(a) Repeat the Schrieffer–Wolff transformation for the case of constant hybridization $V_{\mathbf{k}} = V$ and particle–hole symmetry to show that the Kondo model with source terms now becomes

$$H_K[\bar{\eta}, \eta] = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\sigma} + J \left(\psi^{\dagger}(0) + V^{-1}\bar{\eta} \right) \vec{\sigma} \left(\psi(0) + V^{-1}\eta \right) \cdot \vec{S}. \tag{16.119}$$

(b) By differentiating this expression with respect to $\bar{\eta}_{\sigma}$, show that in the Kondo model the original f-electron operator has now become a *composite operator* involving a combined conduction electron and spin-flip, as follows:

$$f_{\alpha} \equiv \frac{\delta H_K[\bar{\eta}, \eta]}{\delta \bar{\eta}_{\alpha}} = \frac{J}{V} \left(\sigma_{\alpha\beta} \cdot \vec{S} \right) \psi(0)_{\beta}. \tag{16.120}$$

When a Fermi liquid develops, it is this object that behaves like a resonant bound-state fermion.

Solution

(a) In the Anderson model, we can absorb the source term into the hybridization, writing it in the form

$$\mathcal{V} = \sum (V\psi^{\dagger}_{\sigma}(0) + \bar{\eta}_{\sigma}) f_{\sigma} + \text{H.c.}, \tag{16.121}$$

so that in the hybridization we have replaced $\psi_{\sigma}(0) \to \psi_{\sigma}(0) + \frac{1}{V}\eta_{\sigma}$. If we now repeat the Schrieffer–Wolff transformation, the spin exchange term in the Kondo model takes the form

$$H_K[\bar{\eta}, \eta] = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\sigma} + J \left(\psi^{\dagger}(0) + V^{-1}\bar{\eta} \right) \vec{\sigma} \left(\psi(0) + V^{-1}\eta \right) \cdot \mathrm{S}. \tag{16.122}$$

(b) If we now differentiate H_K with respect to $\bar{\eta}$, we obtain

$$f_{\sigma} \equiv \left. \frac{\delta H_K[\bar{\eta}, \eta]}{\delta \eta_{\sigma}} \right|_{\eta, \bar{\eta}=0} = \frac{J}{V} \left[(\vec{\sigma} \cdot \vec{S}) \psi(0) \right]_{\sigma}. \tag{16.123}$$

16.9 "Poor man's" scaling

We now apply the scaling concept to the Kondo model. This was originally carried out by Anderson and Yuval [12–14] using a method formulated in the time rather than the energy domain. The method presented here follows Anderson's "poor man's" scaling approach [31, 32], in which the evolution of the coupling constant is followed as the bandwidth of the conduction sea is reduced. The Kondo model is written

$$H = \sum_{|\epsilon_k| < D} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + H^{(I)}$$

$$H^{(I)} = J(D) \sum_{|\epsilon_k|,|\epsilon_{k'}|<D} c^{\dagger}_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k'\beta} \cdot \vec{S}_f, \tag{16.124}$$

where the density of conduction electron states $\rho(\epsilon)$ is taken to be constant. The poor man's renormalization procedure follows the evolution of $J(D)$ that results from reducing D by progressively integrating out the electron states at the edge of the conduction band. In the poor man's procedure, the bandwidth is not rescaled to its original size after each renormalization. This avoids the need to renormalize the electron operators so that, instead of (16.84), $H(D') = \tilde{H}_L$.

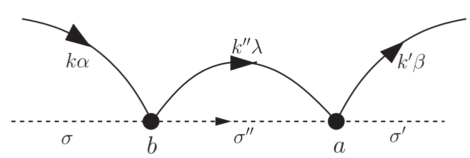
To carry out the renormalization procedure, we integrate out the high-energy spin fluctuations using the t-matrix formulation for the induced interaction ΔH, derived in the previous section. Formally, the induced interaction is given by

$$\Delta H_{ab} = \frac{1}{2}[T_{ab}(E_a) + T_{ab}(E_b)],$$

where

$$T_{ab}(E) = \sum_{\lambda \in |H\rangle} \left[\frac{H^{(I)}_{a\lambda} H^{(I)}_{\lambda b}}{E - E^H_\lambda} \right],$$

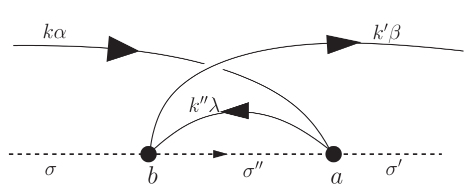
where the energy of state $|\lambda\rangle$ lies in the range $[D', D]$. There are two possible intermediate states that can be produced by the action of $H^{(I)}$ on a one-electron state: either (I) the electron state is scattered directly or (II) a virtual electron–hole pair is created in the intermediate state. In process I, the t-matrix can be represented by the Feynman diagram



for which the t-matrix for scattering into a high-energy electron state is

$$\begin{aligned} T^{(I)}(E)_{k'\beta\sigma';k\alpha\sigma} &= \sum_{\epsilon_{k''} \in [D-\delta D, D]} \left[\frac{1}{E - \epsilon_{k''}} \right] J^2 (\sigma^a \sigma^b)_{\beta\alpha} (S^a S^b)_{\sigma'\sigma} \\ &\approx J^2 \rho \delta D \left[\frac{1}{E - D} \right] (\sigma^a \sigma^b)_{\beta\alpha} (S^a S^b)_{\sigma'\sigma}. \end{aligned} \tag{16.125}$$

In process II,



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the formation of a particle–hole pair involves a conduction electron line that crosses itself, leading to a negative sign. Notice how the spin operators of the conduction sea and antiferromagnet reverse their relative order in process II, so that the t-matrix for scattering into a high-energy hole state is given by

$$T^{(II)}(E)_{k'\beta\sigma';k\alpha\sigma} = -\sum_{\epsilon_{k''}\in[-D,-D+\delta D]} \left[\frac{1}{E-(\epsilon_k+\epsilon_{k'}-\epsilon_{k''})}\right] J^2(\sigma^b\sigma^a)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma}$$
$$= -J^2\rho\delta D\left[\frac{1}{E-D}\right](\sigma^b\sigma^a)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma}, \tag{16.126}$$

where we have assumed that the energies ϵ_k and $\epsilon_{k'}$ are negligible compared with D. Adding (16.125) and (16.126) gives

$$\delta H^{int}_{k'\beta\sigma';k\alpha\sigma} = \hat{T}^{(I)} + \hat{T}^{(II)} = -\frac{J^2\rho|\delta D|}{D}[\sigma^a,\sigma^b]_{\beta\alpha}S^aS^b$$
$$= -\frac{1}{2}\frac{J^2\rho|\delta D|}{D}\overbrace{[\sigma^a,\sigma^b]_{\beta\alpha}}^{2i\epsilon^{abc}\sigma^c}\overbrace{[S^a,S^b]}^{i\epsilon^{abd}S^d}$$
$$= \frac{J^2\rho|\delta D|}{D}\overbrace{\epsilon^{abc}\epsilon^{abd}}^{2\delta_{cd}}\sigma^c_{\beta\alpha}S^d$$
$$= 2\frac{J^2\rho|\delta D|}{D}\vec{\sigma}_{\beta\alpha}\cdot\vec{S}_{\sigma'\sigma}. \tag{16.127}$$

