Kondo Breakdown and Hybridization Fluctuations in the Kondo-Heisenberg Lattice

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We study the deconfined quantum critical point of the Kondo-Heisenberg lattice in three dimensions using a fermionic representation for the localized spins. The mean-field phase diagram exhibits a zero temperature quantum critical point separating a spin liquid phase where the hybridization vanishes and a Kondo phase where it does not. Two solutions can be stabilized in the Kondo phase: namely, a uniform hybridization when the band masses of the conduction electrons and the spinons have the same sign, and a modulated one when they have opposite sign. For the uniform case, we show that above a very small temperature scale, the critical fluctuations associated with the vanishing hybridization have dynamical exponent $z = 3$, giving rise to a resistivity that has a $T \log T$ behavior. We also find that the specific heat coefficient diverges logarithmically in temperature, as observed in a number of heavy fermion metals.

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A large number of experiments have been performed on metallic heavy fermion compounds close to a zero temperature phase transition [a quantum critical point (QCP)] driven by an applied magnetic field, chemical doping, or pressure [1]. In the quantum critical regime, the thermodynamics and transport properties are very unusual, violating the predictions of the Landau Fermi liquid theory of metals. The resistivity is quasilinear in temperature over several decades, and in many cases the specific heat coefficient diverges logarithmically as the temperature is decreased. These unusual observations have motivated many theoretical studies that have attempted to capture these effects. Most theories [2–5] are based on the assumption that at the QCP, the Fermi liquid is destabilized by spin density wave formation, and therefore the critical fluctuations are magnetic in nature. In $d = 3$, these theories fail to capture simultaneously the linear temperature dependence of the resistivity and the divergence of the specific heat coefficient at low temperatures [6]. More recently the problem has been approached from another perspective which takes the point of view that at the QCP, magnetic fluctuations suppress the formation of the heavy Fermi liquid, driving the effective Kondo temperature of the lattice (T_K) to zero [6–9]. In this picture, the QCP is a bicritical point where the metal experiences fluctuations due to the vanishing energy scale T_K as well as the paramagnons. One feature that distinguishes between these two classes of theories is that the first predicts the Fermi volume to change smoothly across the QCP, while the second predicts an abrupt change [6].

In this Letter we explore the possibility that in the quantum critical regime, the unusual behavior in thermodynamics and transport is due to critical fluctuations, but of a nonmagnetic order parameter associated with the vanishing energy scale T_K, and not due to paramagnons. The order parameter we advocate is the field σ associated with the hybridization between the localized spins and the conduction electrons [10,11]. At the QCP, the effective Kondo temperature for the lattice goes to zero, leading to a "Kondo breakdown" of the heavy Fermi liquid. The critical fluctuations of σ are gapless excitations, and we study how these fluctuations influence the properties of the metal using the formalism of the large N Kondo-Heisenberg model.

Beyond the mean-field level, the Kondo-Heisenberg model can be treated as a lattice gauge theory. Senthil *et al.* [8] have examined the effect of the gauge fluctuations in this model, while Coleman *et al.* [9] studied the zero temperature transport anomalies. In our Letter, we find a number of novel effects associated with the fluctuations of the σ field which were not discovered in these earlier studies.

At the Kondo breakdown QCP where $\langle\sigma\rangle = 0$, we observe two new phenomena: (1) σ can order at a finite wave vector leading to spatial modulations of the Kondo hybridization analogous to the Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) state of superconductivity [12]; (2) the presence of multiple energy scales, spread over a very large range in energy. The lowest scale is extremely small (of order 1 mK), above which, up to an ultraviolet cutoff of order the single ion Kondo temperature, the critical fluctuations of σ exhibit a dynamical exponent $z = 3$. This gives rise to a marginal Fermi liquid–like behavior for the conduction electrons in $d = 3$, with a resistivity that goes as $T \log T$. A logarithmic dependence is also found for the specific heat coefficient from both the gauge and σ fluctuations.

