$$f_{j\sigma} \to e^{i\phi_j} f_{j\sigma}, \qquad V_j \to e^{i\phi_j} V_j, \qquad \lambda_j \to \lambda_j - i\dot{\phi}_j(\tau). \tag{17.57}$$

Read–Newns gauge transformation

It is often useful to use this invariance to choose a gauge in which V_j is real and gauge neutral. We do this by absorbing the phase of the hybridization $V_j = |V_j|e^{i\phi_j}$ into the f-electron. Let us examine how the action at site j transforms when we redefine the f-electrons to absorb this phase:

$$\begin{aligned} S_K(j) &= \int_0^\beta d\tau \left[f^\dagger_{j\sigma}(\partial_\tau + \lambda_j) f_{j\sigma} + \left(\overbrace{|V_j|e^{-i\phi_j}}^{\bar{V}_j} c^\dagger_{j\sigma} f_{j\sigma} + \overbrace{|V_j|e^{i\phi_j}}^{V_j} f^\dagger_{j\sigma} c_{j\sigma} \right) + N\frac{|V_j|^2}{J_K} - \lambda_j Q \right] \\ &\xrightarrow{f_j \to e^{i\phi_j} f_j} \int_0^\beta d\tau \left[f^\dagger_{j\sigma}(\partial_\tau + \lambda_j + i\dot{\phi}_j) f_{j\sigma} + |V_j| \left(c^\dagger_{j\sigma} f_{j\sigma} + f^\dagger_{j\sigma} c_{j\sigma} \right) \right. \\ &\qquad \left. + N\frac{|V_j|^2}{J_K} - \lambda_j Q \right]. \end{aligned} \tag{17.58}$$

In our starting model, the constraint field was constant, but in this *radial gauge* it has acquired a time dependence derived from the precession of phase ϕ. If we define the dynamical variable $\lambda_j(\tau) = \lambda_j + i\dot{\phi}_j$, this becomes

$$\begin{aligned} S_K(j) = \int_0^\beta d\tau & \left[f^\dagger_{j\sigma}[\partial_\tau + \lambda_j(\tau)] f_{j\sigma} + |V_j| \left(c^\dagger_{j\sigma} f_{j\sigma} + f^\dagger_{j\sigma} c_{j\sigma} \right) \right. \\ & \left. + N\frac{|V_j|^2}{J_K} - \lambda_j(\tau) Q \right] + \overbrace{iQ \int_0^\beta d\tau \dot{\phi}_j}^{iQ\Delta\phi_j = i2\pi Qn}. \end{aligned} \tag{17.59}$$

The remainder term comes from making the change of variables in the constraint term $\lambda_j = \lambda_j(\tau) - i\dot{\phi}_j$. Fortunately, this term is an exact integral, and since the change in the phase of the hybridization is an integral multiple of 2π it adds an overall phase $e^{i2\pi nQ} = 1$ to the path integral, and hence can be dropped. In this radial gauge, the Read–Newns path integral becomes

$$\begin{aligned} Z &= \int \mathcal{D}[|V|, \lambda] \int \mathcal{D}[\psi^\dagger, \psi] \exp\Big[- \overbrace{\int_0^\beta (\psi^\dagger \partial_\tau \psi + H[|V|, \lambda])}^{S[|V|\lambda,\, \psi^\dagger, \psi]} \Big] \\ H[|V|, \lambda] &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_j \left[|V_j| \left(c^\dagger_{j\sigma} f_{j\sigma} + f^\dagger_{j\sigma} c_{j\sigma} \right) \right. \\ &\qquad \left. + \lambda_j (n_{fj} - Q) + N\frac{|V_j|^2}{J} \right]. \end{aligned} \tag{17.60}$$

Read–Newns path integral: radial gauge

By absorbing the phase, the constraint field becomes a dynamical potential field, integrated along the entire imaginary axis (see Example 17.2 for details). Subsequently, when we use the radial gauge we will drop the modulus sign. The interesting feature about this Hamiltonian is that, with the real hybridization, the conduction and f-electrons now transform under a single global $U(1)$ gauge transformation, i.e. the f-electrons have become *charged*. We will return to this issue in Sections 17.8 and18.6.

17.4.1 The effective action

We now develop the large-N expansion by calculating the effective action. We'll begin without fixing the gauge. The interior fermion integral in the path integral (17.60) defines an effective action $S_E[\bar{V}, V, \lambda]$ by the relation

$$\exp\left[-NS_E[\bar{V}, V, \lambda]\right] \equiv Z_E[\bar{V}, V, \lambda] = \int \mathcal{D}[\psi^\dagger, \psi] \exp\left[-S[\bar{V}, V, \lambda, \ \psi^\dagger, \psi]\right], \quad (17.61)$$

where we have defined $Z_E = e^{-NS_E}$. Using (17.56),

$$S = \int_0^\beta d\tau \left[\sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} (\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} + \sum_j \left(f^\dagger_{j\sigma} (\partial_\tau + \lambda_j) f_{j\sigma} + (\bar{V}_j c^\dagger_{j\sigma} f_{j\sigma} + V_j f^\dagger_{j\sigma} c_{j\sigma}) \right.\right.$$
$$\left.\left. + N \frac{\bar{V}_j V_j}{J} - \lambda_j Q \right) \right]. \quad (17.62)$$

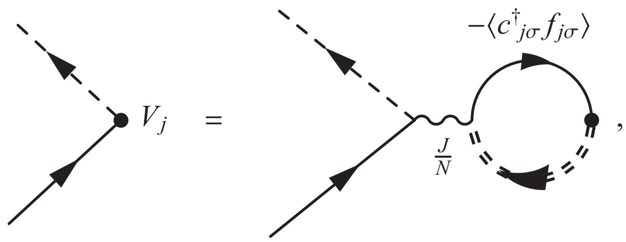
The extensive growth of the effective action with N means that at large N the integration in (17.56) is dominated by its stationary points:

$$Z = \int \mathcal{D}[\lambda, \bar{V}, V] \exp\left[-NS_E[\bar{V}, V\lambda]\right] \approx \left. \exp\left[-NS_E[\bar{V}, V, \lambda]\right]\right|_{\text{saddle point}}. \quad (17.63)$$