In this way we see that the virtual emission of a high-energy electron and hole generates an antiferromagnetic correction to the original Kondo coupling constant:

$$J(D-|\delta D|) = J(D) + 2J^2\rho\frac{|\delta D|}{D} = J(D) - 2J^2\rho\frac{\delta D}{D}, \tag{16.128}$$

since we have reduced the bandwidth, $\delta D = -|\delta D|$. In other words,

$$\frac{\partial J\rho}{\partial \ln D} = -2(J\rho)^2 \tag{16.129}$$

or, in terms of the dimensionless coupling constant $g = \rho J$,

$$\frac{\partial g}{\partial \ln D} = \beta(g) = -2g^2 + O(g^3). \tag{16.130}$$

Now since $\beta(g=0) = 0$ at $g = 0$, scaling comes to halt: we say that $g = 0$ is a *fixed point*. It is instructive to rewrite the scaling equation in the form

$$\frac{\partial \ln g}{\partial \ln(D_0/D)} = 2g + O(g^2), \tag{16.131}$$

where D_0 is the initial bandwidth. From this form, we see that the direction of the scaling depends on the sign of $g = J\rho$ (see Figure 16.16). As we reduce the size D of the cut-off,

- for antiferromagnetic $g > 0$, the magnitude of g grows. We say that the fixed point is *repulsive*. In other words, spin fluctuations antiscreen the antiferrromagnetic interaction, causing it to grow at low energies.
- for ferromagnetic $g < 0$, scaling reduces the magnitude of g, driving one ever closer to the weak coupling fixed point at $g = 0$. In this case, the fixed point is attractive and spin fluctuations screen the interaction, causing J to scale logarithmically slowly to zero at low energies.

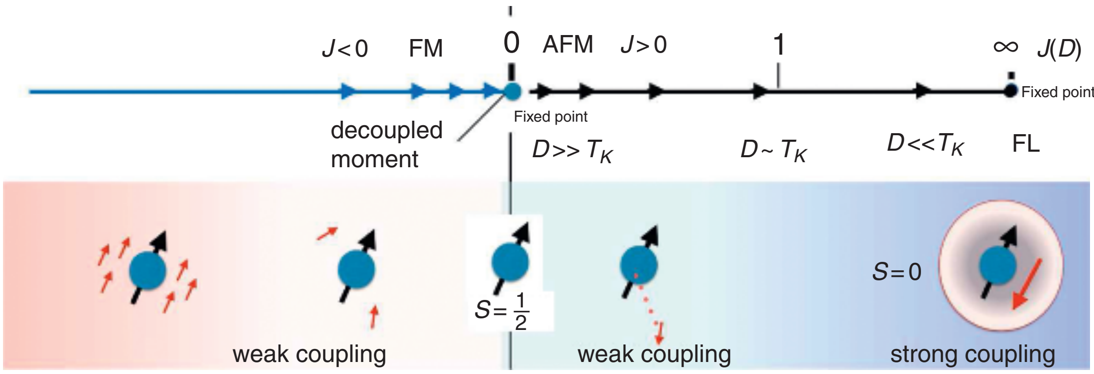


Fig. 16.16 Schematic illustration of renormalization group flow in the Kondo model. For $J < 0$ (ferromagnetic), the coupling constant scales to an attractive fixed point at $J = 0$, forming a decoupled local moment. For $J > 0$ (antiferromagnetic), scaling proceeds from a repulsive weak-coupling fixed point, via a crossover to an attractive strong-coupling fixed point in which the local moment is screened by the conduction electrons, removing its internal degrees of freedom to form a Fermi liquid. In the diagram, FM = ferromagnet, AFM = antiferromagnet, and FL = Fermi liquid.

To examine these two cases in more detail, we integrate the scaling equation between the initial bandwidth D_0 and D', writing

$$\int_{g_0}^{g(D)} \frac{dg'}{g'^2} = -2 \int_{\ln D_0}^{\ln D'} d \ln D'' \tag{16.132}$$

or

$$\left(\frac{1}{g_0} - \frac{1}{g(D')} \right) = -2 \ln(D'/D_0), \tag{16.133}$$

where $g_0 = J\rho = g(D_0)$ is the unrenormalized coupling constant at the original bandwidth D_0. In this case,

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D_0}{D'}}. \tag{16.134}$$

Let us look at the ferromagnetic and antiferromagnetic cases seperately.

Ferromagnetic interaction, $g < 0$

In this case,

$$g(D') = -\frac{|g_o|}{1 + 2|g_o| \ln(D_0/D')}, \tag{16.135}$$

which corresponds to a very gradual decoupling of the local moment from the surrounding conduction sea. The interaction is said to be marginally irrelevant, because it scales logarithmically to zero, and at all scales the problem remains perturbative.

Antiferromagnetic interaction, $g > 0$

For the antiferromagnetic case ($g > 0$), the solution to the scaling equation is

$$g(D') = \frac{g_o}{1 - 2g_o \ln(D/D')} = \frac{1}{2}\frac{1}{\ln(D'/D_0) + \frac{1}{2g_0}} = \frac{1}{2}\frac{1}{\ln\left[\frac{D'}{D_0\exp(-1/(2g_0))}\right]}, \tag{16.136}$$

where we have divided numerator and denominator by $2g_0$. It follows that

$$2g(D') = \frac{1}{\ln(D'/T_K)},$$

where we have introduced the Kondo temperature

$$T_K = D_0 \exp\left[-\frac{1}{2g_o}\right]. \tag{16.137}$$

The Kondo temperature T_K is an example of a dynamically generated scale.

