# Dynamics of disordered heavy-fermion systems

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Dynamics of the disordered heavy-fermion model of Miranda *et al.* are calculated using an expression for the spectral function of the Anderson model that is consistent with quantum Monte Carlo results. We compute $\Sigma(\omega)$ for three distributions of Kondo scales including the distribution of Bernal *et al.* for $UCu_{5-x}Pd_x$. The corresponding low-temperature optical conductivity shows a low-frequency pseudogap, a negative optical mass enhancement, and a linear in frequency transport scattering rate, consistent with results in $Y_{1-x}U_xPd_3$ and $UCu_{5-x}Pd_x$. The formalism is strictly valid for a dilute system of Kondo scatterers like $Y_{1-x}U_xPd_3$, but the leading frequency behavior at low $T$ (much lower than bulk $T_K$) hold for lattice systems as well. [S0163-1829(97)50330-4]

*Introduction.* Over the past four decades, the Fermi-liquid paradigm has been the key to our understanding of metallic behavior. In Fermi-liquid theory we assume a 1:1 correspondence between the low-lying eigenstates of the interacting system to those of the noninteracting electron gas. This leads to a magnetic susceptibility that is weakly temperature dependent, a specific heat linear in $T$, and a low temperature resistivity that is quadratic.

However, recently there has been a great deal of experimental interest in disordered heavy-fermion compounds[1] (e.g. $Y_{1-x}U_xPd_3$, $UCu_{5-x}Pd_x$), where strong electronic correlations preclude Fermi-liquid behavior. The non-Fermi-liquid behavior in these compounds is characterized by a linear resistivity at low $T$, a logarithmic low temperature divergence of the susceptibility and the specific heat coefficient, an optical conductivity with a low frequency pseudogap and a linear transport scattering rate at low frequencies.[1–3] Several models have been proposed to explain these experimental results. Among them are theories based upon proximity to a zero temperature quantum critical point[4] and those which explain the impurity to lattice crossover effects in the multichannel Kondo model.[5]

Dobrosavljević *et al.*[6] investigated a dilute system of magnetic impurities in a disordered metal. Since disorder can give rise to a distribution of the local density of states of the conduction electrons, a distribution of Kondo scales $P(T_K)$ is induced that could be singular enough to produce $\chi$ and $\gamma$ that diverge as $T \rightarrow 0$, a strongly non-Fermi-liquid behavior. More recently, Bernal *et al.*[7] have shown that this $P(T_K)$ is not appropriate for the $U$-doped heavy-fermion systems. They propose an alternative spread of Kondo scales, and use it to calculate the thermodynamics of these alloys. Miranda *et al.*[8] have recently shown that the underlying mechanism behind the non-Fermi-liquid transport and thermodynamics is the presence of a finite number of unquenched low-$T_K$ spins, along with an essentially constant $P(T_K)$ at low $T_K$. This gives a linear in $T$ low temperature resistivity.

*Formalism.* We stay within this phenomenological framework and calculate dynamical quantities such as the optical conductivity and self-energy. Our analysis is strictly valid only in systems with a *dilute* collection of Kondo centers, like $Y_{1-x}U_xPd_3$, but the leading frequency dependence of the dynamical quantities (at low $T$) should apply to concentrated systems like $UCu_{3.5}Pd_{1.5}$ as well.[9] We begin by concentrating on the Kondo regime of the Anderson impurity model, where $d$-electrons occupy the conduction band, and $f$-electrons provide the magnetic impurities for the spin-spin scattering processes. In the low temperature limit this model corresponds precisely to the Fermi-liquid picture of Landau. The electronic density of states has a resonance at the Fermi level, giving significant impurity contributions to the specific heat and magnetic susceptibility. Following Doniach and Sunjic,[10] Frota and Oliveira[11] argued that the Doniach-Sunjic form, modified to account for the $\pi/2$ phase shift, should describe the shape of Kondo resonance. Their expression is in agreement with their results for the Kondo resonance obtained from numerical renormalization group calculations,[12] as well as low-temperature quantum Monte Carlo (QMC) results analytically continued with the maximum entropy method (MEM).[13,14]

