Non-Fermi-Liquid States of a Magnetic Ion in a Metal

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A model of a local orbital coupled through repulsive interactions to both the hybridizing and the screening channels of a conduction band is solved by Wilson's renormalization group method. At particle-hole symmetry we find non-Fermi-liquid lines of critical points when the interaction in the screening channel is above a critical value. Away from particle-hole symmetry the system displays two stable Fermi-liquid fixed points of different symmetries, separated by a non-Fermi-liquid quantum critical point, in the mixed-valence regime. The behavior in the vicinity of this point is consistent with the marginal Fermi-liquid hypothesis.

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The experimental results [1] on the Cu-O-based metals have raised two important related issues: what is the description of the normal state, which does not appear to fit into the Landau Fermi-liquid phenomenology, and what is the mechanism responsible for the superconductive pairing. Here we investigate the low-energy properties of a model relevant to the physics of the Cu-O materials, which sheds light on both issues.

A general description of magnetic impurities in metals was given by Friedel [2] and later by Anderson [3] in a model with local interactions. The Anderson Hamiltonian for a magnetic impurity in a metal and the related Kondo Hamiltonian have been exactly solved by a variety of methods. At low energies $\omega \ll T_K$ (T_K is the Kondo temperature) the excitation spectrum of these models is that of a local Fermi liquid [4,5]. We show that a more general model displays local non-Fermi-liquid properties and local pairing interactions over a range of parameters. This generalization is the single impurity version of one of the multiband models proposed to describe the physics of the Cu-O compounds [6], in the same sense in which the Anderson model is the single impurity version of the single-band Hubbard model.

Our model is specified by the Hamiltonian

$$H = \sum_{k,\sigma,l} \varepsilon_{kl} c^{\dagger}_{k\sigma l} c_{k\sigma l} + \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + t \sum_{k,\sigma} (d^{\dagger}_{\sigma} c_{k\sigma 0} + \text{H.c.}) + \sum_{k,k',l} V_{kk'l} (n_d - 1) \left(\sum_{\sigma} c^{\dagger}_{k'\sigma l} c_{k\sigma l} - 1 \right). \quad (1)$$

The first four terms in Eq. (1) represent the usual Anderson model while the last term takes into account the finite-range interactions between the local "d orbital" and electrons in the conduction band. These interactions are expanded in appropriate symmetry channels l about the impurity site [7]. As required by symmetry, the non-degenerate "d orbital" hybridizes only with one channel, $l = 0$, hereafter called the "hybridizing" channel. All other channels will be referred to as "screening" channels. The chemical potential is set to zero; for $\varepsilon_d = -U/2$ the Hamiltonian is particle-hole symmetric. The spinless version of this model, which is just the generalized resonant level model, has recently been discussed in [8] and displays a (Kosterlitz-Thouless) transition from a Fermi-liquid to a non-Fermi-liquid state as the interaction parameters are varied.

We have solved the model of Eq. (1) by the numerical renormalization group (NRG) method, devised by Wilson [4] in the course of his solution of the Kondo problem and used subsequently in the study of the Anderson Hamiltonian [9] and several other problems. Wilson's method solves the recursion relation for the discretized N-th iteration Hamiltonian, H_N:

$$H_{N+1} = \Lambda^{1/2} H_N + \sum_{l,\sigma} (f^{\dagger}_{N+1\sigma l} f_{N\sigma l} + \text{H.c.}), \quad (2)$$

where Λ is the step size of the logarithmic discretization of the energy. $f_{0\sigma l}$ is the Wannier orbital for the conduction electrons in the l-th channel at the impurity site; $f_{N\sigma l}$ are mutually orthogonal orbitals peaking further and further away from the impurity [4]. We have considered $V_{kk'l} = V_l$ so that the many-body interactions are present only in H_0. Since this simplification does not lead to a change of symmetry, we expect no qualitative differences in the results.