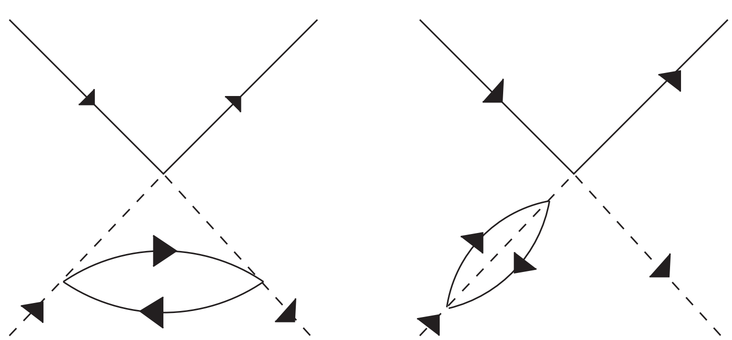
Were we to take this equation literally, we would say that g diverges at the scale $D' = T_K$. This interpretation is too literal, because the scaling has only been calculated to order g^2. Nevertheless it does show that the Kondo interaction can only be treated perturbatively at energies large compared with the Kondo temperature. We also see that, once we have written the coupling constant in terms of the Kondo temperature, all reference to the original cut-off energy scale vanishes from the expression. This cut-off independence of the problem is an indication that the physics of the Kondo problem does not depend on the high-energy details of the model: there is only one relevant energy scale, the Kondo temperature.

By calculating the higher-order diagrams shown in Figure 16.17, it is straightforward, though somewhat technical (see Exercise 16.8), to show that the beta function to order g^3 is given by

$$\frac{\partial g}{\partial \ln D} = \beta(g) = -2g^2 + 2g^3 + O(g^4). \tag{16.138}$$

One can integrate this equation to obtain

$$\ln\left(\frac{D'}{D}\right) = \int_{g_o}^{g} \frac{dg'}{\beta(g')} = -\frac{1}{2}\int_{g_o}^{g} dg'\left[\frac{1}{g'^2} + \frac{1}{g'} + O(1)\right], \tag{16.139}$$



Diagrams contributing to the third-order term in the beta function. See Exercise 16.8. **Fig. 16.17** where we have expanded the numerator in $\frac{1}{\beta(g)} \approx -\frac{1}{g^2(1-g)} - \frac{1}{g^2}(1+g) + O(1)$. A better estimate of the temperature T_K where the system scales to strong coupling is obtained by setting $D' = T_K$ and $g = 1$ in this equation, which gives

$$\ln\left(\frac{T_K}{D}\right) = -\frac{1}{2}\int_{g_0}^{1} dg' \left[\frac{1}{g'^2} + \frac{1}{g'}\right] = -\frac{1}{2g_o} + \frac{1}{2}\ln 2g_o + O(1), \tag{16.140}$$

where we have dropped the terms of order unity on the right-hand side. Thus, up to a prefactor, the dependence of the Kondo temperature on the bare coupling constant is given by

$$T_K = D_0\sqrt{2g_o}e^{-\frac{1}{2g_o}}. \tag{16.141}$$

The square-root $\sqrt{g_0}$ dependence on the coupling constant is often dropped in qualitative discussions, but it is important for more quantitative comparisons.

Example 16.6 Consider the symmetric Anderson model. At energy scales greater than $U/2$ the impurity is mixed-valent. However, once the cut-off $D \sim U/2$, one must carry out a Schrieffer–Wolff transformation.

(a) Show that the Kondo coupling constant of the symmetric Anderson model is $g_0 = J\rho = 4\Delta/(\pi U)$, where $\Delta = \pi\rho V^2$ is the bare resonant level width of the Anderson model.
(b) Using (16.141) with a cut-off $D = U/2$, derive the following form (16.72) for the Kondo temperature of the symmetric Anderson model:

$$T_K = \sqrt{\frac{2U\Delta}{\pi}}\exp\left(-\frac{\pi U}{8\Delta}\right).$$

Solution

(a) In the symmetric Anderson model, $E_f = -U/2$. Assuming that the hybridization $V_k = V$ is constant, then from (16.108) the Kondo coupling constant is given by

$$g_0 = J\rho = V^2\rho\left[\frac{1}{E_f + U/2} + \frac{1}{-E_f}\right] = 4\frac{V^2\rho}{U} = \frac{4\Delta}{\pi U}, \tag{16.142}$$

where $\Delta = \pi\rho V^2$.
(b) Using (16.141) with $D = U/2$, we obtain

$$T_K = \frac{U}{2}\sqrt{\frac{8\Delta}{\pi U}}\exp\left(-\frac{8\Delta}{\pi U}\right) = \sqrt{\frac{2U\Delta}{\pi}}\exp\left(-\frac{\pi U}{8\Delta}\right). \tag{16.143}$$

16.9.1 Kondo calculus: Abrikosov pseudo-fermions and the Popov–Fedatov method

The awkward feature of spin operators is that they do not satisfy Wick's theorm, so that we cannot treat them directly in a Feynman diagram expansion. Kondo calculus requires that we overcome this difficulty, and a variety of methods have been developed. One tool that is particularly useful is the Abrikosov pseudo-fermion representation [44], in which the spin operator, is factorized in terms of a spin-$\frac{1}{2}$ fermion field $f^\dagger_\sigma$, as follows:

$$\vec{S} = f^\dagger_\alpha \left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta} f_\beta. \tag{16.144}$$

This has the advantage that one can now take advantage of Wick's theorem. In Abrikosov's representation of a spin-$\frac{1}{2}$ operator, the up and down states are now represented by the states

$$|\sigma\rangle = f^\dagger_\sigma |0\rangle \qquad (\sigma = \uparrow, \downarrow). \tag{16.145}$$

However, in using the f-electron one has inadvertently expanded the Hilbert space, introducing two unphysical states: the empty state $|0\rangle$ and the doubly occupied state $|\uparrow\downarrow\rangle = f^\dagger_\downarrow f^\dagger_\uparrow |0\rangle$, which need to be eliminated by requiring that

$$n_f = 1. \tag{16.146}$$

Conveniently, this constraint commutes with the spin operator, and hence is a constant of the motion, provided the f-electrons only enter as spin operators in the Hamiltonian. An ingenious way of imposing this constraint has been developed by Popov and Fedotov [53]. Their method introduces a complex chemical potential for the pseudo-fermions:

$$\mu = -i\pi \frac{T}{2}.$$

The partition function of the Hamiltonian is written as an unconstrained trace over the conduction and pseudofermion Fock spaces:

$$Z = \mathrm{Tr}\left[e^{-\beta(H + i\pi \frac{T}{2}(n_f - 1))}\right]. \tag{16.147}$$

Now since the Hamiltonian conserves n_f, we can divide this trace into contributions from the d^0, d^1, and d^2 subspaces, as follows:

$$Z = e^{i\pi/2} Z(f^0) + Z(f^1) + e^{-i\pi/2} Z(f^2).$$

But since $S_f = 0$ in the f^2 and d^0 subspaces, $Z(f^0) = Z(f^2)$, so that the contributions to the partition function from these two unwanted subspaces exactly cancel. In the Popov–Fedotov approach, the bare f-propagators have the form

$$\mathcal{G}_f(i\tilde{\omega}_n) = \frac{1}{i\omega_n + \mu} = \frac{1}{i\omega_n - i\pi T/2} = \frac{1}{i2\pi T(n + \frac{1}{4})}, \tag{16.148}$$

corresponding to a shifted Matsubara frequency $\tilde{\omega}_n = 2\pi T(n + \frac{1}{4})$. You can test this method by applying it to a free spin in a magnetic field (see Example 16.7). The method can also be extended to deal with spin-1 operators using $-\mu = i\pi T/3$.