If we identify $NS_E = -\ln Z_E$, so that $N\delta S_E = -\delta Z_E/Z_E$, then, differentiating (17.61) with respect to $\bar{V}_j$ and λ_j, we see that the saddle-point conditions impose the self-consistent relations

$$\frac{\delta NS_E}{\delta \bar{V}_j(\tau)} = \frac{1}{Z_E} \int \mathcal{D}[\psi^\dagger, \psi] \overbrace{\left(c^\dagger_{j\sigma}(\tau) f_{j\sigma}(\tau) + \frac{NV_j(\tau)}{J} \right)}^{\delta S/\delta \bar{V}_j(\tau)} e^{-S} = \langle c^\dagger_{j\sigma} f_{j\sigma} \rangle(\tau) + \frac{N}{J} V_j(\tau) = 0$$
$$\frac{\delta NS_E}{\delta \lambda_j(\tau)} = \frac{1}{Z_E} \int \mathcal{D}[\psi^\dagger, \psi] \left(n_f(j, \tau) - Q \right) e^{-S} = \langle n_f(j, \tau) \rangle - Q = 0, \quad (17.64)$$

where repeated spin indices imply summation. The second equation in (17.64) is the satisfaction of the constraint, on the average. The first relation, which can be written $V_j = -\frac{J}{N} \langle c^\dagger_{j\sigma} f_{j\sigma} \rangle$, is recognized as the mean-field self-consistency associated with the Hubbard–Stratonovich factorization. We can denote this self-consistency by the Feynman diagram



indicating that the condensation of the boson V is self-consistently induced by an anomalous hybridization. Fortunately, we will not have to solve these equations by explicitly calculating the expectation values; instead, as we found in previous chapters (see Section 13.3), they are implicity imposed by finding the stationary point of the action.

In practice, we shall seek static solutions, using the radial gauge to absorb the phase of the hybridization, so that $\bar{V}_j(\tau) = V_j(\tau) = |V_j|$, $\lambda_j(\tau) = \lambda_j$. In this case the saddle-point partition function $Z_E[V,\lambda]$ is simply the partition function of the static mean-field Hamiltonian $H_{MF} = H[V,\lambda]$, $Z_E = \mathrm{Tr}e^{-\beta H_{MF}}$. Now we may write the action in the form

$$S = \int_0^\beta d\tau \left[\sum_\sigma \psi^\dagger_\sigma (\partial_\tau + \underline{h})\, \psi_\sigma + \sum_j \left(N\frac{V_j^2}{J} - \lambda_j Q \right) \right], \tag{17.65}$$

where the matrix $\underline{h}[V,\lambda]$ is a mean-field Hamiltonian, read off from (17.56). For instance, in a tight-binding representation,

$$H[V,\lambda] = \sum_{i,j,\sigma} \left(c^\dagger_{i\sigma},\quad f^\dagger_{i\sigma} \right) \overbrace{\begin{bmatrix} (t_{ij} - \mu\delta_{ij}) & \bar{V}_j\delta_{ij} \\ V_j\delta_{ij} & \lambda_j\delta_{ij} \end{bmatrix}}^{\underline{h}[V,\lambda]} \begin{pmatrix} c_{j\sigma} \\ f_{j\sigma} \end{pmatrix} + \sum_j \left(N\frac{|V_j|^2}{J} - \lambda_j Q \right), \tag{17.66}$$

where the t_{ij} are the hopping matrix elements obtained by Fourier transforming $\epsilon_{\mathbf{k}} = \sum_{\mathbf{R}_{ij}} (t(\mathbf{R}_{ij}) - \mu\delta_{ij}) e^{-i\mathbf{k}\cdot\mathbf{R}_{ij}}$.

Since the action is Gaussian in the Fermi fields, the Fermi integral can be carried out using (12.142) in terms of the determinant of the action:

$$\begin{aligned} \int \mathcal{D}[\psi^\dagger, \psi] \exp\left[-\int_0^\beta d\tau \sum_\sigma \psi^\dagger_\sigma \left(\partial_\tau + \underline{h}\right) \psi_\sigma \right] &= \left(\det\left[\partial_\tau + \underline{h}\right]\right)^N \\ &= \exp\left[N \ln\det\left[\partial_\tau + \underline{h}\right]\right] \\ &= \exp\left[N \mathrm{Tr}\ln\left[\partial_\tau + \underline{h}\right]\right], \end{aligned} \tag{17.67}$$

where the power N derives from the N identical integrals over each spin component of ψ_σ. In the last line, we have replaced $\ln\det \to \mathrm{Tr}\ln$. Thus

$$NS_E[V,\lambda] = N\left[-\mathrm{Tr}\ln\left(\partial_\tau + \underline{h}\right) + \sum_j \int_0^\beta d\tau \left(\frac{|V_j|^2}{J} - \lambda_j q \right) \right]. \tag{17.68}$$

Since $Z_E = e^{-\beta F_{MF}} = e^{-NS_E}$, where F_{MF} is the mean-field free energy, it follows that

$$F_{MF}[V,\lambda] = \frac{1}{\beta} S_E[V,\lambda] = -\frac{N}{\beta} \mathrm{Tr}\ln\left(\partial_\tau + \underline{h}[V,\lambda]\right) + \sum_j \left(\frac{N|V_j|^2}{J} - \lambda_j Q \right). \tag{17.69}$$

