Weak-localization effects in heavy-fermion systems

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(Received 25 March 1991)

We examine the effect of a random potential acting on the conduction electrons in the Anderson-lattice model of a heavy-fermion (HF) compound (treated to leading order in the $1/N$ expansion). The model is of relevance to diluting normal-metal sites of an HF system. We go beyond coherent-potential-approximation treatments by summing up the Langer-Neal ladder series responsible for weak-localization effects. We find the heavy-fermion mass-enhancement factor enters into the frequency-dependent components in the ac conductivity but not in the static parts. This suggests that some weak-localization effects may be significantly enhanced in HF systems.

I. INTRODUCTION

Heavy-fermion (HF) systems continue to raise as many questions as they leave unanswered. Among the many unsolved questions relating to their ground states is the problem of the effect of disorder. In the Fermi-liquid regime it has been known for some time that small amounts of doping of the HF compound can lead to enormous changes in the residual resitivity.[1-3] Various theoretical approaches to the disorder problem have been formulated.[4,5] These start in general from a scheme that gives good qualitative agreement of the single impurity and lattice limits of the rare-earth concentration, such as the Kondo boson formulation, and incorporate the effect of disorder via either a coherent-potential-approximation (CPA) -type treatment,[4] or use in one dimension (1D) an exact diagonalization procedure to handle the randomness.[5]

Experimentally, the scattering from impurities in the HF state is enormous, as if each impurity is scattering at the unitarity limit.[3] This has given rise to the "Kondo-hole" concept.[2] Since the ground state at each Ce ion in the spin-compensated Kondo lattice is itself producing a phase shift of $\pi/2$ in the coherent regime, replacing a Ce ion with a nonmagnetic ion is equivalent to introducing a scattering phase shift of $-\pi/2$ relative to the background. This elegant description does not, however, explain why very similar changes in ρ_0 arise when the normal host sites are the ones to suffer disorder. Recent experiments on UPt_3 samples with a residual resistivity of $\sim 1\ \mu\Omega$ cm found changes of $\sim 10\ \mu\Omega$ cm per atomic percent.[4]

The fact that such changes are independent of whether the host or rare-earth sites are being doped suggests that the host disorder problem be examined somewhat closely. It would certainly seem to be a much more tractable problem than trying to treat rare-earth site disorder, since it would appear to involve only potential scattering, and perhaps local changes in the hybridization as well. This latter aspect will affect the Kondo processes at a particular site quite significantly and therefore we shall only focus here on simple random potential scattering of the conduction electrons by the disordered host sites. This restriction allows us to explore effects beyond the coherent potential approximation and study the quantum interference effects associated with weak localization.[6] Our effort is directed towards an understanding of the differences and similarities between simple metals and HF systems with regard to the very fundamental questions associated with disorder, and the interplay with many-body interaction effects.

Our approach in this paper will be to resum perturbation theory in the random potential affecting the conduction electron states by keeping the set of Langer-Neal[7] or maximally crossed diagrams known to give diffusive behavior in the density fluctuation spectrum. The remainder of the problem, namely the part associated with the heavy-fermion aspects, will be treated in the mean-field Kondo boson manner known to become accurate for large values of the spin degeneracy. We will not include the interference between diffusive electron propagation and the Kondo effect, or the effect on quasiparticle scattering on the diffusion pole behavior itself. We shall regard weak disorder as a probe of the dynamics of the HF state, at least as a starting point from which to incorporate the above features later.

In the next section we formulate the Hamiltonian of the problem and recap on the large-N mean-field description, including to very lowest order, the effects of potential scattering (as given by Millis and Lee[8]). In the following section we represent the conductivity tensor in the usual Kubo manner and relate it to conduction electron Green's functions. We sum the set of maximally crossed diagrams, obtaining the diffusion pole behavior and calculate the low-frequency behavior of the electrical conductivity. In the final section we shall discuss the consequences of our result for experiments.