Example 16.7 Test the Popov–Fedotov trick [53]. Consider the magnetization of a free electron with Hamiltonian

$$H = \epsilon_\sigma f^\dagger_\sigma f_\sigma. \tag{16.149}$$

Show that with $\epsilon_\sigma = -\sigma B$ you obtain the wrong field dependence of the magnetization $M = \tanh\left(\frac{B}{2T}\right)$, but that with the Popov–Fedotov form $\epsilon_\sigma = -\sigma B + \frac{i\pi T}{2}$ you recover the Brillouin formula for a free spin,

$$M = \tanh\left(\frac{B}{T}\right). \tag{16.150}$$

Solution

If we write

$$F = -T \sum_{\sigma=\pm} \ln\left[1 + e^{-\beta\epsilon_\sigma}\right], \tag{16.151}$$

then the magnetization is given by

$$M = -\frac{\partial F}{\partial B} = \sum_\sigma \sigma f(\epsilon_\sigma). \tag{16.152}$$

If we evaluate this expression with $\epsilon_\sigma = -\sigma B$, we obtain the wrong form for the magnetization:

$$M = \frac{1}{e^{-\beta B}+1} - \frac{1}{e^{\beta B}+1} = \frac{(e^{\beta B} - e^{-\beta B})}{2 + 2\cosh\beta B}. \tag{16.153}$$

We can see the problem: the extra contribution to the partition function from the empty and doubly occupied sites gives $Z = 2 + 2\cosh\beta B$ rather than $Z = 2\cosh\beta B$. If we simplify this expression, we obtain

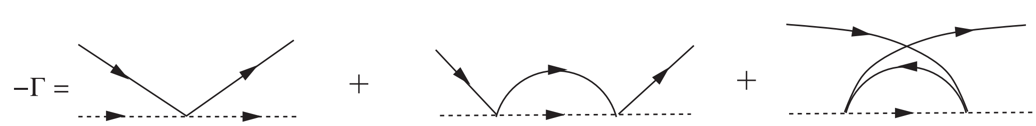
$$M = \frac{\sinh\beta B}{1+\cosh\beta B} = \frac{2\sinh(\beta B/2)\cosh(\beta B/2)}{2\cosh^2(\beta B/2)} = \tanh\left(\frac{B}{2T}\right),$$

which has the wrong field dependence. By contrast, if we use $\epsilon_\sigma = -\sigma B + \frac{i\pi T}{2}$ we obtain

$$M = \frac{1}{ie^{-\beta B}+1} - \frac{1}{ie^{\beta B}+1} = \frac{(e^{\beta B} - e^{-\beta B})}{2\cosh\beta B} = \tanh\left(\frac{B}{T}\right), \tag{16.154}$$

recovering the Brillouin function.

Example 16.8 Explicitly calculate the Kondo scattering amplitude



to second order in J, using the Popov–Fedotov scheme. By examining the scattering amplitude on the Fermi surface, show that the Kondo coupling constant is logarithmically enhanced according to the formula

$$J\rho \rightarrow J\rho + 2(J\rho)^2 \ln\left[\frac{De^{\pi/2-\psi(\frac{1}{2})}}{2\pi T}\right], \tag{16.155}$$

where $\psi(x)$ is the digamma function.

Solution

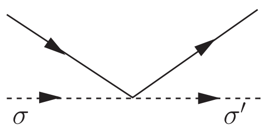
We represent the conduction electron and f-electron propagators by the diagrams

$$= G_c(i\omega_n, \mathbf{k}) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}$$

$$= G_f(i\omega_n) = \frac{1}{i\omega_n - \lambda_f}, \tag{16.156}$$

where $\lambda_f \equiv i\frac{\pi T}{2}$ is the imaginary chemical potential that cancels the doubly occupied and empty states. The first-order Kondo scattering amplitude is given by

$\Gamma_0 =$

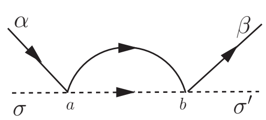


$$= -J\left(\vec{\sigma}_{\beta\alpha} \cdot \vec{S}_{\sigma'\sigma}\right) \qquad \left(\vec{S}_{\sigma'\sigma} \equiv \left(\frac{\vec{\sigma}}{2}\right)_{\sigma'\sigma}\right). \tag{16.157}$$

Here the minus sign derives from the Feynman rules for an interaction vertex, and we have used the shorthand $\vec{S} \equiv \frac{\vec{\sigma}}{2}$ for the f-electron spin matrix elements.

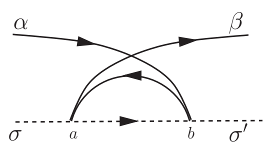
The second-order scattering processes are given by

$\Gamma_I =$



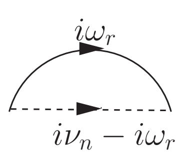
$$= J^2\left(\sigma^b\sigma^a\right)_{\beta\alpha}\left(S^bS^a\right)_{\sigma'\sigma}\pi_1(i\nu_n) \tag{16.158}$$

$\Gamma_{II} =$



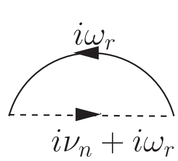
$$= -J^2\left(\sigma^a\sigma^b\right)_{\beta\alpha}\left(S^bS^a\right)_{\sigma'\sigma}\pi_2(i\nu_n), \tag{16.159}$$

where $i\nu_n$ is the total energy in the particle–particle and particle–hole channels, respectively. Note the -1 prefactor in Γ_{II} and the inversion of the order of the conduction electron Pauli matrices, which both derive from the crossing of the incoming and outgoing conduction electron lines. Here,



$$= \pi_1(i\nu_n) = T\sum_{i\omega_r,\mathbf{k}} \frac{1}{i\omega_r - \epsilon_{\mathbf{k}}}\frac{1}{i\nu_n - i\omega_r - \lambda_f}, \tag{16.160}$$

and



$$= \pi_2(i\nu_n) = -T\sum_{i\omega_r,\mathbf{k}} \frac{1}{i\omega_r - \epsilon_{\mathbf{k}}}\frac{1}{i\nu_n + i\omega_r - \lambda_f} \tag{16.161}$$

are the Kondo polarization bubbles in the particle–particle and particle–hole channels, respectively.

