Kondo Effect in Disordered Systems

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We consider a system of dilute magnetic impurities placed in a disordered metal, and examine the modifications of the Kondo temperature T_K due to the presence of disorder. Our calculations, based on a slave-boson approach, show that the probability distribution $P(T_K)$ for Kondo temperatures can be related to the local-density-of-states fluctuations induced by localization effects. The resulting $P(T_K)$ is shown to be sufficiently singular to induce diverging magnetic susceptibility χ as $T \to 0$, a non-Fermi-liquid behavior.

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From a general point of view, there are several reasons why the disordered Kondo problem can be expected to be of central importance to the physics of dirty metals. Experimentally, several classes of disordered metals have recently been found that display unusual non-Fermi-liquid features. In all these examples, ranging from doped semiconductors [1] to Kondo alloys [2] to high-T_c materials [3], local magnetic moments and disorder are simultaneously present. The resulting χ and γ are found to increase as the temperature is lowered, and no saturation is observed down to the lowest available temperatures. The Kondo temperature T_K, representing a crossover temperature to a Fermi-liquid behavior, thus appears to be considerably depressed, possibly even made to vanish.

In the context of metal-insulator transitions (MITs) [4], the Kondo problem is of considerable importance. In particular, at $T > T_K$, spin-flip scattering plays an important role, as it introduces a cutoff in the triplet (spin-diffusion) channel, and thus modifies the overall symmetry, i.e., the universality class of the localization problem [4]. On the other hand, for $0 < T < T_K$, Kondo screening effectively eliminates the local moment, and the spin-diffusion channel remains "massless," and contributes to localization. Therefore, not only the thermodynamics but also the transport properties near the MIT can be expected to be very sensitive to possible modifications of T_K in the presence of disorder.

In this Letter we address the question of how T_K will be modified by disorder by examining the single-impurity Kondo problem in the presence of a random distribution of nonmagnetic impurities. This problem has been previously addressed. Bhatt and Fisher [5] recently used Lifshitz-type reasoning to argue that there is a distribution of Kondo temperatures in a disordered system and that some of the local moments will not be Kondo screened even at the lowest temperatures. In earlier work, Okhawa, Fukuyama, Yosida [6] and Suga, Kasai, and Okiji [6] have used a high-temperature perturbation theory to examine the Kondo effect in weakly disordered systems. They found that the perturbation expansion was singular, and that the singularity was related to the moments of the local density of states. In our study, we will be particularly concerned with trying to identify possible *universal* mechanisms for T_K degradation. In this spirit, we will *ignore* the disorder-induced modification of the Kondo coupling J which is a local quantity, expected to be sensitive to the microscopic details of disorder, and thus strongly system dependent. This is the type of T_K degradation effect considered by Bhatt and Fisher [5].

By now, it is recognized that the low-temperature behavior of a Kondo spin is correctly described by the slave-boson mean-field-theory method [7]. In this technique, the spin-$\frac{1}{2}$ operator $\mathbf{S}$ is written in terms of fermion operators $\chi_s^\dagger$ and χ_s ($s = \uparrow, \downarrow$) as $\mathbf{S} = \frac{1}{2}\sum_{s,s'} \chi_s^\dagger \sigma_{ss'} \chi_{s'}$, with the additional constraint $n_\chi = \sum_s \chi_s^\dagger \chi_s = 1$. Using a functional integral representation, this constraint is enforced by introducing a Lagrange multiplier field $\lambda(\tau)$, and the Kondo interaction is decoupled by introducing an auxiliary field $s(\tau)$. A mean-field solution (which is formally exact in the large-N formulation of the problem) is then obtained by finding the saddle-point of the action in terms of the fields λ and s. The trivial saddle point ($s = 0$, $\lambda = 0$) is always present, but it becomes unstable at $T = T_K$, and a nontrivial solution appears, which corresponds to singlet binding of the local moment and a conduction electron.

This phase transition, which happens at $T = T_K$ in mean field theory, is washed out by fluctuations and turns into a smooth crossover, as established by more accurate RG computations [8]. Nevertheless, a mean-field calculation of T_K correctly predicts the temperature scale of this crossover, which at the same time represents the characteristic energy scale of the ground state.