II. FORMULATION

The full Anderson-lattice model[8] in the boson representation with random potential scattering present is given by

$$H = H' + H_{\text{const}} + H_{\text{pot}} , \tag{1}$$

where

$$H' = \sum_{k,m} \varepsilon_k c^\dagger_{km} + \sum_{i,m} E_0 f^\dagger_{km} f_{km} + V \sum_{k,i,m} (e^{i\mathbf{k}\cdot\mathbf{R}_i} c^\dagger_{k,m} f_{im} b^\dagger_i + \text{H.c.}) \tag{2}$$

describes the conduction electron states (labeled by creation operators $c^\dagger_{km}$, where k,m denote the momentum and spin label), the bare f-electron states (labeled by $f^\dagger_{i,m}$, where i is a site index), and hybridization between these, with mixing element V, with the creation (or destruction) of an empty site (labeled by a boson operator $b^\dagger_i$). The electron energies are given by ε_k, and E_0 denotes the bare f-level position. The restriction to states involving zero or single f occupancy is handled by adding a term

$$H_{\text{const}} = \sum_i \lambda_i \left[\sum_m f^\dagger_{im} f_{im} + b^\dagger_i b_i - Q_i \right] , \tag{3}$$

where λ is a Lagrange multiplier for site i and Q_i is the total charge at site i. Since the constraint that

$$Q_i = n^i_F + n^i_b = 1 \tag{4}$$

is satisfied at all times by virtue of the fact that $[H', Q_i] = 0$, λ_i can be chosen to be time independent.

The potential scattering term in the Hamiltonian is written

$$H_i = \sum_{k,k'} V_I c^\dagger_{km} c_{k'm} , \tag{5}$$

which acts only on the conduction electrons. Following Millis and Lee[8] we rescale the hybridization, boson operators, and total charge by appropriate powers of the spin degeneracy $N = 2j+1$, where j is the magnetic quantum number. Assuming broken symmetry in the rescaled Bose field and in the Lagrange multiplier leads at leading $1/N$ order to the Hamiltonian being replaced by

$$H = H_0 + H_{\text{pot}} + H_{\text{int}} + H_A , \tag{6}$$

where

$$H_0 = \sum_{k,m} [\varepsilon_k c^\dagger_{km} c_{km} + \varepsilon_f f^\dagger_{km} f_{km} + Va(c^\dagger_{km} f_{km} + \text{H.c.})] + \text{boson terms} , \tag{7}$$

and H_A, H_{int} contain coupling to Bose fluctuations as well as coupling to the zero point boson terms. By insisting that these latter terms are cancelled by the leading order Hartree-like contribution from H_{int} (see Ref. 8 for details) the values of a and ε_f (the broken symmetry expectation values of $b^\dagger_i$ and λ_i) are determined. The fermion term shown above is trivially diagonalized with the result that the conduction electron propagation to leading order in $1/N$ is given by

$$G_c(k,i\omega) = \left[i\omega - \varepsilon_k - \frac{V^2\alpha^2}{(i\omega - \varepsilon_f)} \right]^{-1} , \tag{8}$$

where the hybridization is renormalized by the quantity

$$a^2 = q_0(1-n_f)\left[1 - \frac{n_f^2 q_0}{4\rho_0 W}\right] \sim q_0(1-n_f) \tag{9}$$

where $q_0 = Q/N$ is the rescaled total charge (taken to be finite) and W denotes the bandwidth, while ρ_0 is the conduction electron density of states at the Fermi level. The mean-field number of f electrons is given by

$$n_f = (1 + \varepsilon_f/\rho_0 V^2)^{-1} , \tag{10}$$

while the parameter ε_f is basically the single impurity Kondo temperature (to leading order in q_0)

$$\varepsilon_f = W\left[1 - \frac{q_0}{\rho_0 W}\right]\exp\left[-\frac{|E_0|}{\rho_0 V^2}\right] = We^{-|E_0|/\rho_0 V^2} = T_k . \tag{11}$$