Our starting point is the large N formulation of the Kondo-Heisenberg model, where N denotes the enlarged spin symmetry group $SU(N)$. It describes a broad band of conduction electrons interacting with localized spins through antiferromagnetic Kondo coupling $J_K > 0$. The localized spins interact with each other via nearest neighbor exchange $J_H > 0$. We work with a representation of the localized spins in terms of Abrikosov pseudofermions $\vec{S}_i = \sum_{\alpha\beta} f^{\dagger}_{i,\alpha} \vec{\sigma}_{\alpha\beta} f_{i,\beta}$, where $(\alpha, \beta) = (1, N)$, with the constraint of $n_f = N/2$ spinons per site i. The interactions which are quartic fermionic terms can be decoupled using Hubbard-Stratonovich fields $\varphi_{ij} \to \sum_\alpha f^\dagger_{i\alpha} f_{j\alpha}$ for the Heisenberg exchange, and $\sigma^\dagger_i \to \sum_\alpha f^\dagger_{i\alpha} c_{i\alpha}$ for the Kondo interaction. Following Ref. [8] we assume that in $d = 3$, φ condenses in a uniform spin liquid phase that gives dispersion to the spinons, which is an essential ingredient for Kondo breakdown to occur (physically we interpret the uniform spin liquid as a mean-field description of the short range magnetic correlations that persist when a magnetic ground state is destroyed by quantum fluctuations). This gives the Lagrangian

$$\mathcal{L} = \sum_{\langle ij\rangle\alpha} [c^\dagger_{i\alpha}(\partial_\tau + t_{ij})c_{j\alpha} + f^\dagger_{i\alpha}(\partial_\tau + \varphi_0 e^{ia_{ij}} + \lambda_i \delta_{ij}) f_{j\alpha}] - \frac{N}{2}\sum_i \lambda_i + \frac{N}{J_K}\sum_i \sigma^\dagger_i \sigma_i + \frac{N\varphi_o^2}{J_H} + \sum_{i\alpha}(c^\dagger_{i\alpha} f_{i\alpha}\sigma_i + \text{H.c.}) \tag{1}$$

(V, the volume of the system, is set to 1). The above Lagrangian has a local $U(1)$ gauge invariance [13]. The Lagrange multiplier λ_i (scalar potential) enforces the constraint $n_f = N/2$ per site. Given a state which satisfies the above constraint, a single hop of a spinon will violate it. Consequently, only simultaneous opposite hops of spinons between two neighboring sites are physically allowed. This implies that the local spinon current operator $J_{fi} = 0$ at each site. The gauge fields a_{ij} (vector potential) associated with the phase of φ_{ij} ensure that this condition is satisfied.

There are two important parameters in Eq. (1). First, $\alpha = \varphi_0/D$, which is the ratio of the spinon to the conduction electron bandwidth D [note from Eq. (1) that for $\sigma = 0$, $\phi_0 = J_H$]. Second, while the spinon band is half-filled due to the constraint (henceforth we assume $N = 2$), the conduction band filling is generic. Without any loss of generality we take the conduction band to be less than half-filled. This implies that the Fermi wave vector of the spinon band k_{F0} is different from that of the conduction band k_F. We denote the mismatch by $q^* = k_{F0} - k_F$. In the following we take α and (q^*/k_F) to be small. We identify αD with the single ion Kondo scale ($T_K^0 = De^{-1/\rho_0 J_K}$) which is typically 10 K in heavy fermions. Assuming $D \sim 10^4$ K, we get $\alpha \sim 10^{-3}$.

At the mean-field level, the parameters φ_0, $\langle\lambda_i\rangle$ and $\langle\sigma_i\rangle$ are determined by minimizing the free energy F. The mean-field phase transition between the spin liquid state $\langle\sigma_i\rangle = 0$ and the heavy Fermi liquid state with a lattice Kondo temperature $T_K \approx \pi\rho_0\langle\sigma_i\rangle^2$ occurs when

$$\frac{\partial^2 F}{\partial|\sigma_q|^2} = \frac{1}{J_K} + \Pi_{\text{fc}}(q, 0) = 0, \tag{2}$$