In order to determine the T_K in the presence of disorder, we follow this procedure and examine the stability of the trivial solution. In the static approximation (mean-field theory), the fields are replaced by their saddle-point values s_0 and $-i\varepsilon_0$, and the action takes the form [7]

$$S = \sum_s \int_0^\beta d\tau \int d\mathbf{r}\, \bar{\psi}_s(\mathbf{r},\tau)\left[\frac{\partial}{\partial\tau} - \mu - \frac{1}{2}\nabla^2 + V(\mathbf{r})\right]\psi_s(\mathbf{r},\tau) + S_{\rm int} + \sum_s \int_0^\beta d\tau\, \bar{\chi}_s(\tau)\left[\frac{\partial}{\partial\tau} + \varepsilon_0 - \mu\right]\chi_s(\tau) - 2\beta\varepsilon_0$$
$$+ s_0 \sum_s \int_0^\beta d\tau\, [\bar{\psi}_s(\mathbf{R},\tau)\chi_s(\tau) + \bar{\chi}_s(\tau)\psi_s(\mathbf{R},\tau)] + \frac{2\beta}{J} s_0^2, \qquad (1)$$

where μ is the chemical potential, β is the inverse temperature, $V(\mathbf{r})$ is the random potential, and S_{int} represent the interactions among the band electrons.

The free energy of the system $F=-T\ln\int D\psi D\chi \times\exp\{-S\}$ can be expanded in powers of the effective hybridization parameter s_0. The Kondo temperature is obtained by identifying the emergence of the nontrivial ($s_0\neq 0$) solution of the saddle-point equation $\partial F/\partial s_0=0$. This occurs when the coefficient of s_0^2 vanishes. Using the definitions of free local moment and the band electron Green's functions, the implicit equation for T_K can be written as

$$\int_{-\infty}^{+\infty} d\varepsilon \frac{1}{\varepsilon} n_F(\varepsilon)\rho(\mathbf{R},\varepsilon) = -\frac{1}{J}, \tag{2}$$

where $n_F(\varepsilon)=\{1+\exp[(\varepsilon-\mu)/T]\}^{-1}$ is the Fermi function, and $\rho(\mathbf{R},\varepsilon)$ is the single-particle density of states (DOS) of the conduction electrons.

In deriving this result, we have considered interacting band electrons in the presence of a *fixed* realization of the random potential $V(\mathbf{r})$. Thus $\rho(\mathbf{R},\varepsilon)$ is a *fully renormalized* single-particle DOS of disordered interacting electrons evaluated for a given realization of the randomness. Note that $\rho(\mathbf{R},\varepsilon)$ is also a *local* DOS, and is consequently expected to be much more sensitive to disorder than its global counterpart $\rho_{\text{gl}}(\varepsilon)=(1/\Omega)\int d\mathbf{R}\,\rho(\mathbf{R},\varepsilon)$. Indeed, while $\rho_{\text{gl}}(\varepsilon)$ is self-averaging [9] in the thermodynamic limit $\Omega\to\infty$, the *local* DOS remains random since it actually measures the position-dependent electronic density, i.e., the wave-function amplitude fluctuations, viz. $\rho(\mathbf{R},\varepsilon)\sim|\psi_\varepsilon(\mathbf{R})|^2$.

In order to relate our results to the measurable quantities, an appropriate averaging over disorder (or equivalently over the positions of the Kondo spins) has to be performed. The simplest procedure would replace the local DOS $\rho(\mathbf{R},\varepsilon)$ by its average value which, at least for noninteracting electrons, would predict T_K to be unaffected by disorder. However, this approach is incorrect since, for sufficiently wide probability distributions, the *typical* behavior is largely unrelated to the average value which can be dominated by rare, statistically insignificant events. We will argue that this is precisely what is happening in our case, and the knowledge of the full *probability distribution* is necessary to correctly predict the experimentally measurable properties of the system.