Now let us calculate the polarization bubbles (16.160) and (16.161). If we reverse the sign of $i\omega_r \to -i\omega_r$ in the internal summation in (16.160) we obtain

$$\pi_1(i\nu_n) = -T\sum_{i\omega_r,\mathbf{k}} \frac{1}{i\omega_r + \epsilon_{\mathbf{k}}} \frac{1}{i\nu_n + i\omega_r - \lambda_f}, \tag{16.162}$$

and assuming a particle–hole symmetric conduction electron density of states, we can replace $\epsilon_{\mathbf{k}} \to -\epsilon_{\mathbf{k}}$, so that

$$\pi_1(i\nu_n) = \pi_2(i\nu_n) = -T\sum_{i\omega_r,\mathbf{k}} \frac{1}{i\omega_r - \epsilon_{\mathbf{k}}} \frac{1}{i\nu_n + i\omega_r - \lambda_f}. \tag{16.163}$$

Now this is a well-known fermion bubble, and we can use our standard method of contour integration to carry out the summation over the internal Matsubara frequency $i\omega_r$, to obtain

$$\pi_2(i\nu_n) = \sum_{\mathbf{k}} \frac{f(\lambda) - f(\epsilon_{\mathbf{k}})}{i\nu_n - (\lambda_f - \epsilon_{\mathbf{k}})} = \int d\epsilon \rho(\epsilon) \frac{f(\lambda) - f(\epsilon)}{i\nu_n - (\lambda_f - \epsilon)}, \tag{16.164}$$

where $\rho(\epsilon)$ is the density of states per spin. The summation over energy in this integral is a bit tricky. If we use a flat density of states, then at zero temperature

$$\pi_2(i\nu_n) = \frac{\rho}{2}\int_{-D}^{D} \frac{\mathrm{sgn}\epsilon}{i\nu_n + \epsilon} = \rho \ln\left(\frac{D}{|\nu_n|}\right),$$

so the frequency provides the lower logarithmic cut-off. When we do the calculation at a finite temperature, we expect that if $T >> |\nu_n|$ then the temperature becomes the cut-off, so that our back-of-the-envelope estimate of this integral is

$$\pi_2(i\nu_n) \sim \rho \ln\left(\frac{D}{\max(|\nu_n|, T)}\right).$$

To calculate the precise form of the integral takes more work, but can be done for a Lorentzian density of states $\rho(\epsilon) = \rho\Phi(\epsilon)$, where $\Phi(x) = D^2/(\epsilon^2 + D^2)$. Here we quote the result (see Appendix 16A):

$$\int d\epsilon\, \Phi(\epsilon)\left(\frac{f(\lambda_f) - f(\epsilon)}{\epsilon - \xi}\right) = \ln\frac{D}{2\pi T} - \psi\left(\frac{1}{2} + \frac{\xi\beta}{2\pi i}\right) - i\frac{\pi}{2}\tanh(\beta\lambda_f/2), \tag{16.165}$$

provided Im $\xi > 0$ (for the opposite sign, one takes the complex conjugate of the above). Putting in $\lambda_f = i\pi T/2$, $\xi = i(\pi T/2 - \nu_n)$, we then obtain

$$\begin{aligned}\pi_2(i\nu_n) = \rho\int d\epsilon\,\Phi(\epsilon)\left[\frac{f(\lambda_f) - f(\epsilon)}{\epsilon - (\lambda_f - i\nu_n)}\right] &= \rho\left[\ln\frac{D}{2\pi T} - \psi\left(\frac{1}{2} + \frac{\pi T/2 - \nu_n}{2\pi T}\right) + \frac{\pi}{2}\right] \\ &= \rho\left[\ln\frac{De^{\pi/2}}{2\pi T} - \psi\left(\frac{1}{2} + \frac{\pi T/2 - \nu_n}{2\pi T}\right)\right] \qquad (\pi T/2 - \nu_n > 0).\end{aligned} \tag{16.166}$$

Strictly speaking, our result only holds for Im $\xi > 0$, i.e. when $\pi/2 - \nu_n = |A| > 0$. The other sign, where $\pi/2 - \nu_n = -|A| < 0$, is obtained by taking the complex conjugate of the result for positive $\pi/2 - \nu_n = |A|$. But since the right-hand side is real, taking the complex conjugate has no effect, so we see that the result only depends on the magnitude $|\pi T/2 - \nu_n|$, enabling us to write

$$\pi_2(i\nu_n) = \rho\left[\ln\frac{De^{\pi/2}}{2\pi T} - \psi\left(\frac{1}{2} + \frac{|\nu_n - \pi T/2|}{2\pi T}\right)\right]. \tag{16.167}$$

Notice that the analytic continuation of this expression contains a branch cut along the line Im $z = i\pi T/2$, a consequence of using a non-Hermitian Hamiltonian (this can be fixed by using a shifted Matsubara frequency for the f-lines). It follows that

$$\pi_2(z) = \begin{cases} \rho\left[\ln\frac{De^{\pi/2}}{2\pi T} - \psi\left(\frac{1}{2} + \frac{z - i\pi T/2}{2\pi iT}\right)\right] & (\text{Im } z > \pi T/2) \\ \rho\left[\ln\frac{De^{\pi/2}}{2\pi T} - \psi\left(\frac{1}{2} - \frac{z^* + i\pi T/2}{2\pi iT}\right)\right] & (\text{Im } z < \pi T/2). \end{cases} \tag{16.168}$$

Adding up the second-order amplitudes, we obtain

$$\begin{aligned} -\Gamma(z_{pp}, z_{ph})_{\beta\sigma';\alpha\sigma} = -J\left(\vec{\sigma}_{\beta\alpha}\cdot\vec{S}_{\sigma'\sigma}\right) &+ J^2\rho[\pi_2(z_{pp})(\sigma^b\sigma^a)_{\beta\alpha} \\ &- \pi_2(z_{ph})(\sigma^b\sigma^a)_{\beta\alpha}]\left(S^bS^a\right)_{\sigma'\sigma}. \end{aligned} \tag{16.169}$$