where $\Pi_{\text{fc}}(q, 0)$ is the static electron-spinon (fc) polarization. We solve this equation for two different situations, the result of which is depicted in Fig. 1. (i) *e-e* case, where both the bands are taken to be electronlike. Linearizing the fermionic dispersions we have $\epsilon_k = v_F(k - k_F)$ for the conduction electrons, and $\epsilon^0_k = \alpha v_F(k - k_F - q^*)$ for the spinons (where $k = |\mathbf{k}|$). For linearized dispersions, $\Pi_{\text{fc}}(q, 0)$ turns out to be q independent. Inclusion of the curvature stabilizes a second order phase transition around $q = 0$, the polarization taking the form $\Pi_{\text{fc}}(q, 0) = \frac{\rho_0}{1-\alpha} \times (\ln\alpha + \frac{1-\alpha^2+2\alpha\ln\alpha}{4(1-\alpha)^2}\frac{q^2}{k_F^2})$, where $\rho_0 = 1/D$ is the conduction electron density of states at the Fermi energy. In this case the $T = 0$ phase transition occurs at a critical Kondo coupling of $J_K^c = 1/[\rho_0 \ln(1/\rho_0 J_H)]$ [14]. (ii) *e-h* case, where the conduction band is taken to be electronlike as before, while the spinon band is holelike with a linearized dispersion $\epsilon^0_k = -\alpha v_F(k - k_F - q^*)$. In this case we find $\Pi_{\text{fc}}(q, 0) = \frac{\rho_0}{1+\alpha}(\ln\frac{\alpha v_F^2|q^{*2} - q^2|}{D^2(1+\alpha)^2} - 2 + \frac{q^*}{q}\ln\frac{q^*+q}{|q^*-q|})$, which has a minimum at $q = 1.2q^*$ independent of α. In this state T_K is modulated, with nodes in space where T_K vanishes. This solution is similar to the spin density wave instability encountered in chromium [15] and in the LOFF state of superconductivity [12,16]. Figure 1(a) shows that for parabolic bands the minimum of the effective potential is lower in the *e-h* case than in the *e-e* case. Thus, for parabolic bands, the modulated solution is more stable [Fig. 1(b)]. However, the question of which solution is realized in real compounds will be material dependent.

We now turn to the fluctuations around the mean-field solution. We present our results for the simpler *e-e* case, leaving the more complex *e-h* case for a later paper. In the quantum critical regime there are two important types of gapless fluctuations, namely, the gauge fluctuations associated with a_{ij} and the critical fluctuations of the Kondo bosons σ.

The gauge fluctuations of this theory have been studied earlier by Senthil *et al.* [8]. Here we summarize the salient points to put our work in perspective. It is convenient to work in the Coulomb gauge $\vec{\nabla}\cdot\vec{a} = 0$, where the vector gauge fields a_μ ($\mu = x, y, z$) are purely transverse [13]. The fluctuations of λ decouple from those of a_μ, and give rise to a screened Coulomb interaction. As such, they are massive and can be neglected. The gauge fields

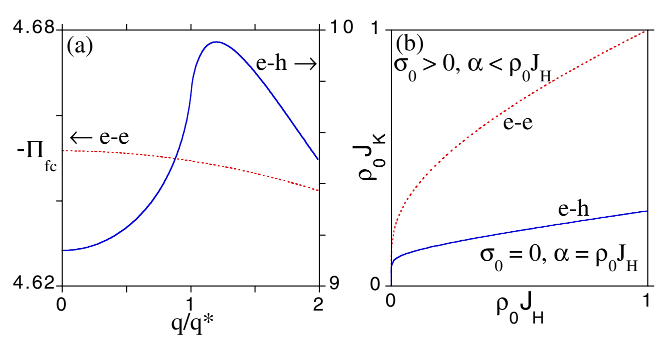

FIG. 1 (color online). (a) q dependence of Π_{fc} ($\alpha = 0.01$ and $q^*/k_F = 0.1$). Note differing scales for the *e-e* and *e-h* cases. (b) Quantum critical point as a function of J_K and J_H for the *e-e* ($q = 0$) and *e-h* ($q = 1.2q^*$) cases.