The qualitative features of the probability distribution $P(\rho)$ (ρ stands for the *local* DOS) are easily obtained from the following simple physical picture. At weak disorder we expect small fluctuations, and the distribution is peaked around $\bar{\rho}=\rho_0$. In the opposite limit, in the insulator, we have localized (bound) states, and the spectrum consists of sharp, δ-function peaks. As the MIT is crossed, these peaks broaden by an amount which measures the tunneling between what at lower energy were the localized states. In the vicinity of the MIT, we thus expect $P(\rho)$ to have large weight at small values of ρ, and a long, but small-amplitude tail at ρ large.

These qualitative considerations are very nicely born out by detailed microscopic calculations based on a field-theoretical nonlinear σ-model approach, which determined *all* the cumulants of the local DOS in a one-loop RG calculation [10,11]. For weak disorder, the distribution was found to be a narrow Gaussian, but with long log-normal tails which nevertheless carry only a small relative weight. For sufficiently strong disorder, i.e., sufficiently close to the MIT, the *whole* distribution becomes log-normal,

$$P(\rho)=\frac{1}{\sqrt{4\pi u}}\frac{1}{\rho}\exp\left\{-\frac{1}{4u}\ln^2\left[\frac{\rho}{\rho_0}e^u\right]\right\}. \tag{3}$$

The result is valid in the region $u\geq 1$, where the parameter u is defined by $u=\int_{l/L}^{1}(d\lambda/\lambda)/g(\lambda)$. Here, $g(\lambda)$ is the scale-dependent dimensionless conductance, λ the momentum rescaling factor, l the mean free path, and L the Thouless length [4] (i.e., the effective size of the system). As the MIT is approached, $u\to\infty$, and most of the weight of $P(\rho)$ shifts to small ρ values, near the peak at $\rho_{\text{typ}}=\rho_0 e^{-u}$, rather than near the average value $\bar{\rho}=\rho_0$, which is not modified. Equation (3) has been obtained for noninteracting electrons, and is valid both in the presence and in the absence of time-reversal symmetry (orthogonal versus unitary ensemble). When the interactions are added, to one-loop order no further corrections are found [12] for any local DOS cumulants, except for the lowest one $\bar{\rho}$, which is reduced as mentioned above. Thus, to one-loop order, we can again use Eq. (2), by simply replacing ρ_0 with its interaction-renormalized value. We stress, however, that all our results are the consequences of the qualitative features of $P(\rho)$ as discussed in the previous paragraph. The log-normal form is useful for obtaining simple analytical expressions.

From the knowledge of $P(\rho)$, we can now obtain the desired *probability distribution* of Kondo temperatures. In a given sample, $\rho(\mathbf{R},\varepsilon)$ will be a random function not only of position $\mathbf{R}$ but also of energy ε. Since the integration in Eq. (2) is carried out over energies, this could reduce the fluctuations. However, the integral in question gets its dominant contribution from an energy interval of order $\Delta\varepsilon\sim T_K$ near the Fermi surface. The low-temperature properties of the system, such as χ and γ, will be dominated by precisely *those* Kondo sites with very low T_K. Using the fact that T_K is *exponentially* small in ρ, it is not hard to see [13] that at low temperatures, to leading order, the energy dependence of the DOS can be ignored. We thus replace $\rho(\mathbf{R},\varepsilon)\to\rho(\mathbf{R},0)\equiv\rho(\mathbf{R})$, the DOS at the Fermi surface (ε is everywhere measured with respect to the Fermi energy $\varepsilon_F=\mu$), and get $T_K(\mathbf{R})=\varepsilon_F\exp\{-1/\rho(\mathbf{R})J\}$. Furthermore, from $P(T_K)=(d\rho/dT_K)P(\rho(T_K))$, we find

$$P(T_K)=(4\pi u)^{-1/2}\frac{1}{T_K\ln(\varepsilon_F/T_K)}\exp\left\{-\frac{1}{4u}\ln^2[\rho_0 J e^{-u}\ln(\varepsilon_F/T_K)]\right\}. \tag{4}$$