At the zeroth iteration, the Hamiltonian is

$$H_0 = \frac{2\Lambda^{1/2}}{\Lambda + 1} \Big[\varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + t \sum_{\sigma} (d^{\dagger}_{\sigma} f_{0\sigma 0} + \text{H.c.}) + \sum_{l,\sigma} 2 g_l (n_d - 1)(f^{\dagger}_{0\sigma l} f_{0\sigma l} - \tfrac{1}{2}) \Big]. \quad (3)$$

Here, $g_l = \rho V_l$ are dimensionless coupling constants and ρ is the one-electron density of states at the Fermi level which we take to be the same in all conduction electron channels, and t defines the bare hybridization width parameter, $\Gamma = \pi\rho t^2$.

First we consider the particle-hole symmetric case, $\varepsilon_d = -U/2$, and include, in addition to the hybridizing channel $l = 0$, a single *spinless* screening channel $l = 1$. For simplicity, we describe the results for interaction V_0 in the $l = 0$ channel taken equal to zero; qualitatively similar results have also been obtained without these restrictions.

For V_1 small compared to the "gap," $U/2$, the spectrum is characteristic of the unstable local moment fixed point at low iterations ($N \lesssim 7$) followed at large N by the strong-coupling (Kondo effect) fixed point. The strong-coupling fixed point corresponds to a renormalized value of the hybridization width parameter $\Gamma = \infty$ (or $\pi/2$ phase shift per spin channel at the impurity) and a pair of leading irrelevant operators, which are characterized by the energy scale T_K [4,9]. The asymptotic low-energy properties are those of a local Fermi liquid.

With increasing V_1, the first effect is the renormalization of the Kondo temperature T_K upwards, which can be seen on closer examination to be due to the renormalization of U downwards. Eventually, the impurity behaves as an effective attractive center, with the charge 0 and 2 states favored over the charge 1 state. The flow after a few iterations is the same as in the Anderson model with $U < 0$. With $U_{\text{eff}} < 0$ and $U_{\text{eff}}/\Gamma > \pi$, the problem at particle-hole symmetry transforms to that of a Kondo effect in a pseudo-spin (τ) channel, with τ_z denoting charge states 0 and 2, and $\tau^{\pm}$ flipping between these states [7].

As V_1 is further increased, the Kondo temperature in the pseudo-spin channel is rapidly depressed. For $V_1 < V_c$, the flow is, however, still to the strong-coupling fixed point (free Fermi fixed point with phase shifts $\pi/2$ in the hybridization channel and 0 in the screening channel) and therefore to Fermi-liquid behavior at low energies. The asymptotic low-energy spectra about the strong-coupling fixed point are described by four leading irrelevant operators:

$$\Lambda^{(N-1)/2}\Bigg[w_1\left(\sum_\sigma f^\dagger_{1\sigma 0}f_{2\sigma 0}+\text{H.c.}\right)+w_2\left(\sum_\sigma f^\dagger_{1\sigma 0}f_{1\sigma 0}-1\right)^2+w_3(f^\dagger_{01}f_{11}+\text{H.c.})$$
$$+w_4\left(\sum_\sigma f^\dagger_{1\sigma 0}f_{1\sigma 0}-1\right)\left(f^\dagger_{01}f_{01}-\frac{1}{2}\right)\Bigg]. \tag{4}$$

The depression of T_K with V_1 can be studied through the variation of the w_i with g_1, obtained by fitting the low-energy spectra. We find that all $w_i \sim T_K^{-1}$ have an essential singularity at $g_1 \to g_{1c}$ of the form

$$w_i \sim e^{(\frac{d}{g_{1c}-g_1})^\alpha}, \tag{5}$$

where the exponent α is found numerically to be close to 1 and g_{1c} and d depend on the values of the initial parameters.

This behavior is analogous to that found in the transition from the antiferromagnetic to ferromagnetic Kondo effect [10], as well as in the multichannel spinless model [8]; w_i is reminiscent of the correlation length at the Kosterlitz-Thouless transition. Indeed, for $V_1 > V_{1c}$, a line of critical points is found.

