambda])}^{S[\bar{V},V,\lambda,\,\psi^\dagger,\psi]}\Bigg]$$

$$H[\bar{V},V,\lambda] = \sum_{\mathbf{k}}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_j\Bigg[\bar{V}_j\left(c^\dagger_{j\sigma}f_{j\sigma}\right) + \left(f^\dagger_{j\sigma}c_{j\sigma}\right)V_j$$
$$+\lambda_j(n_{fj}-Q) + N\frac{\bar{V}_jV_j}{J}\Bigg], \tag{17.56}$$

Read–Newns path integral for the Kondo lattice

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

The importance of the Read–Newns path integral is that it 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 cannot be dealt with in perturbation theory. Bound states induce long-range temporaral correlations in scattering and, indeed, once the hybridization condenses, the interaction lines break up into independent anomalous scattering events, denoted by



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