PSEUDOGAP EFFECTS IN HEAVY FERMIONS CLOSE TO A QUANTUM PHASE TRANSITION

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Neutron-scattering experiments on heavy fermions close to a magnetic quantum critical point are suggestive of an anomalous local dynamical spin susceptibility. The possibility that this anomaly arises due to a single-particle pseudogap is explored through a study of the Kondo model with a power-law density of states, a problem which exhibits a zero-temperature phase transition at a finite Kondo coupling. The critical properties at the transition are sensitive to particle-hole (a)symmetry, but in all cases are consistent with a simple scaling form for the free energy. The local spin susceptibility at the critical coupling exhibits an anomalous temperature exponent which varies continuously with the power of the pseudogap.

A number of heavy-fermion metals exhibit non-Fermi-liquid behaviors near a zero-temperature ($T=0$) magnetic ordering transition. [1] Neutron-scattering experiments on one such system, $CeCu_{6-x}Au_x$, highlight an unusual energy dependence of the spin susceptibility [2,3] which extends over a wide range of momenta, suggesting that the *local* susceptibility is anomalous, [3] contrary to the predictions of spin-fluctuation theory. [4] We show here that an anomalous local susceptibility can arise from a pseudogap in the single-particle spectrum. A pseudogap might be generated in quantum-critical systems by superconducting fluctuations, e.g., in $CePd_2Si_2$ and $CeIn_3$, [5] or by some other mechanism. [6]

We study a variant of the Kondo Hamiltonian for a single spin-$\frac{1}{2}$ impurity,

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} + H\tau^z_{\sigma\sigma})\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + (H+h)\, S^z + \sum_{\sigma\sigma'} c^\dagger_{0\sigma} \left(\frac{J_0}{2} \vec{S}\cdot\vec{\tau}_{\sigma\sigma'} + V_0 \delta_{\sigma\sigma'} \right) c_{0\sigma'}. \tag{1}$$

Here $\tau^i_{\sigma\sigma'}$ is a Pauli matrix, H is the uniform magnetic field, [7] h is a local field coupling only to the impurity spin $\vec{S}$, $c^\dagger_{0\sigma}$ creates a spin-σ electron at the impurity site, $J_0 > 0$ is the (antiferromagnetic) Kondo coupling, and V_0 characterizes the potential scattering from the impurity. The conduction-band dispersion $\epsilon_{\mathbf{k}}$ is assumed to give rise to the pseudogapped density of states [8,9]

$$\rho(\epsilon) = \rho_0 |\epsilon|^r, \quad |\epsilon| \le 1, \quad \text{and} \quad \rho(\epsilon) = 0, \quad |\epsilon| > 1. \tag{2}$$

In a metal ($r = 0$), any $J_0 > 0$ leads to quenching of the impurity moment at sufficiently low temperatures.[10] With a pseudogap ($r > 0$), however, quenching occurs[8] only if $J_0 > J_c(V_0, r)$. Depending on the value of r, this threshold behavior is associated with either one or two fixed points.[11] For $r \lesssim 0.375$, potential scattering is irrelevant, and there exists a single, particle-hole-symmetric fixed point at $V_0 = 0$, $J_0 = J_c(0, r)$. For $r \gtrsim 0.375$, potential scattering is relevant, and a particle-hole-asymmetric fixed point exists at $V_0 = V_c(r)$, $J_0 = J_c(V_c, r)$. Over the range $0.375 \lesssim r < \frac{1}{2}$, the symmetric fixed point remains accessible for zero bare potential scattering; whereas for $r \geq \frac{1}{2}$, $J_c(0, r) = \infty$, i.e., Kondo quenching of the impurity is completely suppressed.

Comparison of the impurity susceptibility $\chi_{\rm imp} = -\partial^2 F_{\rm imp}/\partial H^2|_{H=h=0}$ and the local susceptibility $\chi_{\rm loc} = -\partial^2 F_{\rm imp}/\partial h^2|_{H=h=0}$, where $F_{\rm imp}$ is the impurity free energy obtained from Eq. (1), provides key insight into the nature of the $T = 0$ phase transition. Numerical renormalization-group (NRG) results[12,11] for $r > 0$ indicate that $\lim_{T\to 0} T\chi_{\rm imp}$ is nonzero for all values of J_0; whereas $\lim_{T\to 0} T\chi_{\rm loc}$ goes continuously to zero as J_c is approached from below and $\lim_{T\to 0} T\chi_{\rm loc} = 0$ for all $J_0 > J_c$.