The mass enhancement is given by $V^2a^2/\varepsilon_f^2 \sim q_0 D/T_k$. We note that if we set $q_0 = 1/N$ the results for $G_c(k,i\omega)$ agree (for $\omega < T_k$) with those obtained from perturbative resummation techniques.[9] The result in this formalism actually appears as

$$G_c(k,i\omega) = \left[i\omega - \varepsilon_k - \frac{T_k}{N\rho_0(i\omega - T_k)} \right]^{-1} . \tag{12}$$

The poles of G_c yield the quasiparticle energies which follow the well known renormalized hybridized band structure.[8] Taking (1) or (2) as the HF Green's function for conduction electrons allows the effects of H_{pot} to be readily calculated perturbatively. To leading order, Dyson's equation yields for the conduction electron-self-energy[8]

$$-\text{Im}\sum_c (k,w) = \frac{\text{sgn}(\omega)}{2\tau_i} = \text{sgn}(\omega)\pi\rho_0 V_I^2 n , \tag{13}$$

which contributes the usual Drude result to the conductivity.

III. DIFFUSION POLE BEHAVIOR AND RELATION TO THE CONDUCTIVITY

The conductivity can be evaluated in the usual Kubo manner since only the conduction electrons in the Anderson Hamiltonian are concerned: In going beyond the usual Boltzmann type of analysis we require higher-order contributions which lead to the following expression for the conductivity tensor:

$$G^j_{\alpha\beta} = \frac{Ne^2}{4m^2\beta}(2\mathbf{k}_\alpha + q_\alpha)(2\mathbf{k}_\beta + q_\beta)\Gamma(\mathbf{k},\mathbf{k}',\mathbf{q};\omega,\omega') , \tag{14}$$
$$G_c(\mathbf{k},i\omega')G_c(\mathbf{k}',i\omega')G_c(\mathbf{k}+\mathbf{q},i\omega+i\omega')G_c(\mathbf{k}'+\mathbf{q},i\omega+i\omega'),$$

which is represented graphically in Fig. 1. As in the usual manner G^j relates the vector potential to the current density. The theory of weak localization tells us that the crucial contributions to Γ are given by the maximally crossed graphs Fig. 2(a) [drawn uncrossed in Fig. 2(b)]. Each graph at finite order in this maximally crossed set is known to be nonanalytic in the impurity concentration.[6,7] Consequently the entire series has to be summed in order

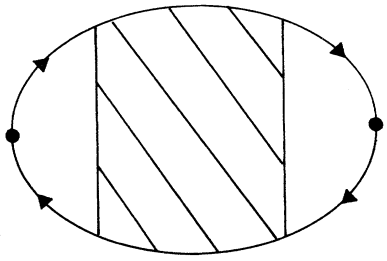

FIG. 1. Two-particle Green's function involved in the conductivity tensor expression.

to obtain a finite result. The uncrossed series of graphs obtained from Fig. 2(a) by reversing the bottom line is easier to visualize since it constitutes a ladder sum. Summing up the ladder series yields for Γ for the result [see Fig. 2(c)]

$$\Gamma(\mathbf{k},\mathbf{k}',\mathbf{q},\omega')=\frac{n|V_I|^2}{[1-X(\mathbf{k}+\mathbf{k}'+\mathbf{q})]}\ , \tag{15}$$