If we switch to the frequency domain, replacing $\partial_\tau \to -i\omega_n$ by a Matsubara frequency, we may also write

$$F_{MF} = -NT \sum_{i\omega_n} \mathrm{Tr}\ln\Big[-\mathcal{G}^{-1}(i\omega_n)\Big] + \sum_j \left(\frac{N|V_j|^2}{J} - \lambda_j Q\right)$$
$$\mathcal{G}^{-1} = (i\omega_n - \underline{h}[V,\lambda]), \tag{17.70}$$

where we have identified $\mathcal{G}^{-1} = (i\omega_n - \underline{h}[V,\lambda])$ with the inverse Green's function. Sometimes, it's convenient to re-express S_E in terms of the eigenvalues E_ζ of the Hamiltonian. If we diagonalize the Hamiltonian, so that $\underline{h} \to E_\zeta \delta_{\zeta\zeta'}$, then $\mathrm{Tr}\ln(-i\omega_n + \underline{h}) = \sum_\zeta \ln(E_\zeta - i\omega_n)$. We can also do the Matsubara sum, under which $-T\sum_{i\omega_n}\ln(E_\zeta - i\omega_n) \to -T\ln(1+e^{-\beta E_\zeta})$, so that the free energy can also be written

$$F_E[V,\lambda] = -NT\sum_\zeta \ln\left(1+e^{-\beta E_\zeta}\right) + \sum_j \left(\frac{N|V_j|^2}{J} - \lambda_j Q\right). \tag{17.71}$$

Equations (17.70) and (17.71) are complementary: the former reflects the path-integral approach, the latter a more conventional mean-field approach. Let us now apply them to the Kondo impurity and lattice models.

Example 17.3 This example shows in detail how to derive the measure of the Read–Newns path integral. The initial Kondo lattice path integral involves static constraint fields λ_j, integrated over a finite range of the imaginary axis: $\lambda_j \in [0, i2\pi T]$, as follows:

$$Z = \prod_j \int_0^{2\pi iT} \frac{d\lambda_j}{2\pi iT} \int \mathcal{D}[V,\psi] \exp\left[-\int_0^\beta (\bar\psi\partial_\tau\psi + H[V,\lambda])\right]. \tag{17.72}$$

By inserting the identity $\int \mathcal{D}[g_j] = 1$ into the Kondo path integral, where $\mathcal{D}[g_j]$ denotes the integration over the entire orbit of gauge transformations $g_j(\tau) = e^{i\phi_j(\tau)}$, show that λ_j is promoted to a dynamical variable $\lambda_j'(\tau) = \lambda_j + i\dot\phi_j(\tau)$, integrated over the entire imaginary axis.

Solution

If we insert the identity $\prod_j \int \mathcal{D}[g_j] = 1$ into the path integral, it becomes

$$Z = \int \mathcal{D}[\lambda, g, V, \psi] e^{-S[\lambda,V,\psi]}. \tag{17.73}$$

At this point, g is just a dummy variable. We need to (a) carry out a gauge transformation to absorb g into the fields, and (b) rewrite the measure of integration in terms of the transformed fields.

(a) Change of variables.
The first step is to show that the action is unchanged by the gauge transformation

$$f_j(\tau) = e^{i\phi_j(\tau)} f'_j(\tau), \qquad V_j(\tau) = e^{i\phi_j(\tau)} V'_j(\tau). \tag{17.74}$$

Under this transformation, the Hamiltonian is unchanged but the f-Berry phase term (see (12.132)) acquires an additional $i\dot{\phi}_j$ term from the time dependence of $g_j(\tau) = e^{i\phi_j(\tau)}$, as follows:

$$f^\dagger(\partial_\tau + \lambda_j)f \longrightarrow f'^\dagger e^{-i\phi_j}(\partial_\tau + \lambda_j)e^{i\phi_j}f' = f'^\dagger(\partial_j + \lambda_j + i\dot{\phi}_j)f'_j. \tag{17.75}$$

To absorb this term we must also transform the λ_j field, introducing the dynamical variable $\lambda'_j(\tau) = \lambda_j + i\dot{\phi}_j(\tau)$. Subtly, under the transformation the constraint term adds a phase shift to the action:

$$\begin{aligned} S[V, \lambda, \psi] &= \int_0^\beta d\tau \sum_j \left[f'^\dagger_j(\partial_\tau + \lambda'_j)f'_j - (\lambda'_j - i\dot{\phi}_j)Q \right] + \cdots \\ &= S[V', \lambda', \psi'] + iQ \sum_j \int_0^\beta d\tau \dot{\phi}_j. \end{aligned} \tag{17.76}$$

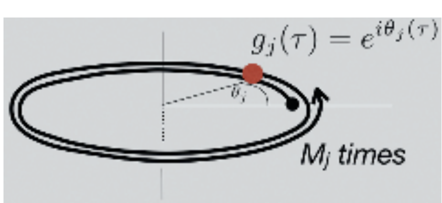
Now $Q \int_0^\beta d\tau \dot{\phi}_j = Q\Delta\phi_j$ is determined by the change in ϕ_j between $\tau = 0$ and $\tau = \beta$. Since $g_j = e^{i\phi_j}$ is periodic in time, $\Delta\phi_j$ is an integer multiple M_j of 2π, and since Q is an integer, the phase shift is a multiple of 2π, leaving e^{-S} invariant:

$$\exp\left(-S[V, \lambda, \psi]\right) = \exp\left(-S[V', \lambda', \psi'] - 2\pi i \sum_j (QM_j) \right) = \exp\left(-S[V', \lambda', \psi']\right). \tag{17.77}$$

(b) Change of measure.
Since the gauge transformation is unitary, the measure for the hybridization and f-electron fields is unchanged (phase factors cancel):

$$\prod_\tau d\bar{V}_j(\tau)dV_j(\tau) = \prod_\tau d\bar{V}'_j(\tau)dV'_j(\tau), \qquad \prod_\tau df^\dagger_j(\tau)df_j(\tau) = \prod_\tau df'^\dagger_j(\tau)df'_j(\tau). \tag{17.78}$$