We can generalize their expression to finite temperatures and get

$$A_f(\omega, T_K) = \frac{1}{\pi\Delta}\mathrm{Re}[i\Gamma_K/(\omega + i\sqrt{\Gamma_K^2 + \gamma^2})]^{1/2}, \quad (1)$$

where $\Delta$ is the $f$-$d$ hybridization energy, and $\Gamma_K = (\pi/2)^2 T_K$ is the half-width of this resonance, $T_K$ being the Kondo temperature. We add a temperature dependent width $\gamma$ to the original expression of Frota and Oliveira,[11] with $\gamma$ determined by fitting to QMC-MEM results.[13] As shown in Fig. 1, this form continues to exhibit remarkable agreement with the shape of the Kondo resonance (the low-frequency peak) obtained from QMC-MEM, *even at finite temperatures*. By comparison with a wide range of Anderson impurity spectra, we were able to obtain the universal function $\gamma(T/T_K)$ for over three decades of $T/T_K$. For $T/T_K \lesssim 0.3$, we use $\gamma(T) = 4.52T$, a value derived from Noziéres'[15] phenomenological Fermi-liquid description of the Kondo problem at low temperatures. The result for $\gamma(T/T_K)$ will be presented in a table of an upcoming publication.

Since we are working in the dilute limit, we assume the impurities to be independent scatterers and disorder average
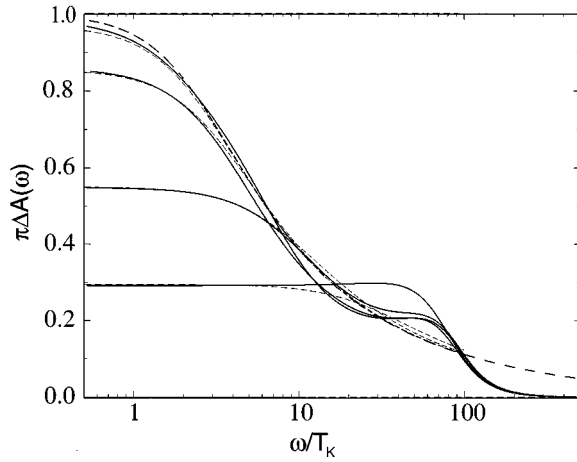
FIG. 1. Spectral function for the $f$-electron in the Kondo limit of the Anderson model. The long-dashed line is the Doniach-Sunjic result (Ref. 11) (true for $T=0$). The dotted lines represent the extension of the Doniach-Sunjic result to finite $T$ which is used for calculating the dynamics in this paper; the solid lines represent QMC-MEM results. $T/T_K = 0.2$, 0.8, 3.2, and 12.8 for the curves from top to bottom. For $T/T_K \lesssim 0.3$, $A_f(\omega, T_k)$ has a width $\gamma = 4.52T$ which comes from Fermi-liquid theory (Ref. 15). For higher $T/T_K$, we adjust $\gamma$ to fit the QMC-MEM data.

over the universal single impurity spectral function [Eq. (1)] to calculate dynamical quantities. The Hilbert transform of $A_f(\omega, T_K)$ then gives the average impurity $t$ matrix

$$t_f(z) = \int dT_K P(T_K) \int d\omega \frac{V^2 A_f(\omega, T_K)}{z - \omega}, \qquad (2)$$

where $V$ is the $f$-$d$ hybridization. Following Miranda et al.[8] we use a dynamical mean-field approximation,[16] which becomes exact in the limit of infinite dimensions, to calculate the lattice self-energy from a concentration $x$ of substitutional Kondo impurities

$$\Sigma(\omega) = \frac{x t_f(\omega)}{1 + x t_f(\omega)\mathcal{G}(\omega)}, \qquad (3)$$

where $\mathcal{G}(\omega)$ describes the average effective medium of the impurity. It is related to the average local host Greens function $G$

$$G(\omega) = \int d\epsilon \frac{N(\epsilon)}{\omega - \epsilon + \mu - \Sigma(\omega)}, \qquad (4)$$

through the relation

$$\mathcal{G}^{-1} = G^{-1} + \Sigma, \qquad (5)$$

where $N(\epsilon) = (1/t^* \sqrt{\pi}) e^{-\epsilon^2/t^{*2}}$ and we set $t^* = 10\,000$ K to establish a unit of energy and temperature. The solutions of Eqs. (1)–(5) then give the full lattice self-energy.