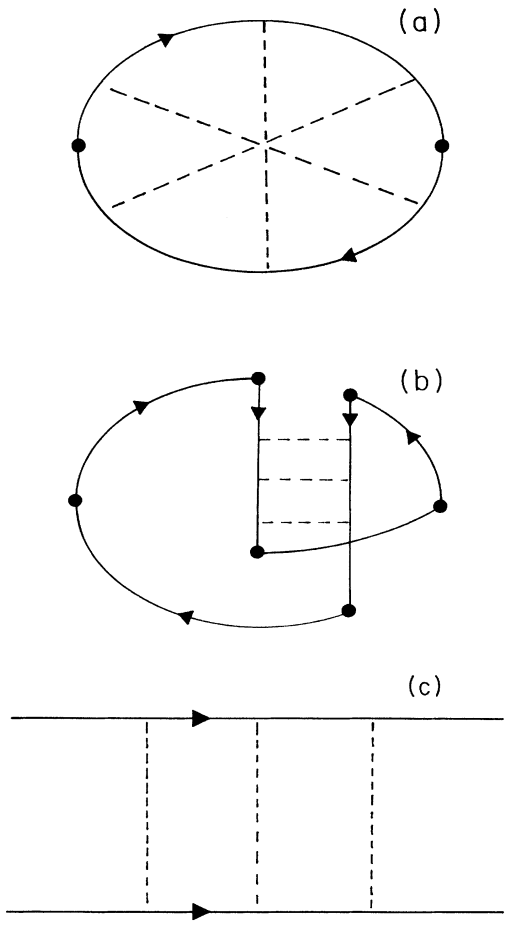

FIG. 2. (a) Maximally crossed diagrams leading to the diffusion pole behavior, drawn uncrossed in (b). The ladder series involved in the determination of Γ is shown in (c).

where

$$X(\mathbf{p},\omega)=n|V_I|^2\sum_{\mathbf{p}'}G_c(\mathbf{p}-\mathbf{p}',i\omega+i\omega')G_c(\mathbf{p}',i\omega') \tag{16}$$

represents the contribution from the intermediate particle-particle ladder rungs. As usual, ω' and $\omega+\omega'$ have to lie on opposite sides of the real axis in order for X to be nonzero. The crucial aspect of the sum in (16) lies in the frequency dependence. Ignoring this (i.e., setting $\omega=0^+$) the remaining momentum-dependent terms are given by the usual result for an unenhanced metal,

$$\begin{aligned}X(p,\omega=0^+)=n|V_I|^2\sum_{\mathbf{p}'}&\left[\frac{i}{2\tau}+\frac{1}{N\rho_0}-\varepsilon_{\mathbf{p}-\mathbf{p}'}\right]^{-1}\\&\times\left[-\frac{i}{2\tau}+\frac{1}{N\rho_0}-\varepsilon'_p\right]^{-1}\\&=1-(v_F\tau)^2p^2/3\ .\end{aligned} \tag{17}$$

The constant terms in the Green's functions make no difference to the result. The mass enhancement has no effect in this term since the analytic properties are determined by $1/2\tau$. On the other hand, we do obtain a significant contribution from expanding $X(p,\omega)$ to leading order in ω. We find this coefficient to be (setting $p=0$)

$$\delta X=(-m^*/m)i\omega\tau nV^2\sum_{\mathbf{p}'}G_c(-\mathbf{p}',\omega+\omega')G(\mathbf{p}',\omega')\ , \tag{18}$$

which is straightforwardly evaluated in the usual manner to give

$$\delta X(0,\omega)=(m^*/m)i\omega i\tau\ . \tag{19}$$

We note the huge enhancement factor m^*/m entering the frequency-dependent term. The overall result of these manipulations is that the $\Gamma(k,k',q,\omega,\omega')$ has the usual diffusion pole dependence

$$\Gamma(\mathbf{k},\mathbf{k}',\omega,\omega')=\frac{n|V_I|^2}{\tau(\omega m^*/m+D|\mathbf{k}+\mathbf{k}'+\mathbf{q}|^2)}\ , \tag{20}$$

where the diffusion constant has its usual value $D=1/3v_F^2\tau$. In keeping with earlier transport results in HF systems the momentum-dependent features are unaffected while frequency-dependent effects are severely affected by the mass enhancement.[8,10] The conductivity tensor then takes the form (for $q=0$)

$$\begin{aligned}G^j_{\alpha\beta}(q=0,i\omega)=+\frac{N_f e^2}{m^2V}k_{F_\beta}k_{F_\beta}\sum_{\mathbf{k}',\mathbf{p}'}&\frac{n|V_I|^2}{\tau(\omega m^*/m+Dp^2)}\\&\times I(\mathbf{p}-\mathbf{k}',\mathbf{k}',\omega)\ ,\end{aligned} \tag{21}$$