a_μ, which act as vectorial Lagrange multipliers to ensure that the local spinon current $J_{fi} = 0$, do not have any intrinsic dynamics of their own. Their dynamics is generated via coupling with the spinon band, and therefore they are overdamped. For frequencies smaller than the spinon bandwidth αD, the transverse gauge field propagator $D_{\mu\nu}(\mathbf{x}, \tau) = \langle T_\tau[a_\mu(\mathbf{x}, \tau)a_\nu(0, 0)]\rangle$ has the standard form $D_{\mu\nu}(q, i\Omega_n) = (\delta_{\mu\nu} - q_\mu q_\nu/q^2)\Pi^{-1}(q, i\Omega_n)$, with $\Pi(q, i\Omega_n) \propto [(q/2k_{F0})^2 + |\Omega_n|/(\alpha v_F q)]$. This is the typical form for excitations with dynamical exponent $z = 3$, which in $d = 3$ are known [17] to give a contribution to the specific heat coefficient $\gamma \equiv -\partial^2 F/\partial T^2 \propto \ln(\alpha D/T)$ and to the static spin susceptibility $\delta\chi_s \propto T^2 \ln(\alpha D/T)$. Finally, when the compact nature of the $U(1)$ gauge group on the lattice is taken into account, the gauge fluctuations convert the finite temperature mean-field transition line into a crossover line [8,18].

In the quantum critical regime, the fluctuations of the complex order parameter fields $(\sigma_i^\dagger, \sigma_i)$ are massless as well (ignoring for the moment the T-dependent mass generated by the quartic $|\sigma|^4$ coupling). The propagator for these fluctuations is defined as $D_\sigma(x, \tau) = \langle T_\tau[\sigma^\dagger(x, \tau)\sigma(0, 0)]\rangle$ with $D_\sigma^{-1}(q, i\Omega_n) = 1/J_K + \Pi_{\rm fc}(q, 0) + \Delta\Pi_{\rm fc}(q, i\Omega_n)$ where

$$\Delta\Pi_{\rm fc}(q, i\Omega_n) = \sum_{\pm} \frac{\rho_0[\mp X_{1\pm}\ln(X_{1\pm}) \pm X_{2\pm}\ln(X_{2\pm})]}{2\alpha v_F q(1-\alpha)} \qquad (3)$$

with $X_{1\pm} = -\alpha i\Omega_n \pm \alpha v_F q - \alpha v_F q^*$, $X_{2\pm} = -i\Omega_n \pm \alpha v_F q - \alpha v_F q^*$, and $\Pi_{\rm fc}(0, 0) = \rho_0 \ln(\alpha)/(1 - \alpha)$ ($\Delta\Pi_{\rm fc}$ is the dynamical part of the fc polarization). The different regimes of $D_\sigma(q, i\Omega_n)$ with their associated dynamical exponents z are summarized in Fig. 2(a). At high energies, one finds $z = \infty$ behavior consistent with quasilocal behavior. But we find physical properties are dominated by the $z = 3$ and $z = 2$ regimes. These two regimes can be understood as follows. Because of the mismatch between the two Fermi surfaces, a minimum momentum is necessary to excite interband (fc) particle-hole pairs. As a result for $\Omega < \alpha v_F(q^* - q)$, excitations of σ do not decay into particle-hole pairs but propagate ballistically with $D_\sigma^{-1}(q, i\Omega_n) \approx \rho_0[q^2/(4k_F^2) - i\Omega_n/E_X]$, i.e., $z = 2$ (where $E_X = \alpha v_F q^*$). This behavior is cut off for frequencies $\Omega > E^*$ with