Next, we show that the remaining measure $\mathcal{D}[\lambda, g] = \mathcal{D}[\lambda']$, with a flat measure of integration over the dynamical variable $\lambda'_j(\tau) = \lambda_j + i\dot{\phi}_j$. Since $\phi_j(\beta) = \phi_j(0) + 2\pi M_j$ is periodic up to a multiple of 2π, we may write



$$\phi_j(\tau) = 2\pi TM_j\tau + \tilde{\phi}_j(\tau), \tag{17.79}$$

which describes a path for $g_j(\tau) = e^{i\phi_j(\tau)}$ that wraps M_j times around the origin. The second term is a periodic function of τ that can be decomposed into its Matsubara

Fourier components, $\tilde{\phi}_j(\tau) = \sum_n \tilde{\phi}_n(j)e^{-i\nu_n\tau}$. The original measure for integrating over the static λ_j and g_j is

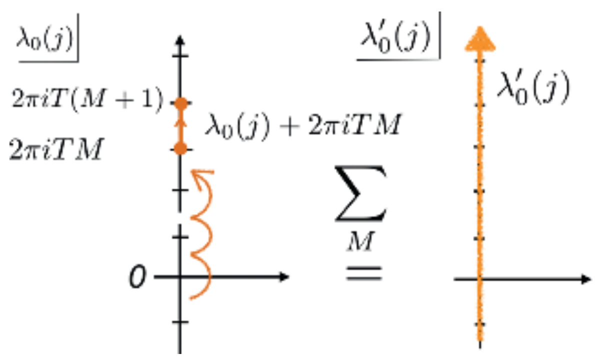
$$\mathcal{D}[\lambda_j, g_j] = \sum_{M_j} \int_0^{2\pi iT} d\lambda_j \prod_\tau d\tilde{\phi}_j(\tau)$$
$$= \sum_{M_j} \int_0^{2\pi iT} d\lambda_j \prod_n d\tilde{\phi}_n(j), \qquad (17.80)$$

where, in the last line, the measure for the integration over $\tilde{\phi}_j$ has been replaced by the integration over its Matsubara Fourier components.

Now the dynamical variable $\lambda'_j(\tau) = \lambda_j + i\dot{\tilde{\theta}}_j = \lambda_j + 2\pi iTM_j + i\dot{\tilde{\phi}}_j(\tau)$ has a Fourier series

$$\lambda'_j(\tau) = \sum_n \lambda'_n(j)e^{-i\nu_n\tau}, \qquad (17.81)$$

where $\lambda'_0(j) = \lambda_j + 2\pi iTM_j$ and $\lambda'_n(j) = i(-i\nu_n)\tilde{\theta}_n(j) = \nu_n\tilde{\phi}_n(j)$. When we integrate over λ_j, the range of the $\lambda'_0(j) = \lambda_j + 2\pi iTM_j$ runs from $2\pi iTM_j$ to $2\pi iT(M_j + 1)$ along the imaginary axis, so that when we sum over all M_j, $\lambda'_0(j)$ runs over the entire imaginary axis (see figure below).



It follows that the combination

$$\sum_{M_j} \int_{2\pi iTM_j}^{2\pi iT(M_j+1)} d\lambda'_0(j) \equiv \int_{-i\infty}^{i\infty} d\lambda'_0(j) \qquad (17.82)$$

gives an unconstrained integral over the static part $\lambda'_0(j)$ of $\lambda'{}_j(\tau)$.

For $n \neq 0$, the Fourier coefficients $\lambda'_n(j) = \nu_n\tilde{\phi}_n(j)$ are directly proportional, so, up to a normalization, their measures are equal, so that

$$\prod_n d\tilde{\phi}_n(j) = \mathcal{N}^{-1} d\phi_0(j) \prod_{n\neq 0} d\lambda'_n(j),$$

where $\mathcal{N}$ is a normalizing factor $\prod_n = \prod_{n\neq 0} \nu_n$ that we shall drop. Thus, by integrating over all possible $\tilde{\phi}_j$, we integrate over all finite frequency Fourier components of $\lambda'_j(\tau)$.

Combining the static and dynamical parts of the measure, it follows that

$$\mathcal{D}[\lambda_j, g_j] \equiv \mathcal{D}[\lambda'{}_j] = \prod_j d\phi_0(j) \prod_n d\lambda'_n(j),$$

and since $\mathcal{D}[V,\psi] = \mathcal{D}[V',\psi']$,

$$\mathcal{D}[g,\lambda,V,\psi] = \mathcal{D}[\phi_0]\mathcal{D}[\lambda',V',\psi'], \tag{17.83}$$

where the measure for the dynamical field λ' is flat and $\mathcal{D}[\phi_0] = \prod_j d\phi_0(j)$ is the integral over the static phases $\phi_0(j)$. Since the action is independent of ϕ_0, we can drop the overall integral over the static phases, enabling us to replace $\mathcal{D}[\phi_0] \to 1$ and write

$$\mathcal{D}[g,\lambda,V,\psi] \equiv \mathcal{D}[\lambda',V',\psi']. \tag{17.84}$$

17.5 Mean-field theory of the Kondo impurity

17.5.1 The impurity effective action

The large-N mean-field theory of the Kondo effect maps the original Hamiltonian onto a self-consistently determined resonant level model, which we will write in the form

$$H_{MF} = \sum_\sigma \left(\cdots c^\dagger_{\mathbf{k}\sigma} \cdots,\ f^\dagger_\sigma\right) \left(\begin{array}{c|c} \epsilon_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'} & \bar{V} \\ \hline V & \lambda \end{array}\right) \begin{pmatrix} \vdots \\ c_{\mathbf{k}'\sigma} \\ \vdots \\ f_\sigma \end{pmatrix} + \frac{NV^2}{J} - \lambda Q. \tag{17.85}$$

In Section 16.4.2 we learned that the single resonance described by this model is located at an energy λ, with a hybridization width $\Delta = \pi\rho V^2$ (see (16.19)). By minimizing the free energy of this system, we need to figure out how λ and Δ are related to the Kondo coupling constant. Let us first evaluate the free energy of the resonance. We can read off $\underline{h}$ from (17.85), so from (17.70), the mean-field free energy is given by

$$F_{MF} = -TN\sum_n \ln\det \left(\begin{array}{c|c} (\epsilon_{\mathbf{k}} - i\omega_n)\delta_{\mathbf{k},\mathbf{k}'} & \bar{V} \\ \hline V & \lambda - i\omega_n \end{array}\right) + \left(\frac{NV^2}{J} - \lambda Q\right). \tag{17.86}$$