The knowledge of this self-energy enables one to calculate physical quantities[17] like transport coefficients and the optical conductivity. In this paper we concentrate on the optical conductivity $\sigma(\omega)$. It is measured in units of $\sigma_0 = e^2 \pi/2\hbar a$, which with $h/e^2 \approx 2.6 \times 10^4$ $\Omega$, varies between $10^{-3}$ and $10^{-2}$ [$(\mu\Omega$ cm$)^{-1}$], depending on the lattice constant $a$.

*Results.* We choose three different distributions $P(T_K)$, corresponding to strong,[6] weak[7] and a phenomenological disorder motivated by Miranda et al.'s[8] argument that the experimental $P(T_K)$ should be relatively constant at low temperatures. We consider the distribution of Kondo scales as arising from a distribution of couplings between the conduction and the $f$-electron spins $P(J)$. For the strongly disordered sample, $P(T_K)$ has the form[6]

$$P_{sd}(T_K) = (4\pi)^{-1/2} \frac{1}{T_K \ln(t^*/T_K)}$$

$$\times \exp\{-0.25\ln^2[0.217e^{-1}\ln(t^*/T_K)]\}, \quad (6)$$

where we have used a bulk Kondo temperature $T_K^0 = 10^2$ K (in most U-based heavy-fermion systems $T_K^0$ varies between 100–200 K). The weak disorder is characterized by a Gaussian distribution $P(J)$ of width $2u = 0.01$, where $u$ is a disorder parameter[6] and a higher value of $u$ corresponds to more disorder. This leads to

$$P_{wd}(T_K) = \frac{1}{\sqrt{0.01\pi}} \frac{1}{0.217 T_K \ln^2(T_K/t^*)}$$

$$\times \exp\left\{-100\left[\frac{1}{0.217\ln(T_K/t^*)} + 1\right]^2\right\}. \quad (7)$$

For the phenomenological spread of Kondo scales, we assume the form

$$P_{ph}(T_K) = \frac{0.01}{e^{(T_K - T_K^0)} + 1}. \qquad (8)$$

This distribution is not based on microscopics; it simply satisfies the experimental criterion of constancy at low $T_K$ and looks qualitatively similar to the $P(T_K)$ for $UCu_{5-x}Pd_x$.[8] Unlike the $1/(T_K \ln T_K)$ divergence of the strongly disordered case, $P_{ph}(T_K)$ has a finite number of spins with $T_K = 0$.

The nature of the disorder gives rise to different physics in each case, as is manifested in the functional form of $\text{Im}\Sigma(\omega)$ (Fig. 2) (these plots are for $T=0$ and $x=0.2$ for all three distributions). For a weakly disordered system, $\text{Im}\Sigma(\omega)$ has the form $-c + \omega^2$ as $\omega \to 0$ where $c$ is a constant.[19] This suggests a finite lifetime for the electrons at the Fermi energy at zero temperature which makes it different from a normal (pure metal) Fermi liquid. But since there are no unquenched spins at $T=0$, the system does form a local Fermi liquid, with a resistivity $\rho(T) \sim \rho(0) - AT^2$. For the case of strong disorder, $P_{sd}(T_K)$ is divergent at low $T_K$. Even though we are on the metallic side of the metal-insulator transition, a large number of spins with very low Kondo temperatures gives a non-Fermi-liquid ground state. For this scenario, we find that $\text{Im}\Sigma(\omega) \sim -c + \omega^{1/4}$ at low $\omega$.