Notice that the logarithmically divergent parts of the particle–hole and particle–particle scattering are the same, while the low-energy parts differ by finite amounts. However, if we examine the onshell scattering on the Fermi surface, i.e. with $z_{ph} = z_{pp} = i\pi T/2$, then we obtain

$$\begin{aligned} -\Gamma &= -J\left(\vec{\sigma}_{\beta\alpha}\cdot\vec{S}_{\sigma'\sigma}\right) + J^2\rho\ln\frac{De^{\pi/2-\psi(1/2)}}{2\pi T}[\sigma^b,\sigma^a]_{\beta\alpha}(S^bS^a)_{\sigma'\sigma} \\ &= -J\left(\vec{\sigma}_{\beta\alpha}\cdot\vec{S}_{\sigma'\sigma}\right) + J^2\rho\ln\frac{De^{\pi/2-\psi(1/2)}}{2\pi T}2i\sigma^c_{\beta\alpha}\overbrace{\epsilon_{bac}(S^bS^a)_{\sigma'\sigma}}^{iS^c} \\ &= -\left[J + 2J^2\rho\ln\frac{De^{\pi/2-\psi(1/2)}}{2\pi T}\right]\left(\vec{\sigma}_{\beta\alpha}\cdot\vec{S}_{\sigma'\sigma}\right), \end{aligned} \tag{16.170}$$

explicitly demonstrating the logarithmic renormalization of the coupling constant.

16.9.2 Universality and the resistance minimum

Provided the Kondo temperature is far smaller than the cut-off, then at low energies it is the only scale governing the physics of the Kondo effect. For this reason, we expect all physical quantities to be expressed in terms of universal functions involving the ratio of the temperature or field to the Kondo scale. For example, the susceptibility

$$\chi(T) = \frac{1}{T}F\left(\frac{T}{T_K}\right) \tag{16.171}$$

and the quasiparticle scattering rate

$$\frac{1}{\tau(T)} = \frac{1}{\tau_o}\mathcal{G}\left(\frac{T}{T_K}\right) \tag{16.172}$$

both display universal behavior. If we change the cut-off of the model, adjusting the bare coupling constant g_0 so that T_K is fixed, the physical quantities will be unchanged. If we replace $g_0 \rightarrow g(D)$ in (16.140), then all models with $J(D)\rho = g(D)$, where

$$\ln\left(\frac{T_K}{D}\right) = -\frac{1}{2g(D)} + \frac{1}{2}\ln 2g(D), \tag{16.173}$$

will have the same Kondo temperature and thus the same low-temperature behavior. However, we can view this another way: as the temperature is lowered, quantum processes become coherent at increasingly lower energies, and the effective cut-off for quantum processes is T. Thus, as the temperature is lowered, the coupling constant g_0 is renormalized to a new value,

$$g_0 \rightarrow g(T), \tag{16.174}$$

where

$$\ln\left(\frac{T_K}{T}\right) = -\frac{1}{2g(T)} + \frac{1}{2}\ln 2g(T). \tag{16.175}$$

In this way, lowering the temperature drives the system along the renormalization trajectory from weak to strong coupling.

We can check the existence of universality by examining these properties in the weak-coupling limit, where $T >> T_K$. Here, we find

$$\frac{1}{\tau(T)} = 2\pi J^2\rho S(S+1)n_i = \frac{2\pi}{\rho}S(S+1)n_i g_0^2 \qquad \left(S = \frac{1}{2}\right) \tag{16.176}$$

$$\chi(T) = \frac{n_i}{T}[1 - 2J\rho] = \frac{n_i}{T}\left[1 - 2g_0\right], \tag{16.177}$$

where n_i is the density of impurities.

Now scaling, if it's correct, implies that at lower temperatures $J\rho \rightarrow J\rho + 2(J\rho)^2 \ln\frac{D}{T}$, so that to next leading order we expect

$$\frac{1}{\tau} = n_i\frac{2\pi}{\rho}S(S+1)\left[J\rho + 2(J\rho)^2\ln\frac{D}{T}\right]^2 \tag{16.178}$$

$$\chi(T) = \frac{n_i}{T}\left[1 - 2J\rho - 4(J\rho)^2\ln\frac{D}{T} + O((J\rho)^3)\right]. \tag{16.179}$$

These results are confirmed in second-order perturbation theory as the result of adding in the one-loop corrections to the scattering vertices. The first result was obtained by Jun Kondo in his pioneering study [9]. Kondo was looking for a consequence of the antiferromagnetic superexchange interaction predicted by Anderson [7], so he computed the electron scattering rate to third order in the magnetic coupling. The logarithm which appears in the electron scattering rate means that, as the temperature is lowered, the rate at which electrons scatter off magnetic impurities rises. It is this phenomenon that gives rise to the famous Kondo resistance minimum.

But we can use universality to go much further, and actually deduce the form of the universal functions $F[x]$ and $\mathcal{G}[x]$ in (16.171) and (16.172), at least in weak coupling when the temperature is large compared with the Kondo temperature, $T/T_K >> 1$. Let us rearrange (16.175) into

$$g(T) = \frac{1}{2\ln\left(\frac{T}{T_K}\right) + \ln 2g(T)}, \tag{16.180}$$

which we may iterate to obtain

$$2g(T) = \frac{1}{\ln\left(\frac{T}{T_K}\right) + \frac{1}{2}\ln\left(\frac{1}{\ln\frac{T}{T_K} + \ln 2g}\right)} = \frac{1}{\ln\left(\frac{T}{T_K}\right)} + \frac{\ln(\ln(T/T_K))}{2\ln^2\left(\frac{T}{T_K}\right)} + \cdots, \tag{16.181}$$

where the expansion has been made assuming $\ln T/T_K >> \ln g$. At high temperature, by substituting $T_K = De^{-1/2J\rho}$ we can check that the leading-order term is simply

$$\begin{aligned} 2g(T) &= \frac{1}{\ln\left(\frac{T}{T_K}\right)} = \frac{1}{\frac{1}{2J\rho} + \ln T/D} = \frac{2J\rho}{1 + 2J\rho\ln T/D} \\ &= 2\left[J\rho + 2(J\rho)^2\ln\left(\frac{D}{T}\right)\right] + O[(J\rho)^3]\,, \end{aligned} \tag{16.182}$$

the leading logarithmic correction to $g(T)$. By using scaling we are thus able to re-sum diagrams far beyond leading-order perturbation theory. Using this expression to make the replacement $J\rho \to g(T)$ in the leading-order perturbation theory (16.176), we obtain

$$\chi(T) = \frac{n_i}{T}\left[1 - \frac{1}{\ln(T/T_K)} - \frac{1}{2}\frac{\ln(\ln(T/T_K))}{\ln^2(T/T_K)} + \cdots\right] \tag{16.183}$$

$$\frac{1}{\tau(T)} = n_i\frac{\pi S(S+1)}{2\rho}\left[\frac{1}{\ln^2(T/T_K)} + \frac{\ln(\ln(T/T_K))}{\ln^3(T/T_K)} + \cdots\right]. \tag{16.184}$$