The behaviors of $\chi_{\rm imp}$ and $\chi_{\rm loc} = 0$ suggest that the $T = 0$ phase transition is continuous, and that the free energy should contain a singular component

$$F_{\rm sing} = T f\left(|J_0 - J_c|/T^a,\ |h|/T^b\right). \tag{3}$$

Note that $F_{\rm sing}$ scales with the local field h, rather than its uniform counterpart H, and that f, a, or b may well be different for $V_0 = 0$ and $V_0 \neq 0$.

Alternatively, one can characterize the critical behavior by a set of exponents β, γ, δ, and x, defined as follows:

$$\begin{aligned} M_{\rm loc}(J_0 < J_c, T = h = 0) &\propto (J_c - J_0)^{\beta}, \quad M_{\rm loc}(J_0 = J_c, T = 0) \propto |h|^{1/\delta}, \\ \chi_{\rm loc}(J_0 > J_c, T = 0) &\propto (J_0 - J_c)^{-\gamma}, \quad \chi_{\rm loc}(J_0 = J_c) \propto T^{-x}. \end{aligned} \tag{4}$$

Here $M_{\rm loc}(h{=}0) = -\partial F_{\rm sing}/\partial h|_{h=0}$ acts as the order parameter for the transition and $\chi_{\rm loc} = -\partial^2 F_{\rm sing}/\partial h^2|_{h=0}$ is the order-parameter susceptibility. Equation (3) implies a pair of scaling relations among the critical exponents, e.g.,

$$\beta = \gamma(1 - x)/(2x), \quad \delta = (1 + x)/(1 - x). \tag{5}$$

Recently we reported[13] critical exponents obtained at particle-hole symmetry, both for the model described in Eq. (1) and for its SU(N) generalization with $N \gg 1$. Here we present side-by-side the exponents at the symmetric and asymmetric critical points of the spin-$\frac{1}{2}$ problem [i.e., for $V_0 = 0$ and $V_0 = V_c(r)$], calculated using NRG methods described in Refs. 10 and 12.

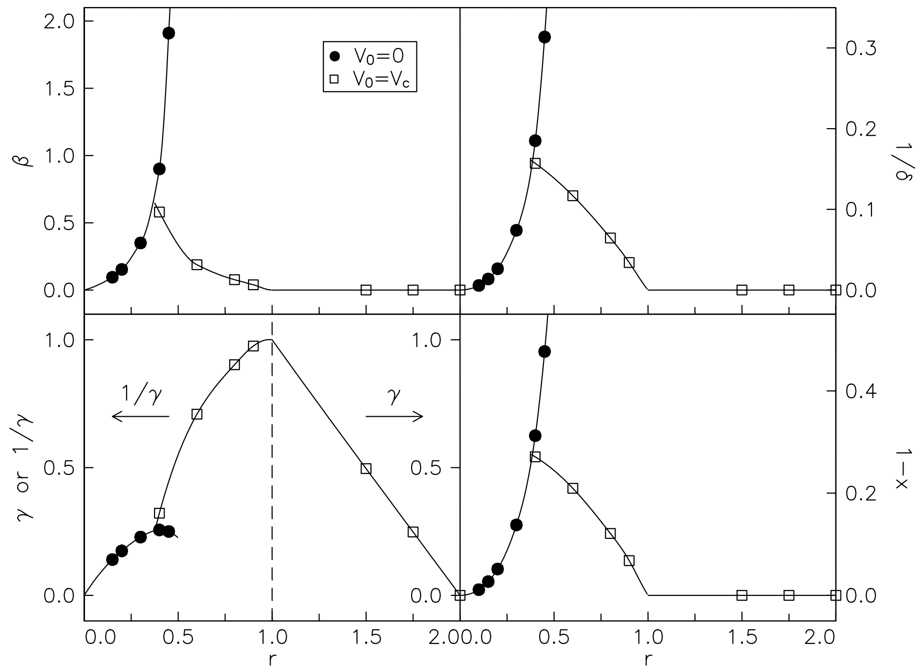

Figure 1: Critical exponents defined in Eqs. (4) plotted vs r, both at and away from particle-hole symmetry (filled and open symbols, respectively). For $r \lesssim 0.375$, the two sets of exponents coincide. Estimated errors are smaller than the symbols. Connecting lines are provided as a guide to the eye.