$$E^* = c\alpha D(q^*/k_F)^3 \quad \text{and} \quad c \sim 10^{-1}, \qquad (4)$$

above which the dynamical exponent z changes from 2 to 3. For most of the phase space, the spectrum for the fluctuations of σ lie within the interband particle-hole continuum, making their dynamics overdamped with $D_\sigma^{-1}(q, i\Omega_n) \approx \rho_0[q^2/(4k_F^2) + \pi|\Omega_n|/(2\alpha v_F q)]$, i.e., $z = 3$. The energy scale in the $z = 3$ regime is $\Gamma_q/E_X \approx q^3/(2\pi k_F^2 q^*)$ which has an infrared cutoff at E^* because of the mismatch vector q^*. The ultraviolet cutoff scale for the $z = 3$ regime is $\alpha v_F(q + q^*)$ which is of order αD for $q \sim k_F$. The energies E^* (infrared) and αD (ultraviolet) appear as crossover scales for any physical property that is affected by the excitations of σ. For a one impurity Kondo scale $\alpha D \sim 10$ K, and $q^*/k_F \sim 10^{-1}$ [19], we estimate $E^* \sim 1$ mK. E^* is therefore a very small energy scale which is essentially unobservable.

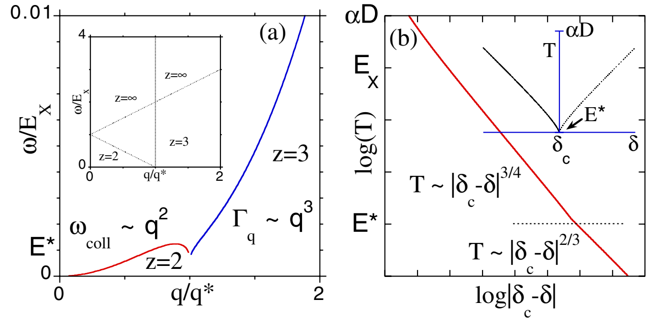

FIG. 2 (color online). (a) Structure of D_σ for the *e-e* case ($\alpha \ll 1$) at the QCP for positive frequencies. z is the dynamical exponent in the various regions, which are delineated by the dashed lines, equal to $\alpha v_F(q^* \pm q)$ and $v_F(q^* \pm q)$. $\omega_{\rm coll}$ is the zero of D_σ^{-1} in the $z = 2$ regime (a propagating mode), and Γ_q is the dispersion of the damped mode in the $z = 3$ regime (maximum of the imaginary part of D_σ). Note the presence of energy scales $E^* \sim 10^{-4}\alpha D$ and $E_X = \alpha v_F q^* \sim 10^{-1}\alpha D$. (b) Phase diagram for the *e-e* case ($\alpha \ll 1$). Note the crossover from $z = 2$ to $z = 3$ behavior at E^* (dotted line). The inset shows the phase diagram on a linear scale. The solid line is the crossover line in the Kondo phase, the dashed line the crossover line in the spin liquid phase.

The crossover lines in T that define the quantum critical region are symmetric around the QCP $\delta = \delta_c$, where $\delta = 1/(\rho_0 J_K)$ [Fig. 2(b)]. These are determined by the T-dependent mass generated by the quartic $|\sigma|^4$ coupling. For $T < E^*$, we find that the leading contribution is from the $z = 2$ regime (proportional to $T^{3/2}$ for $d = 3$), so that the crossover temperature $T \propto |\delta - \delta_c|^{2/3}$, while for $T > E^*$ the $z = 3$ regime dominates giving a crossover temperature $T \propto |\delta - \delta_c|^{3/4}$ for $d = 3$.

Next we examine the contribution to the free energy from the fluctuations of σ. We find that the leading contribution is entirely due to the $z = 3$ regime since it comes from a much larger phase space volume (the $z = 2$ contribution is similar to that of a gapless magnon mode). For $E^* < T < \alpha D$, we find $F(T) \sim \int n_B {\rm Im} \ln(D_\sigma^{-1}) \sim -k_F^3 T^2/(9\alpha D)\ln(\alpha D/T)$, which is a typical result for $z = 3$ excitations. This implies a contribution to the specific heat coefficient $\gamma \sim 2k_F^3/(9\alpha D)\ln(\alpha D/T)$, which adds to a similar contribution from the transverse gauge fluctuations. For $T < E^*$, the infrared cutoff sets in, and the specific heat coefficient from the σ fluctuations saturates. This regime is then dominated by the logarithmic contribution from the transverse gauge fields [17].