$P_{ph}(T_K)$, the distribution of Kondo scales that is relevant to $UCu_{5-x}Pd_x$, is intermediate between these two cases. It gives us an $\text{Im}\Sigma(\omega)$ that behaves like $-c + |\omega|$ as $\omega \to 0$. This behavior can be understood through the following simple argument. Oliveira's expression for the $f$-electron spectral function at $T=0$ can be expanded near $\omega=0$ to give a form $A_f(\omega, T_K) \sim 1 - \alpha(\omega/T_K)^2$, where $\alpha$ is a constant.
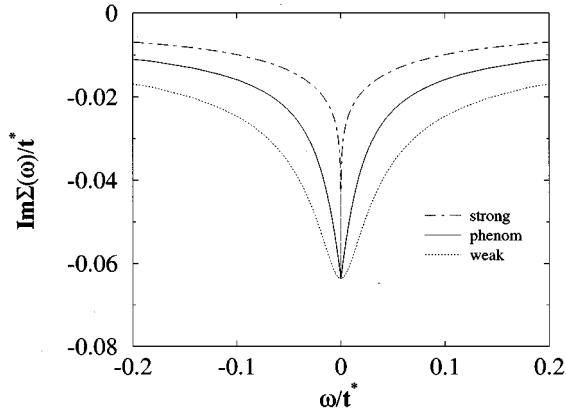
FIG. 2. Imaginary part of the conduction electron self-energy when $T=0$ and $x=0.2$. The three different curves denote different distributions of disorder. The lowest one corresponds to very weak disorder $[P(T_K)\to 0$ as $T_K\to 0]$ and at low $\omega$ has the form $\text{Im}\Sigma(\omega)\propto -c+\omega^2$, giving a local Fermi liquid with $\rho(T)=\rho(0)-AT^2$. The highest one is for strong disorder (still metallic), with a $\omega^{1/4}$ dependence as $\omega\to 0$. The one in the middle corresponds to a phenomenological distribution of Kondo scales suitable for the heavy-fermion systems. It approaches the form $\text{Im}\Sigma(\omega)\propto -c+|\omega|$ as $\omega\to 0$. This strongly hints towards a linear resistivity at low $T$ in these compounds.

Given that $P_{ph}(T_K)\approx$ const at low $T_K$, $\int_0^\infty A_f(\omega,T_K)P_{ph}(T_K)dT_K$ gets its dominant contribution from the region where $T_K\gtrsim \omega$. If we change the lower limit of the integral from 0 to $\omega$ and make use of the fact that $P_{ph}(T_K)$ has a finite upper cutoff ($\sim 100$ K), $\text{Im}\Sigma(\omega)$ turns out to be $-c+|\omega|$. A similar argument was employed by Miranda et al.[8] to calculate the resistivity. Averaging $\omega$ over a region of width $k_BT$ near the Fermi surface replaces $|\omega|$ by $T$, giving a resistivity linear in temperature which is observed experimentally in $Y_{1-x}U_xPd_3$ and $UCu_{3.5}Pd_{1.5}$.[1] This result is confirmed by direct calculation of the resistivity (not shown).