Using the result $\det\begin{pmatrix} D & C \\ B & A\end{pmatrix} = \det D \det\left[A - BD^{-1}C\right]$, we can integrate out the conduction electrons to write

$$F_{MF} = -TN\sum_n \ln\left[-i\omega_n + \lambda + \sum_{\mathbf{k}} \frac{|V|^2}{i\omega_n - \epsilon_{\mathbf{k}}}\right] + \left(\frac{NV^2}{J} - \lambda Q\right) + F_C, \tag{17.87}$$

where $F_C = -TN\sum_{\mathbf{k},n}\ln(\epsilon_{\mathbf{k}} - i\omega_n)$ is the conduction electron free energy. Using the large-bandwidth approximation, $\sum_{\mathbf{k}} \frac{|V|^2}{i\omega_n - \epsilon_{\mathbf{k}}} = -i\Delta\,\mathrm{sgn}(\omega_n) \equiv \Delta_n$ (see (16.29)), this becomes

$$F_{MF}[V,\lambda] = -\frac{N}{\beta}\sum_n \ln\left[-i\omega_n + \lambda + i\Delta_n\right] e^{i\omega_n 0^+} + N\left(\frac{|V|^2}{J_K} - \lambda Q\right) + F_C. \tag{17.88}$$

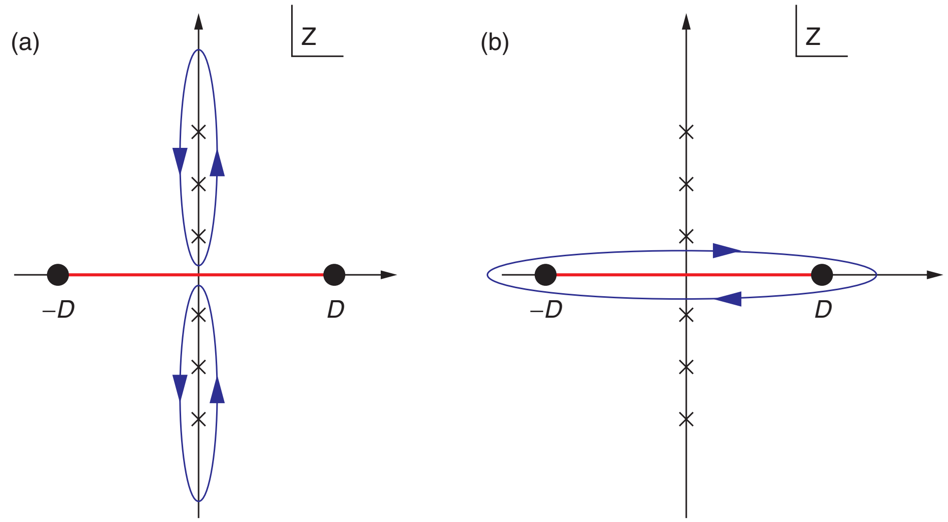


Fig. 17.7 Contour used in evaluating free energy: (a) undistorted contour; (b) contour distorted to run around branch cut in the f-electron Green's function.

We now carry out the Matsubara summation by the standard method, replacing $-T\sum_n F(i\omega_n) \rightarrow \oint \frac{dz}{2\pi i} f(z)F[z]$, where the contour runs counterclockwise around the poles in the Fermi function (Figure 17.7(a)). Now the logarithm contains a branch cut along the real axis, where $\Delta_n = \Delta \mathrm{sgn}(\mathrm{Im}\, z)$ jumps from $i\Delta$ below the real axis to $-i\Delta$ above it. If we introduce a finite bandwidth D, this branch cut runs from $z = -D$ to $z = +D$.

Distorting the contour to run clockwise around this branch cut (Figure 17.7(b)) we obtain

$$
\begin{aligned}
F_{MF}[V,\lambda] &= N\int_{-D}^{D} \frac{d\omega}{2\pi i} f(\omega)\left(\ln[-\omega+\lambda-i\Delta] - \ln[-\omega+\lambda+i\Delta]\right) \\
&\quad + N\left(\frac{|V|^2}{J_K} - \lambda Q\right) + F_C \\
&= -N\int_{-D}^{D} d\omega f(\omega) \overbrace{\left(\frac{1}{\pi}\mathrm{Im}\ \ln[\lambda + i\Delta - \omega]\right)}^{\delta_f(\omega)/\pi} + N\left(\frac{|V|^2}{J_K} - \lambda Q\right) + F_C,
\end{aligned}
\tag{17.89}
$$

where we have made the identification $\delta(\omega) = \mathrm{Im}\ \ln[\lambda + i\Delta - \omega] = \tan^{-1}\left(\frac{\Delta}{\lambda-\omega}\right)$ as the scattering phase shift of the impurity (see (16.33)). We then obtain

$$
F_{MF}[V,\lambda] = -N\int_{-D}^{D} d\omega \left(\frac{\delta_f(\omega)}{\pi}\right) f(\omega) + N\left(\frac{|V|^2}{J_K} - \lambda Q\right) + F_C. \tag{17.90}
$$

We can give this result a simple interpretation: the effect of the resonant phase shift changes the allowed momenta of the radial partial-wave states, which in turn causes the one-particle eigenstates of the continuum to move by a fraction δ_f/π of the energy-level spacing $\Delta\epsilon$ according to the relation (see (16.205)) $\tilde{\epsilon}_k = \epsilon_k - \frac{\delta(\epsilon_k)}{\pi}\Delta\epsilon$, where k labels the eigenstates. The corresponding change in the free energy of the continuum is then

$$\Delta F = \sum_k \frac{\partial}{\partial \epsilon_k}\left(-T \ln\left[1+e^{-\beta\epsilon_k}\right]\right)\left[-\frac{\delta_f(\epsilon_k)}{\pi}\Delta\epsilon\right] = -\sum_k f(\epsilon_k)\frac{\delta(\epsilon_k)}{\pi}\Delta\epsilon$$
$$\equiv -\int d\epsilon \frac{\delta_f(\epsilon)}{\pi} f(\epsilon), \tag{17.91}$$

where we have replaced the discrete summation by an integral. The first term in (17.90) is precisely this shift in the continuum free energy.