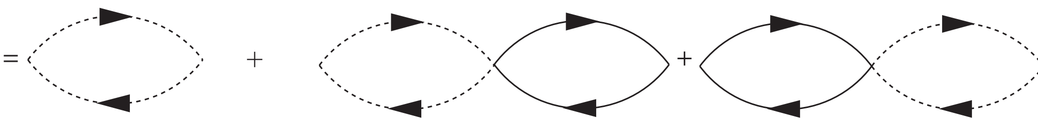
From the second result, we see that the electron scattering rate has the scale-invariant form in (16.172)

$$\frac{1}{\tau(T)} = \frac{1}{\tau_0}\mathcal{G}(T/T_K), \tag{16.185}$$

where $\frac{1}{\tau_0} \propto \frac{n_i}{\rho}$ represents the intrinsic scattering rate off the Kondo impurity. The quantity $1/\rho$ is essentially the Fermi energy of the electron gas, and $1/\tau_0 \sim \frac{n_i}{\rho}$ is the unitary scattering rate, the maximum possible scattering rate that is obtained when an electron experiences a resonant $\pi/2$ scattering phase shift. From this result, we see that, at absolute zero, the electron scattering rate will rise to the value $\frac{1}{\tau(T)}|_{T=0} = \frac{n_i}{\rho}\mathcal{G}(0)$, indicating that at strong coupling the scattering rate is of the same order as the unitary scattering limit. We shall now see how this same result comes naturally out of a strong-coupling analysis.

Example 16.9

(a) Use the Popov–Fedotov scheme to compute the leading correction to the impurity magnetic susceptibility, given by the diagrams

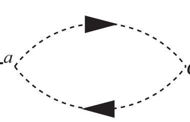
$\chi =$ 

$$= \frac{\mu_B^2}{T}\left[1 - 2J\rho + O(J^2)\right]. \tag{16.186}$$

(b) Based on scaling arguments, what is the form of the J^2 correction to the susceptibility?
(c) What diagrams are responsible for the logarithmic correction to the susceptibility?

Solution

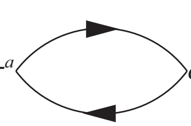
(a) For these calculations, let us temporarily set $\mu_B = 1$. We need to calculate the f-electron susceptibility, given by

$\chi_f \delta^{ab} = \sigma^a$  $\sigma^b = -T \sum_{i\omega_n} \mathrm{Tr}[\sigma^a G_f(i\omega_n)\sigma^b G_f(i\omega_n)] = \chi_f \delta^{ab}.$ (16.187)

So

$$\begin{aligned}\chi_f &= -2T\sum_{i\omega_n} \frac{1}{(i\omega_n - \lambda_f)^2} = \frac{\partial}{\partial \lambda_f} \overbrace{2T\sum_{i\omega_n} \frac{1}{i\omega_n - \lambda_f}}^{-f(\lambda_f)} \\ &= 2\left(-\frac{\partial f(\lambda_f)}{\partial \lambda_f}\right) = \frac{2f_\lambda(1-f_\lambda)}{T} = \frac{1}{T},\end{aligned} \tag{16.188}$$

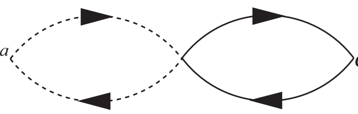
where the factor of 2 derives from the trace over the spin degrees of freedom and we have used $f_\lambda(1 - f_\lambda) = 1/[(i + 1)(-i + 1)] = \frac{1}{2}$. Similarly, the conduction electron susceptibility given by

$\chi_c \delta^{ab} = \sigma^a$  $\sigma^b = -T \sum_{\mathbf{k}, i\omega_n} \mathrm{Tr}\left[\sigma^a G_{\mathbf{k}}(i\omega_n)\sigma^b G_{\mathbf{k}}(i\omega_n)\right]$

$$\begin{aligned}&= -2\delta^{ab} T \sum_{\mathbf{k}, i\omega_n} \frac{1}{(i\omega_n - \epsilon_{\mathbf{k}})^2} = 2\delta^{ab} \sum_{\mathbf{k}} \frac{\partial}{\partial \epsilon_{\mathbf{k}}} \overbrace{T\sum_{i\omega_n} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}}^{-f(\epsilon_{\mathbf{k}})} \\ &= 2\delta^{ab} \sum_{\mathbf{k}} \left(-\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\right) = 2\rho\delta^{ab}.\end{aligned} \tag{16.189}$$

Now the first-order diagrams are given by

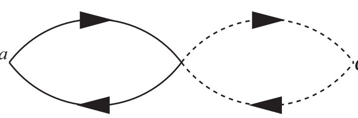
$$\chi_A \delta^{ab} = \sigma^a$$



$$\sigma^b = (\chi_f \delta^{ac})\left(-\frac{J}{2}\right)(\chi_c \delta^{cb}) = -\frac{J\rho}{T} \tag{16.190}$$

and

$$\chi_B \delta^{ab} = \sigma^a$$



$$\sigma^b = (\chi_c \delta^{ac})\left(-\frac{J}{2}\right)(\chi_f \delta^{cb}) = -\frac{J\rho}{T}. \tag{16.191}$$

Adding the results together, the first-order correction to the impurity susceptibility is given by

$$\chi = \frac{\mu_B^2}{T}(1 - 2J\rho) + O((J\rho)^2), \tag{16.192}$$

where we have reinstated μ_B.