Figure 3 shows the temperature dependence of the optical conductivity of the phenomenologically disordered system. Consistent with what is seen in $Y_{1-x}U_xPd_3$ and $UCu_{3.5}Pd_{1.5}$ (Ref. 2), the Drude-like peak is recovered when $T\gtrsim 100$ K, since spins with essentially all possible values of $T_K$ are participating in the dynamics at this temprature. The inset lists the zero temperature optical conductivities for the three distributions of Kondo scales. All are characterized by a vanishing Drude weight at low $T$, along with a finite frequency peak. As the disorder is increased, this peak moves towards lower frequencies, concomitant with the decrease in the average value of $T_K$ (which is different than $T_K^0$). The Drude peak at $T=0$ is recovered from the weak disorder case if $u\to 0$ in $P(J)$, giving $P_{wd}(T_K)\propto \delta(T_K-T_K^0)$ ($T_K^0$ is the bulk value), which takes us to the single Kondo scale physics. The identical $T=0$ dc value of the conductivity in all three cases is a consequence of the Friedel sum rule at the Fermi level and is an artifact of our framework (we are always in the unitarity limit). $\sigma(\omega=0,T=0)$ would be different if the values of $x$ are chosen to be different in the three cases.
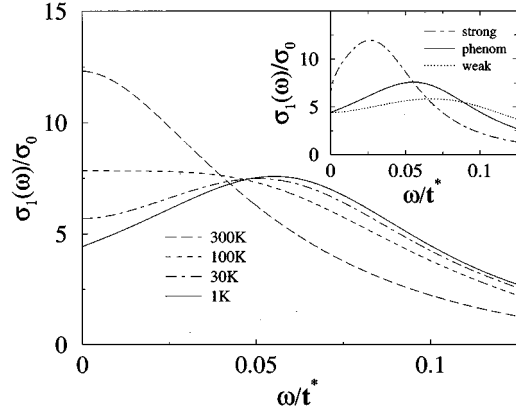
FIG. 3. Optical conductivity for the phenomenological distribution of Kondo scales at a few temperatures when $x=0.2$. At very low temperatures a finite number of unquenched spins preempt the formation of a Fermi liquid. The interesting feature is the development of a Drude peak as we go from temperatures much below the bulk Kondo value ($T_K^0\approx 100$ K) to those much above it. The inset shows the conductivity for the three different $P(T_K)$ when $T=0$. The absence of a Drude peak is conspicuous in all three cases.

The optical conductivity of metals, even non-Fermi-liquid metals, is usually analyzed by rewriting it in a generalized Drude form[2]

$$\sigma(\omega)=\frac{\omega_p^2}{4\pi}\frac{1}{\Gamma(\omega)-i\omega(1+\lambda(\omega))}, \qquad (9)$$
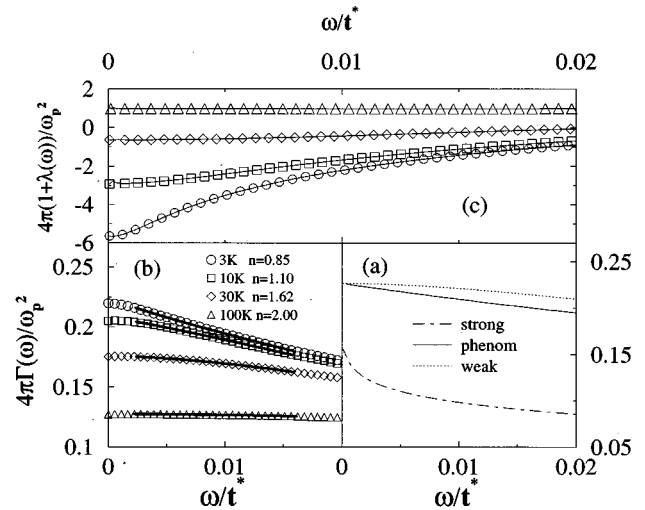
FIG. 4. (a) Frequency dependence of the scattering relaxation rate $\Gamma(\omega)$ at $T=0$ for the three different $P(T_K)$ when $x=0.2$. Note that $\Gamma(\omega)$ is linear in $\omega$, and therefore consistent with experiment (Ref. 2), only for the phenomenological distribution of Kondo scales. $\Gamma(\omega)$ corresponding to weak disorder has an $\omega^2$ behavior as $\omega\to 0$, suggesting the formation of a local Fermi liquid. (b) $\Gamma(\omega)$ for $P_{ph}(T_K)$ at different temperatures; in each case the solid line is a fit to the form $\Gamma(\omega)=\Gamma_0(1-(T/T_0)^n-(\omega/\omega_0)^n)$. We see that up until 10 K, we have a scattering rate that is roughly linearly decreasing in $\omega$ and $T$. (c) Optical mass enhancement for $P_{ph}(T_K)$ at different temperatures [symbols are the same as (b)]. At low temperatures $1+\lambda(0)<0$ indicative of a non-Fermi liquid.

where $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$. We calculate the transport relaxation rate $\Gamma(\omega)$ and the optical mass enhancement $[1+\lambda(\omega)]$ for the three distributions of Kondo scales. However, as shown in Fig. 4(a), only the phenomenological distribution results in a linear in frequency zero temperature $\Gamma(\omega)$, consistent with what is seen in $Y_{1-x}U_xPd_3$ and $UCu_{3.5}Pd_{1.5}$.[2] In each case, we find that the low frequency optical mass enhancement $1+\lambda(0)$ is negative (however, in the case of weak disorder a positive mass is recovered as $u \to 0$).