Example 17.4

(a) Diagonalize the impurity resonant level Hamiltonian

$$H_{MF} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} V[c^\dagger_{k\sigma} f_\sigma + f^\dagger_\sigma c_{k\sigma}] + \lambda \sum_\sigma n_{f\sigma} \tag{17.92}$$

and compute the scattering phase shift of the resonant level.

(b) Show that injection of an f-state into the continuum induces a resonant correction to the total the density of states:

$$\rho \to \rho^*(E) = \rho + \frac{1}{\pi}\frac{\Delta}{(E-\lambda)^2+\Delta^2}. \tag{17.93}$$

Solution

(a) To diagonalize the Hamiltonian, we write it in the form

$$H = \sum_{\gamma\sigma} E_\gamma a^\dagger_{\gamma\sigma} a_{\gamma\sigma}, \tag{17.94}$$

where the quasiparticle operators a_γ are related to the original operators via the one-particle eigenstates, $a^\dagger_{\gamma\sigma} = \sum_k c^\dagger_{k\sigma}\langle k|\gamma\rangle + f^\dagger_\sigma \langle f|\gamma\rangle \equiv \sum_k \alpha_k c^\dagger_{k\sigma} + \beta f^\dagger_\sigma$. Now if we denote the amplitudes of the one-particle eigenstates $|\gamma\rangle$ by $\langle\eta|\gamma\rangle \equiv (\cdots\langle k'|\gamma\rangle\cdots, \langle f|\gamma\rangle)$, then since $h_{\eta\eta'}\langle\eta'|\gamma\rangle = \langle\eta|H|\gamma\rangle = E_\gamma\langle\eta|\gamma\rangle$ it follows that the amplitudes $\langle\eta|\gamma\rangle$ must satisfy the eigenvalue equation

$$\underline{h}\cdot\begin{pmatrix}\vdots\\ \alpha_{\mathbf{k}}\\ \vdots\\ \beta\end{pmatrix} = \left(\begin{array}{c|c} \epsilon_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'} & \bar{V} \\ \hline V & \lambda \end{array}\right)\begin{pmatrix}\vdots\\ \alpha_{\mathbf{k}'}\\ \vdots\\ \beta\end{pmatrix} = E_\gamma \begin{pmatrix}\vdots\\ \alpha_{\mathbf{k}}\\ \vdots\\ \beta\end{pmatrix} \tag{17.95}$$

or

$$\epsilon_k\alpha_k + V\beta = E_\gamma\alpha_k$$
$$V\sum_{k'}\alpha_{k'} + \lambda\beta = E_\gamma\beta. \tag{17.96}$$

(If you like, you can rederive this by expanding the quasiparticle operators on both sides of (17.94) in terms of the conduction and f-electron fields, carrying out the commutator and then comparing coefficients of $c^\dagger_{k\sigma}$ and $f^\dagger_\sigma$ (see Example 14.3).) Solving for α_k using the first equation, and substituting into the second, we obtain

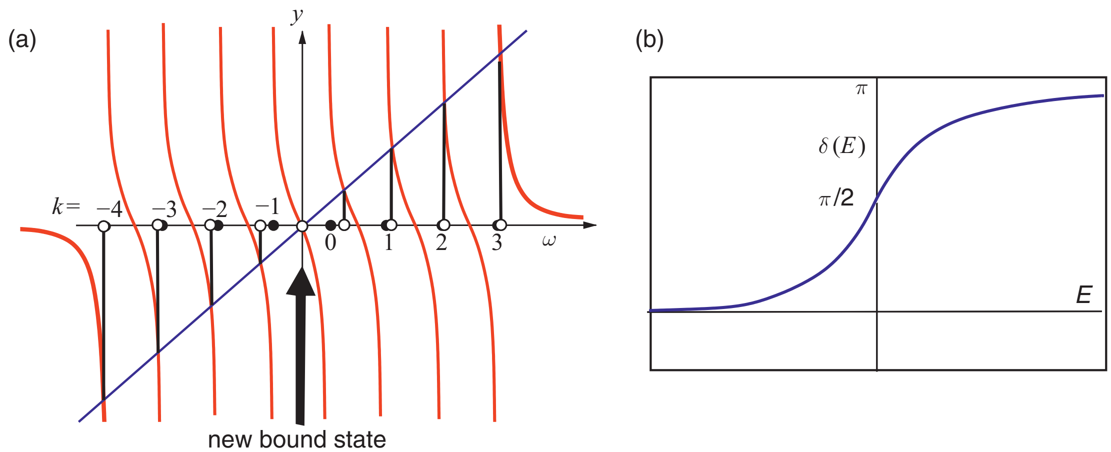


Fig. 17.8 (a) Graphical solution of the equation $y = \lambda + \sum_k \frac{V^2}{y-\epsilon_k}$, for eight equally spaced conduction electron energies for a resonance located at $\lambda = 0$ (arrow). Notice how the injection of a bound state at $y = 0$ displaces electron band states away from the Fermi surface, increasing the number of eigenstates by one. (b) Energy dependence of the scattering phase shift.

$$E_\gamma - \lambda - \sum_k \frac{V^2}{E_\gamma - \epsilon_k} = 0. \tag{17.97}$$

We can recognize this solution as a pole of the f-Green's function, $G_f(E_\gamma)^{-1} = 0$ (see (16.23) and (16.25)).