Equation (4) is the central result of this Letter. The first thing that we note about this distribution is that $P(T_K)$ *diverges at* $T_K \to 0$, so we have a large number of spins with very low Kondo temperature. We can be more specific, and calculate the low-temperature form of χ and γ. For a given spin at site $\mathbf{R}$, its contribution to both χ and γ is $\sim 1/T$ for $T_K(\mathbf{R}) < T$, and so the dominant contribution at low T comes from the same sites. Thus we can write $\chi \sim (1/T) n_{\rm fr}(T)$ (and similarly for γ), where we have defined an *effective number of free spins* by $n_{\rm fr}(T) = \int_0^T dT_K P(T_K)$. Introducing the quantity $x_{\max} = -(1/\sqrt{4u}) \ln[\rho_0 J e^{-u} \ln(\varepsilon_F/T)]$, we can rewrite this as

$$n_{\rm fr}(T) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{x_{\max}(T)} dx\, e^{-x^2} = \tfrac{1}{2}\{1 + \mathrm{erf}[x_{\max}(T)]\}. \quad (5)$$

At low temperatures $n_{\rm fr}(T) \sim T^{\alpha(T)}$, with $\alpha(T) \to 0$ as $T \to 0$, i.e., it vanishes, but slower than any power. We conclude that χ and γ *diverge* as $T \to 0$—a strongly non-Fermi-liquid behavior.

It is interesting to estimate the *size* of this anomaly for some typical values of the parameters. By using a Fermi energy of $\varepsilon_F \sim 10^4$ K, a bare Kondo temperature of $T_K^0 \sim 10^2$ K, and working in the strongly disordered (but still metallic) region $u \sim 1$, we obtain $n_{\rm fr}(T) \sim (40\text{–}60)\%$ at temperatures $T \sim 10^{-4}$–1 K. We note the extremely slow temperature dependence, resulting from the $\ln\ln T$ dependence of $x_{\max}(T)$.

We thus find a strikingly *large* fraction, of the order of 50% of pseudo-free spins at temperatures by orders of magnitude lower than the bare Kondo temperature T_K^0. Our results are valid only in the region $u \geq 1$, i.e., in the strongly disordered region. For weak disorder, $P(\rho)$ still has the long, log-normal tails leading to the divergence of χ and γ. However, the size of this effect is expected to be extremely small, so for weak disorder the anomalies become important only at physically unattainable temperatures. In fact, for finite systems and weak disorder, there will exist a minimum Kondo temperature $T_{K_{\min}}$ of the order of the T_K^0 below which Fermi-liquid behavior will occur. On the other hand, the region of strong disorder $u \geq 1$, where our results apply, is not restricted to the infinitesimal vicinity of the MIT; for example, in the orthogonal case, $u = \ln(\sigma_0/\sigma)$, and so $u \sim 1$ corresponds to the conductivity being $\sim 60\%$ of its bare value σ_0. Thus, our effect is expected to be observable in sufficiently dirty, but still metallic samples.

The interaction corrections enhance the anomalies even further, by reducing $\bar{\rho}$. As the MIT is approached, $\bar{\rho}$ vanishes [4] as a power law $\bar{\rho} \sim \rho_0 e^{-\delta u}$ ($u \to \infty$ at the MIT), characterized by an exponent $\delta \sim 1$. If these interaction corrections are incorporated, only a small quantitative change (increase) is obtained as compared to the noninteracting case.

It is interesting to examine also the critical behavior of $n_{\rm fr}(T)$ as the MIT is approached. To examine this, let us vary the parameter u (disorder) and fix T. Since $x_{\max}(T) \sim \frac{1}{2}\sqrt{u}$ at $u \gg 1$, we conclude that $n_{\rm fr}(T) \to 1$ as $u \to \infty$. Of course, the MIT is a zero-temperature transition, so $u \to \infty$ only as $T \to 0$. To examine the true $T \to 0$ limit, we imagine that we are exactly *at* the MIT, but at finite temperature T. In this case, e^{-u} vanishes as a power of the temperature. Using this form in Eq. (5), and letting $T \to 0$, we confirm that $n_{\rm fr}(T) \to 1$ at the MIT. We thus conclude that *all* the Kondo spins become effectively free as the MIT is approached.