where I is the product of the four Green's functions

$$I(\mathbf{p}-\mathbf{k}',\mathbf{k},\omega)=\frac{1}{\beta}\sum_{\omega'} G_c(\mathbf{p}-\mathbf{k},\omega')G_c(\mathbf{k}',\omega') \times G_c(\mathbf{p}-\mathbf{k}',\omega+\omega')G_c(\mathbf{k}',\omega+\omega') , \tag{22}$$

and, since the dominant region of importance in the $\mathbf{p}$ integration is over the long-wavelength region $p<1/V_F\tau \ll k_F$, we may replace $I(\mathbf{p}-\mathbf{k}',k',\omega)$ by its value at $p=0$,

$$\sum_{\mathbf{k}'} I(-\mathbf{k}',\mathbf{k}',\omega)=\frac{1}{\beta}\sum_{\omega_1}\frac{\Theta(-\omega')\Theta(\omega+\omega')4\pi\rho_0}{(\omega+1/\tau)^3} . \tag{23}$$

We note that for small frequencies the important energy scale is τ^{-1}, so that our final expression for the conductivity tensor becomes

$$G^j_{\alpha\beta}(q=0,i\omega)=i\omega\frac{N_f e^2}{\pi V}\sum_{\mathbf{p}}\left[p^2+\frac{\omega}{D}\frac{m^*}{m}\right]^{-1}\delta_{\alpha\beta} , \tag{24}$$

since the electric field at frequency ω is proportional to the vector potential by a factor $i\omega$, we finally obtain after analytic continuation $i\omega\rightarrow\omega+i\delta$ the frequency-dependent conductivity for an isotropic HF system

$$\sigma_{\text{maxcrossed}}(0,\omega)=-\frac{N_f e^2}{\pi V}\sum_{\mathbf{p}}\left[p^2-\frac{i\omega}{D(m^*/m)}\right]^{-1} , \tag{25}$$

due to summing up the interfering Langer-Neal graphs. To this must be added the regular ohmic contribution

$$\sigma_{\text{ohm}}=ne^2\tau/m , \tag{26}$$

which is unaffected by mass-enhancement processes (these cancel from both the collision time and effective mass).

The important feature to note in (25) is the appearance at the mass-enhancement factor multiplying the frequency. As is well known, the frequency-dependent conductivity increases with increasing frequency as $(\omega\tau)^{1/2}$ in 3D signaling the destruction of the coherent backscattering effects responsible for localization.[11] In the present problem this term is substantially enhanced as a result of being multiplied by the mass-enhancement factor, so that the conductivity increase can be written

$$\delta\sigma/\sigma_0=\frac{3\sqrt{6}}{4(k_F l)^2}\sqrt{(m^*/m)\omega\tau} . \tag{27}$$

Consequently such an increase may be observable in a HF system, although it competes with the Drude falloff. However, it may be possible to observe other features associated with the frequency-dependent aspects of the localization problem which should be similarly enhanced in a HF system. It should be noted that at the present level of calculation the frequency dependence shows a universal dependence on the mass enhancement. A number of HF properties reveal such a one scale universality,[12] not only at the mean-field level but also calculated to one-loop order.

In conclusion, we have developed an approach to the interplay between localization and interaction by working in a model where the interaction effects are treated as fundamental and the disorder aspects are treated perturbatively by resumming maximally crossed graphs arising from the randomness. We find that although no particular difference (compared with usual weak localization) arises in the dc conductivity, the frequency dependence is significantly enhanced. The model should be applicable to heavy-fermion systems in which the normal-metal sites are replaced by impurities or made vacant as a result of radiation bombardment.

ACKNOWLEDGMENTS

The author wishes to thank Meigan Aronson, Jim Allen, Steven Dierker, Stuart Field, and Rombout Hoogerbeets for helpful discussions and acknowledges financial support from the Horace P. Rackham Foundation.

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