The solutions of the eigenvalue equation (17.97) are illustrated graphically in Figure 17.8. Suppose the energies of the conduction sea are given by the $2M$ discrete values

$$\epsilon_k = \left(k + \frac{1}{2}\right)\Delta\epsilon \qquad (k \in \{-M, \ldots M-1\}), \tag{17.98}$$

distributed symmetrically above and below the Fermi energy. Consider the particle–hole case when the f-state is exactly half-filled, i.e. when $\lambda = 0$. From the diagram, we see that one solution to the eigenvalue equation corresponds to $E_\gamma = 0$, i.e. the original $2M$ band-electron energies have been displaced to both lower and higher energies, forming a band of $2M + 1$ eigenvalues: the resonance has injected one new eigenstate into the band. Each new eigenvalue is shifted infinitesimally relative to the original conduction electron energies, according to

$$E_\gamma = \epsilon_\gamma - \Delta\epsilon \frac{\delta(E_\gamma)}{\pi}, \tag{17.99}$$

where $\delta(E_\gamma) \in [0, \pi]$ is the resonant scattering phase shift.

Let us now determine the dependence of $\delta[E]$ on the conduction electron energy. Substituting the phase shift into the eigenvalue equation (17.97), we obtain

$$E_\gamma = \lambda + \sum_{n=\gamma+1-M}^{\gamma+M} \frac{V^2}{\Delta\epsilon(n - \frac{\delta_\gamma}{\pi})} \rightarrow \lambda + \frac{\Delta}{\pi} \sum_{n=-\infty}^{\infty} \frac{1}{(n - \frac{\delta_\gamma}{\pi})}. \tag{17.100}$$

Here we have identified $\rho \equiv \frac{1}{\Delta\epsilon}$ as the conduction electron density of states, writing $\Delta = \pi V^2/\Delta\epsilon = \pi V^2 \rho$ as the resonance level width. We have also taken the liberty of extending the bounds of the summation to infinity. Using contour integration methods, recognizing that $\cot z$ has poles at $z = \pi n$ of strength one,

$$\sum_{n=-\infty}^{\infty} \frac{\pi}{(\pi n - \delta_\gamma)} = \sum_n \oint_{poles\, z=\pi n} \frac{dz}{2\pi i} \frac{\pi \cot z}{z - \delta_\gamma}$$
$$= -\oint_{pole\, at\, z=\delta_\gamma} \frac{dz}{2\pi i} \frac{\pi \cot z}{z - \delta_\gamma} = -\pi \cot \delta(E_\gamma). \quad (17.101)$$

Using this result, (17.100) becomes

$$E_\gamma = \lambda - \Delta \cot \delta[E_\gamma] \Rightarrow \tan \delta[E_\gamma] = \frac{\Delta}{\lambda - E_\gamma}. \quad (17.102)$$

(b) From (17.99) we deduce that

$$\frac{d\epsilon}{dE} = 1 + \frac{\Delta\epsilon}{\pi} \frac{d\delta(E)}{dE}$$
$$= 1 + \frac{1}{\pi\rho} \frac{d\delta(E)}{dE}, \quad (17.103)$$

where $\rho = 1/\Delta\epsilon$ is the density of states in the continuum. The new density of states $\rho^*(E)$ is given by $\rho^*(E)dE = \rho d\epsilon$, so that

$$\rho^*(E) = \rho(0)\frac{d\epsilon}{dE} = \rho + \rho_i(E), \quad (17.104)$$

where

$$\rho_i(E) = \frac{1}{\pi} \frac{d\delta(E)}{dE} = \frac{1}{\pi} \frac{\Delta^2}{(E - \lambda)^2 + \Delta^2} \quad (17.105)$$

corresponds to the enhancement of the conduction electron density of the states due to injection of the resonant bound state.

17.5.2 Minimization of free energy

With the results from the previous section, let us now calculate the free energy and minimize it to self-consistently evaluate λ and Δ. The shift in the free energy due to the Kondo effect is then

$$\Delta F = -N \int_{-D}^{D} \frac{d\epsilon}{\pi} f(\epsilon) \mathrm{Im} \ln[\xi - \epsilon] - \lambda Q + \frac{N\Delta}{\pi J \rho}, \quad (17.106)$$

where we have introduced the complex number $\xi = \lambda + i\Delta$ whose real and imaginary parts represent the position and width of the resonant level, respectively. This integral can be done at finite temperature, but for simplicity let us carry it out at $T = 0$, when the Fermi function becomes a step function, $f(x) = \theta(-x)$. This gives

$$\Delta E = \frac{N}{\pi} \mathrm{Im}\left[(\xi - \epsilon) \ln \left[\frac{\xi - \epsilon}{e} \right] \right]_{\epsilon=-D}^{\epsilon=0} - \lambda Q + \frac{N\Delta}{\pi J \rho}$$
$$= \frac{N}{\pi} \mathrm{Im}\left[\xi \ln \left[\frac{\xi}{eD} \right] - D \ln \left[\frac{D}{e} \right] \right] - \lambda Q + \frac{N\Delta}{\pi J \rho}, \quad (17.107)$$