$\Gamma(\omega)$ for the phenomenological distribution at several different temperatures is plotted in Fig. 4(b). Here, consistent with Degiorgi $et\ al.$[2] we fit the relaxation rate to $\Gamma(\omega) = \Gamma_0(1 - (T/T_0)^n - (\omega/\omega_0)^n)$ in the low frequency region. We find that $T_0 \approx 85$ K and $\omega_0 \approx 0.09t^*$, and are roughly constant in temperature. At high temperatures, $\Gamma(\omega)$ and $1+\lambda(\omega)$ [Fig. 4(c)] are weakly frequency dependent, $1+\lambda(\omega) > 0$ and $n = 2.00$, as expected for a Fermi liquid. Thus, as seen in Fig. 3, a Drude peak is recovered in $\sigma_1(\omega)$. As the temperature is lowered, $\Gamma(\omega)$ and $1+\lambda(\omega)$ become strongly frequency dependent, $1+\lambda(0) < 0$, and $n \approx 1$, features which we believe should be viewed as characteristic of a non-Fermi liquid. A very similar sequence of features are seen in $Y_{1-x}U_xPd_3$ and $UCu_{3.5}Pd_{1.5}$.[2]

$Conclusion.$ Within the Kondo disorder model,[6–8] we calculate dynamics for $dilute$ U-based heavy-fermion systems. As mentioned in the Introduction, this calculation is very well justified for a system with dilute Kondo scatterers $(Y_{1-x}U_xPd_3)$ at all temperatures. For a concentrated Kondo lattice system like $UCu_{3.5}Pd_{1.5}$, only the leading temperature ($\omega$) dependence applies (not the numerical prefactor). When temperature ($\omega$) becomes comparable to $T_K^0$, self-consistent modifications to $P(T_K)$ presumably are significant for the lattice.

We observe a linear resistivity at low $T$ consistent with Ref. 8, the lack of a Drude peak and a low-frequency pseudogap in the real part of the optical conductivity, a negative low temperature optical mass, and a linear in frequency optical dynamical scattering rate. All these features are observed in $Y_{1-x}U_xPd_3$ and $UCu_{3.5}Pd_{1.5}$.[1,2] It is also straightforward to compute the spin-relaxation rate in NMR ($1/T_1$), which will be addressed in an upcoming publication. Thus, we conclude that the phenomenological distribution of Kondo scales model is sufficient to describe the dynamics of these disordered systems. It is important to stress that Kondo disorder is not the sole possible explanation of non-Fermi-liquid behavior in these systems.[4,5] In fact, it has recently been shown that the two-channel Kondo lattice model displays remarkably similar optical properties.[18] However, it remains to be seen if an appropriate two-channel Kondo model can accurately describe the transport and optical properties of $dilute$ systems such as $Y_{1-x}U_xPd_3$.

$Note\ added\ in\ proof.$ Recently, we received an unpublished paper by Miranda $et\ al.$ (since published[20]) where scaling arguments are employed to calculate the Green's functions and magnetic dynamic susceptibility.

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[19] Strictly speaking, since $P_{wd}(T_K)$ has a weak divergence like $1/(T_K \ln^2 T_K)$ as $T_K \to 0$, the corresponding $Im\Sigma(\omega)$ also will contain a term like $\omega^\alpha$ with $\alpha < 1$. However, the prefactor of this term is proportional to the relative weight of this singularity, which for our choice of parameters is about $10^{-7}$. Hence, the term with the fractional power gets suppressed by the quadratic term for all experimentally accessible temperatures and frequencies.

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