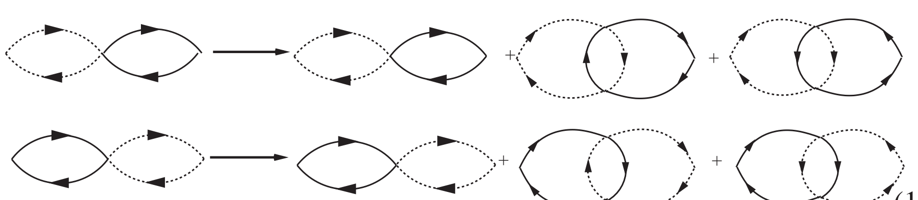
(b) We expect the second-order corrections to the susceptibility to be obtained by renormalizing the coupling constant. Following the results of Example 16.7, the renormalization is given by

$$J\rho \to J\rho + 2(J\rho)^2 \ln\left[\frac{D}{T}\right]. \tag{16.193}$$

Since the renormalization group only provides leading logarithmic accuracy, we have dropped the dimensionless constants inside the logarithm. We therefore expect that the second-order corrections to the susceptibility will take the form

$$\begin{aligned}\chi(T) &= \frac{\mu_B^2}{T}\left[1 - 2\left(J\rho + 2(J\rho)^2 \ln\left[\frac{D}{T}\right]\right)\right] \\ &= \frac{\mu_B^2}{T}\left[1 - 2J\rho + 4(J\rho)^2 \ln\left[\frac{D}{T}\right]\right] + O[(J\rho)^3].\end{aligned} \tag{16.194}$$

(c) The logarithmic corrections to the susceptibility derive from the vertex insertions into the first-order diagrams, given by



(16.195)

There are other contributions to the susceptibility, such as self-energy corrections and corrections to the external magnetic vertex, but none will be logarithmically divergent corrections. Moreover, the conservation of spin will mean that many self-energy and vertex corrections will cancel one another.

Using (16.224), it follows that

$$M = \tilde{\chi}_s = \frac{\delta_\uparrow}{\pi} - \frac{\delta_\downarrow}{\pi} = 2\frac{\alpha - \Phi\rho}{\pi} = \tilde{\gamma} - (\chi_c - \tilde{\gamma}) = 2\tilde{\gamma} - \chi_c, \tag{16.227}$$

from which the Yamada–Yoshida identity

$$2\tilde{\gamma} = \chi_c + \chi_s \tag{16.228}$$

follows. Notice that, if we restore μ_B, then $\chi_s \to \chi_s/\mu_B^2 = \tilde{\chi}_s$.

(c) Notice that, in the non-interacting impurity ($U = 0$), $\chi_c = \tilde{\chi}_s = \gamma$. In the limit that $U < 0$ is large and negative, the spin susceptibilty is suppressed to zero, so that the charge Wilson ratio is

$$\frac{\chi_c}{\tilde{\gamma}} = 2. \tag{16.229}$$

This is a result of the charge Kondo effect.

16.10.3 Experimental observation of the Kondo effect

Experimentally, there is now a wealth of observations that confirm our understanding of the single-impurity Kondo effect. Here is a brief itemization of some of the most important observations (Figure 16.19).

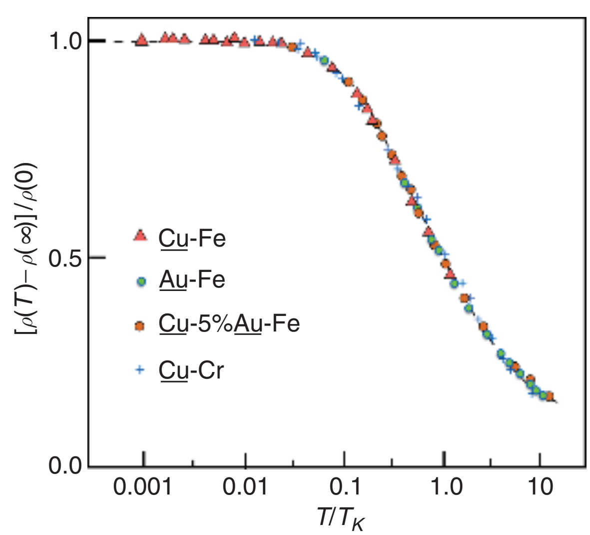


Fig. 16.19 Temperature dependence of excess resistivity associated with scattering from an impurity spin [54]. The resistivity saturates at the unitarity limit at low temperatures, due to the formation of the Kondo resonance. The notation A-M denotes dilute magnetic impurities M dissolved in host metal A. Reprinted and adapted Figure VII. 14 from R. M. White and T. Geballe, Long-range order in solids, in *Solid State Physics*, ed. H. Ehrenreich, F. Seitz, and D. Turnbull, vol. 15, p. 283, 1979. Copyright 1979 Elsevier.

- A resistance minimum appears when local moments develop in a material. For example, in $Nb_{1-x}Mo_x$ alloys, a local moment develops for $x > 0.4$, and the resistance is seen to develop a minimum beyond this point [2, 5].
- Universality is seen in the specific heat $C_V = \frac{n_i}{T} F(T/T_K)$ of metals doped with dilute concentrations of impurities. Thus the specific heat of Cu-Fe (iron impurities in copper) can be superimposed on the specific heat of Cu-Cr, with a suitable rescaling of the temperature scale [54].
- Universality is observed in the differential conductance of quantum dots [55, 56] and spin-fluctuation resistivity of metals with a dilute concentration of impurities [57]. Actually, both properties are dependent on the same thermal average of the imaginary part of the scattering t-matrix:

$$\begin{aligned} \rho_i &= n_i \frac{ne^2}{m} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) 2\,\mathrm{Im}\,[T(\omega)] \\ G &= \frac{2e^2}{\hbar} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \pi\rho\,\mathrm{Im}\,[T(\omega)]. \end{aligned} \tag{16.230}$$

Putting $\pi\rho \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \mathrm{Im}\,T(\omega) = t(\omega/T_K, T/T_K)$, we see that these properties have the form

$$\begin{aligned} \rho_i &= n_i \frac{2ne^2}{\pi m \rho} t(T/T_K) \\ G &= \frac{2e^2}{\hbar} t(T/T_K), \end{aligned} \tag{16.231}$$

where $t(T/T_K)$ is a universal function. This result is born out by experiment (Figure 16.19).

16.11 Multi-channel Kondo physics

In practice, magnetic moments in real materials exhibit many different variants on the original $S = \frac{1}{2}$ Kondo model, a point first emphasized by Philippe Nozières and André Blandin [18]. Here we end with a brief discussion of two important variants of the original $SU(2)$ Kondo spin model:

- The multi-channel Kondo model, in which the spin interacts with k different screening channels.
- The spin-S Kondo model, in which the impurity has spin $S > \frac{1}{2}$. This is important in multi-electron orbitals, in which the localized electrons are coupled together to form a large spin S by the Hund's interaction.

The k-channel spin-S Kondo model (Figure 16.20) which incorporates both of these features is written

$$H = J \sum_{\lambda=1}^{k} \vec{\sigma}_\lambda(0) \cdot \vec{S} + \sum_{\substack{k,\sigma=\pm \\ \lambda=1,k}} \epsilon_k c^\dagger_{k\lambda\sigma} c_{k\lambda\sigma}. \tag{16.232}$$