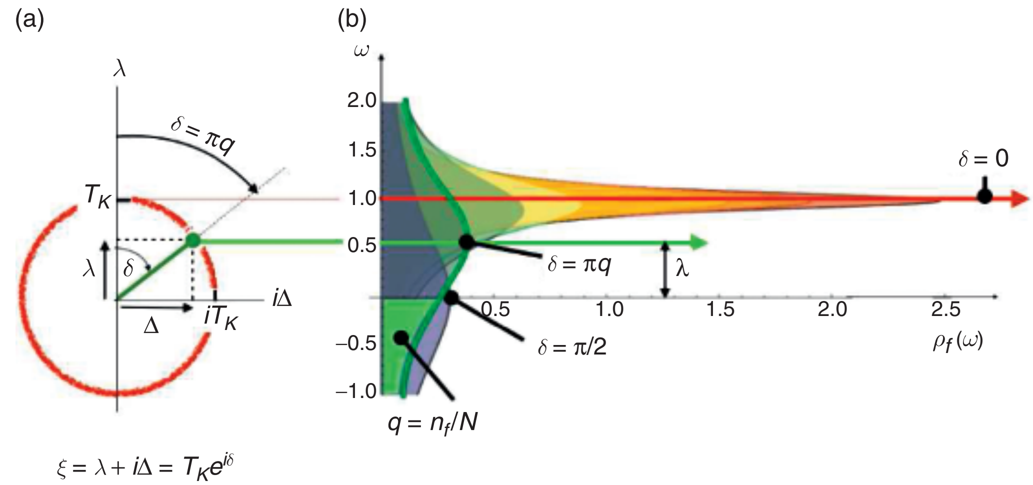


Fig. 17.9 Illustrating the mean-field solution to the impurity Kondo model. (a) Showing how the real and imaginary parts of the resonant level position $\xi = \lambda + i\Delta$ lie on a circle of radius T_K, with a phase shift $\delta = \pi q = \pi n_f/N$. (b) Showing the corresponding f density of states $\rho_f(\omega)$ for a range of different occupancies.

where we have expanded $(\xi + D)\ln\left[\frac{D+\xi}{e}\right] \to D\ln\left[\frac{D}{e}\right] + \xi \ln D$ to obtain the second line. We can further simplify this expression by noting that

$$-\lambda Q + \frac{N\Delta}{\pi J\rho} = -\frac{N}{\pi}\mathrm{Im}\left[\xi \ln\left[e^{-\frac{1}{\rho J}+i\pi q}\right]\right], \tag{17.108}$$

where $q = Q/N$, so that

$$\Delta E = \frac{N}{\pi}\mathrm{Im}\left[\xi \ln\left[\frac{\xi}{eT_K e^{i\pi q}}\right]\right], \tag{17.109}$$

where we have dropped the constant term and introduced the Kondo temperature $T_K = De^{-\frac{1}{J\rho}}$. The stationary point $\partial E/\partial\xi = 0$ is given by (see Figure 17.9)

$$\xi = \lambda + i\Delta = T_K e^{i\pi q} \qquad \left\{ \begin{array}{rcl} T_K & = & \sqrt{\lambda^2 + \Delta^2} \\ \tan(\pi q) & = & \frac{\Delta}{\lambda}. \end{array} \right. \tag{17.110}$$

Notice the following:

- The phase shift $\delta = \pi q$ is the same in each spin scattering channel, reflecting the singlet nature of the ground state. The relationship between the filling of the resonance and the phase shift $Q = \sum_\sigma \frac{\delta_\sigma}{\pi} = N\frac{\delta}{\pi}$ is Friedel's sum rule.
- The energy is stationary with respect to small variations in λ and Δ. It is only a local minimum once the condition $\partial E/\partial\lambda = 0 \equiv (\langle \hat{n}_f \rangle - Q)$ is imposed, which gives $\lambda = \Delta\cot(\pi q)$ and hence

$$\Delta E = \frac{N}{\pi}\left[\Delta \ln\left[\frac{\Delta}{eT_K \sin\pi q}\right]\right]. \tag{17.111}$$

Plotted as a function of V, this is the classic “Mexican hat” potential, with a minimum where $\partial E/\partial V = 0$ at $\Delta = \pi\rho|V|^2 = T_K \sin\pi q$ (Figure 17.9).

- According to (17.104), the enhancement of the density of states at the Fermi energy is

$$\begin{aligned}\rho^*(0) &= \rho + \frac{\Delta}{\pi(\Delta^2+\lambda^2)} \\ &= \rho + \frac{\sin^2(\pi q)}{\pi T_K}\end{aligned} \tag{17.112}$$

per spin channel. When the temperature is changed or a magnetic field is introduced, one can neglect changes in Δ and λ, since the free energy is stationary. This implies that, in the large-N limit, the susceptibility and linear specific heat are those of a non-interacting resonance of width Δ. The change in linear specific heat $\Delta C_V = \Delta\gamma T$ and the change in the paramagnetic susceptibility $\Delta\chi$ are given by

$$\begin{aligned}\Delta\gamma &= \left[\frac{N\pi^2 k_B^2}{3}\right]\rho_i(0) = \left[\frac{N\pi^2 k_B^2}{3}\right]\frac{\sin^2(\pi q)}{\pi T_K} \\ \Delta\chi &= \left[N\frac{j(j+1)(g\mu_B)^2}{3}\right]\rho_i(0) = \left[N\frac{j(j+1)(g\mu_B)^2}{3}\right]\frac{\sin^2(\pi q)}{\pi T_K}.\end{aligned} \tag{17.113}$$

Notice how it is the Kondo temperature that determines the size of these two quantities. The dimensionless Wilson ratio of these two quantities is

$$W = \left[\frac{(\pi k_B)^2}{(g\mu_B)^2 j(j+1)}\right]\frac{\Delta\chi}{\Delta\gamma} = 1.$$

At finite N, fluctuations in the mean-field theory can no longer be ignored. These fluctuations induce *interactions* among the quasiparticles, and the Wilson ratio becomes

$$W = \frac{1}{1-\frac{1}{N}}.$$

The dimensionless Wilson ratios of a large variety of heavy-electron materials lie remarkably close to this value.

17.6 Mean-field theory of the Kondo lattice

17.6.1 Diagonalization of the Hamiltonian

We can now make the jump from the single-impurity problem to the lattice. The virtue of the large-N method is that, while approximate, it can be readily scaled up to the lattice. We'll now recompute the effective action for the lattice, using equation (17.70). Let us assume that the hybridization and constraint fields at the saddle point are uniform, with $V_j = V$ and $\lambda_j = \lambda$ at every site. In fact, even if we start with a $V_j = Ve^{-i\phi j}$ with a different phase at each site, we can always absorb the phase ϕ_j using the Read–Newns gauge transformation (17.57) to absorb the additional phase onto the f-electron field. We