We now calculate the self-energy of the conduction electrons due to the hybridization fluctuations ($c \rightleftharpoons f + \sigma$). This is defined as $\Sigma_c(k, i\omega_n) = T\sum_{\omega_n, q} G_f(k + q, i\omega_n + i\Omega_n)D_\sigma(q, i\Omega_n)$, where $G_f^{-1}(k, i\omega_n) = (i\omega_n - \epsilon_k^0)$ is the inverse propagator of the spinons. As in the case of the free energy, we find that the leading contribution is due to the $z = 3$ regime of $D_\sigma(q, i\Omega_n)$. At $T = 0$ and for $E^* < \omega < \alpha D$, we find $\mathrm{Im}\Sigma_c(k_F, \omega) \sim k_F^2/(6\pi\alpha v_F \rho_0)\omega$. The temperature dependence of $\mathrm{Im}\Sigma_c(k_F, \omega = 0, T)$ involves a frequency integral weighted by the factor $n_B + n_F = 1/\sinh(\Omega/T)$. This makes the integral logarithmically divergent in the infrared, which is cut off by E^*. For $E^* < T < \alpha D$ we find

$$\mathrm{Im}\,\Sigma_c(k_F, \omega = 0, T) \sim k_F^2/(6\pi\alpha v_F \rho_0) T \ln(2T/E^*). \quad (5)$$

For $\omega, T < E^*$, the self-energy is Fermi liquid–like.

We turn to the T dependence of the static spin susceptibility $\chi_s(T)$. At the mean-field level, we find what is usual for band fermions, namely, a constant part plus a T^2 term. To calculate the correction beyond mean field ($\delta\chi_s$) due to the Kondo bosons, we note that in a magnetic field B, there is an additional $[B/(\alpha D)]^2$ contribution to $D_\sigma^{-1}(q, i\Omega_n)$. This gives $\delta\chi_s(T) \propto T^{4/3}$ for $E^* < T < \alpha D$, and a T^2 dependence below E^* [so below E^* the $T^2 \ln(T)$ contribution due to the gauge bosons dominates].

Finally we discuss the temperature dependence of the resistivity, ρ, that is obtained in the quantum critical regime. Equation (5) gives the T dependence of the inverse lifetime $\tau_c^{-1} \propto \mathrm{Im}\Sigma_c(T)$ of the conduction electrons. For one band models experiencing $q \simeq 0$ scattering, this lifetime cannot be associated with the transport lifetime, τ_{tr}, because the leading contribution to the self-energy comes from forward scattering processes which are not effective in relaxing the current. Consequently, when vertex corrections are taken into account, τ_{tr}^{-1} acquires an additional temperature dependence proportional to $q^2 \sim T^{2/z}$. However, our model consists of two bands, one of light particles (the conduction electrons) which scatter from very heavy particles (the spinons) [20]. As such, the charge neutral spinons act as an effective bath for the relaxation of the conduction electron current (the other charge carrying modes, the complex σ bosons, have overdamped dynamics, and therefore the current is mostly carried by the conduction electrons). The first nonzero vertex correction involves two σ boson exchange processes. Such a correction is small by a factor of α. Therefore τ_{tr} can be identified with τ_c, and for $E^* < T < \alpha D$ we find

$$\delta\rho(T) \equiv \rho(T) - \rho(0) \propto T \ln(2T/E^*). \quad (6)$$

For $T < E^*$, $\delta\rho(T) \propto T^2$, but E^* is extremely small (~1 mK). Thus, the Kondo-Heisenberg model captures one of the most mysterious features of quantum criticality in heavy fermion compounds, namely, the quasilinear resistivity observed for most compounds over a large temperature range.

In conclusion, we studied the Kondo breakdown QCP of the Kondo-Heisenberg model in $d = 3$. Over a large temperature range, we find that the critical fluctuations have a dynamical exponent $z = 3$, giving rise to marginal Fermi liquid behavior for the conduction electrons. The specific heat coefficient has a $\log(1/T)$ dependence, while the resistivity has a $T \log T$ behavior. The Kondo-Heisenberg model is characterized by multiple energy scales, and as such shows great promise in explaining the various subtleties associated with heavy fermion quantum critical behavior.

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