So far we have examined the effect of disordered conduction electrons on the local moments. Another important question concerns the feedback effect of these local moments on the transport properties of the conduction electrons. In particular the moments with $T_K(\mathbf{R}) < T$ will contribute to spin-flip scattering and will thus induce a "mass" (cutoff) in the spin-diffusion (triplet) channel [4]. The simplest estimate of this effect would give the corresponding scattering time $1/\tau_s \sim n_{\rm fr}(T)$, which, at strong disorder, is a large fraction of the spins, yielding strong spin-flip scattering near the MIT, even at low temperatures.

Such an estimate, however, ignores the fact that those very sites with $T_K(\mathbf{R})$ low correspond to having also low $\rho(\mathbf{R}) \sim |\psi(\mathbf{R})|^2$, i.e., low conduction electron density, an effect that would reduce the spin-flip scattering. To be slightly more specific, at the level of the Born approximation (for local-moment–electron scattering), the scattering rate for a given site is proportional to the local DOS $\rho(\mathbf{R})$. By adding the contribution from all the sites with $T_K < T$, taking into account the DOS dependence leads us to define an effective number (fraction) of spins that induce spin-flip scattering of the band electrons by $n_{\rm sc}(T) = (1/\rho_0)\int_0^T dT_K \rho(T_K) P(T_K)$. The integral can be evaluated as before, and we find $n_{\rm sc}(T) = \frac{1}{2}\{1 + \mathrm{erf}[x_{\max}(T) - \sqrt{u}]\}$.

It is particularly interesting to examine the behavior of $n_{\rm sc}(T)$ as the MIT is approached. Since $x_{\max} \approx \frac{1}{2}\sqrt{u}$ at $u \gg 1$, the argument of the error function is $\approx -\frac{1}{2}\sqrt{u} \to -\infty$ as $u \to +\infty$. Thus we find that $n_{\rm sc}(T) \to 0$ at the MIT. The local moments seem to decouple from the conduction electrons, as in the phenomenological "two-fluid model" of Si:P of Paalanen *et al.* [14]. More specifically, by using an asymptotic expansion of the error function, we find that the triplet "mass" $M_t \sim 1/\tau_s$ vanishes as a power of the distance from the critical point. The validity of our estimate of $1/\tau_s$ should be confirmed by more detailed calculations. More importantly, our simple calculations indicate a new scenario for the MIT: The mass (cutoff) M_t which acts as a symmetry-breaking field vanishes as the MIT is approached. This may modify the critical behavior of the conductivity.

In summary, in this paper, we have examined the behavior of magnetic impurities in disordered electronic systems. The modifications of the Kondo temperature were

evaluated as a result of localization and interaction effects. Our calculations show that the probability distribution for Kondo temperatures is so singular that it can induce divergences for both the linear specific heat $\gamma = c/T$ and the magnetic susceptibility χ as $T \to 0$, even *inside* the metallic phase. Such non-Fermi-liquid behavior is not present in the absence of randomness and results directly from disorder-induced fluctuations of the electronic system. Since the localization and interaction effects that we have considered describe the *long-wavelength* (hydrodynamic) fluctuations, we expect them to be the dominant mechanisms in the vicinity of the MIT.

In this study several potentially important aspects of dirty metals have been omitted. We have assumed the existence of local moments in the metal. There is some evidence that disorder itself can play an important role in their formation [15]. Second, we have not examined the effects of the interactions of local moments. In the presence of short-ranged interactions, based on the results of Bhatt and Lee [16], we expect the power-law singularities of χ and γ to persist, although the exponents could be modified. Bhatt and Fisher [5] have given arguments suggesting that the long-ranged RKKY interactions could change the power-law singularity discussed here to a weaker logarithmic singularity. However, even if these arguments are correct, the importance of the RKKY interactions will be diminished as the MIT is approached, since their long-range nature stems directly from the electronic wave functions being extended in the metallic phase [17].

In any case, finding a universal mechanism for T_K degradation although perhaps not sufficient is certainly a necessary requirement for any general theory that attempts to explain the non-Fermi-liquid features observed in a number of dirty metals.

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