In all cases, $M_{\rm loc}$ and $\chi_{\rm loc}$ behave as described in Eqs. (4), establishing the continuous nature of the phase transition. The critical exponents satisfy the general scaling relations [Eqs. (5)] to within the estimated random errors (which are smaller than 0.5% for δ and x, 2% for γ, and 5% for β). This agreement supports the validity of the scaling hypothesis presented in Eq. (3).

The critical exponents are plotted in Fig. 1. A striking feature is the difference between the symmetric and asymmetric exponents for $r \gtrsim 0.375$. The trends with increasing r followed by β, δ, and x for $V_0 = 0$ are all reversed for $V_0 = V_c$. Indeed, for $r \geq 1$, all three exponents revert to their $r = 0$ values. By contrast, γ generally decreases as r increases from 0 to 2, irrespective of the potential scattering. We reiterate, however, that in every case the four exponents are completely consistent with our scaling ansatz for the free energy.

In summary, we have computed the critical exponents of the power-law Kondo problem, both at and away from particle-hole symmetry. We find that the temperature exponent of the local spin susceptibility at the $T = 0$ phase transition [x defined in Eqs. (4)] varies with the power of the pseudogap, and takes an anomalous value for all $0 < r < 1$. The possible relevance of our result for heavy fermions can be seen within the dynamical mean-field approach, [14] which maps a lattice system onto an impurity coupled self-consistently to a fermionic bath. The development of a pseudogap in the lattice will show up as a pseudogap in the effective impurity problem. Should this impurity problem lie near criticality, our results imply the existence of an anomalous local dynamical spin susceptibility. Thermodynamic and transport measurements on quantum-critical heavy fermion systems have found no suppression of the spectral weight. However, tunneling or photoemission experiments are needed to test more directly the existence of a single-particle pseudogap of the type discussed in this paper.

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References

1. *Proceedings of the ITP Conference on Non-Fermi Liquid Behavior in Metals, Santa Barbara, USA, 17–21 June 1996*, eds. P. Coleman, B. Maple, and A. J. Millis, *J. Phys.: Condens. Matter* **8** (1996).
2. A. Rosch, *et al.*, *Phys. Rev. Lett.* **79**, 159 (1997); O. Stockert, *et al.*, *ibid.* **80**, 5627 (1998).
3. A. Schroder, *et al.*, *Phys. Rev. Lett.* **80**, 5623 (1998).
4. J. Hertz, *Phys. Rev.* B **14**, 1165 (1976); A. J. Millis, *ibid.* **48**, 7183 (1993).
5. N. D. Mathur, *et al.*, *Nature* **394**, 39 (1998), and references therein.
6. For discussion of pseudogaps in the underdoped cuprates, see, e.g., *Proceedings of the International Conference on Materials and Mechanisms of Superconductivity, Beijing, Feb. 1997*, *Physica* C **282-287** (1997).
7. We work with units in which $k_B = 1$ and $g\mu_B = 1$.
8. D. Withoff and E. Fradkin, *Phys. Rev. Lett.* **64**, 1835 (1990).
9. All band energies are expressed in units of the half-bandwidth and measured from the Fermi energy, $\epsilon = 0$.
10. A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, England, 1993).
11. C. Gonzalez-Buxton and K. Ingersent, *Phys. Rev.* B **57**, 14254 (1998), and references therein.
12. K. Chen and C. Jayaprakash, *J. Phys.: Condens. Matter* **7**, L491 (1995).
13. K. Ingersent and Q. Si, preprint cond-mat/9810226.
14. A. Georges, *et al.*, *Rev. Mod. Phys.* **68**, 13 (1996), and references therein.