Our results can be understood from the fixed point Hamiltonians for $g_1 > g_{1c}$. As distinct from the fixed point Hamiltonian in the Kondo problem, these fixed points are characterized by the full kinetic energy E_K (no exclusion of the impurity site, i.e., no $\pi/2$ phase shift) and finite interactions g_i^* in the hybridizing and screening channels:

$$H^* = E_K + g_0^*(n_d-1)\left(\sum_\sigma f^\dagger_{0\sigma 0}f_{0\sigma 0}-1\right)$$
$$+g_1^*(n_d-1)(f^\dagger_{01}f_{01}-\tfrac{1}{2}) \tag{6}$$

with only $n_d = 0, 2$ allowed. Note that there is zero hybridization at the fixed point, so spectra with different n_d are decoupled. g_i^* are determined by fitting the asymptotic spectra. The stability of this fixed point is studied by considering the leading operator

$$O = w\Lambda^{(N-1)/2}(f^\dagger_{0\uparrow 0}f^\dagger_{0\downarrow 0}d_\downarrow d_\uparrow + \text{H.c.}), \tag{7}$$

which couples the $n_d = 0$ and $n_d = 2$ sectors, of H^*. To study the dimensionality of O, consider $H^*_{n_d=0}$ and $H^*_{n_d=2}$, which are H^* in the $n_d = 0$ and $n_d = 2$ sectors, respectively. Because $H^*_{n_d=0}$ is a sum of three commuting Hamiltonians, its eigenstates can be written as $|n_d = 0\rangle = |i\uparrow\rangle|j\downarrow\rangle|m1\rangle|\Omega\rangle$, where $|\Omega\rangle$ denotes the empty d orbital, $|i\sigma\rangle$ represents excited states of the Fermi sea of spin σ electrons in the hybridizing channel, and $|m1\rangle$ the excited states of the Fermi sea in the screening channel. Similarly, the ground state of $H^*_{n_d=2}$ is $|n_d = 2\rangle = |0\uparrow\rangle|0\downarrow\rangle|01\rangle d^\dagger_\uparrow d^\dagger_\downarrow|\Omega\rangle$. The matrix elements of O in the fixed point basis can then be easily evaluated following considerations analogous to those used in the x-ray edge problem [11]:

$$\langle n_d = 0|O|n_d = 2\rangle \sim \Lambda^{\frac{N-1}{2}\alpha}, \tag{8}$$

where the anomalous dimension of the operator O, $\alpha = 2\delta_0/\pi - (\delta_0/\pi)^2 - \frac{1}{2}(\delta_1/\pi)^2$, is written in terms of the phase shifts at the fixed point, $\delta_l = \tan^{-1}(\pi g_l^*/A_\Lambda)$ with $A_\Lambda = \frac{1+\Lambda^{-1}}{1-\Lambda^{-1}}\frac{\ln\Lambda}{2}$. Therefore, $g^* = g_{1c}$ corresponds to $\alpha = 0$, where O is marginal, while for $g^* > g_{1c}$, $\alpha < 0$ and O becomes an irrelevant operator. The form (8) has also been verified by fitting the low-lying numerical eigenvalues and is consistent with the results of the multi-

channel spinless model [8].

For $\alpha \leq 0$ the singular scale invariant low energy behavior of various correlation functions can be estimated as in Ref. [8]. The (pair) susceptibility behaves like $\sim T^{-(\alpha+1)}$, while the contribution to the resistivity of the conduction electrons due to scattering at the impurity site is $\sim c_0 + c_1 T^{2\alpha}$, where the c's are constants.

We next consider the particle-hole asymmetric problem. Especially interesting for application to the copper-oxide problem is the mixed-valence regime [12], where n_d fluctuates between ~ 0 and ~ 1 (or 1 and 2) in the ground state (corresponding to Cu^+ and Cu^{++} states, respectively). For such cases, U is taken as ∞. It is also convenient to rewrite the interaction terms (proportional to V_l) in Eq. (1) in the form

$$\sum_{k,k',l} V_l \left(n_d - \frac{1}{2}\right)\left(\sum_\sigma c^\dagger_{k'\sigma l} c_{k\sigma l} - 1\right) \qquad (9)$$

so that V_l do not affect the relative positions of the $n_d = 0$ and $n_d = 1$ states. Mixed-valence behavior then occurs for $|\varepsilon_d| \leq \Gamma, U \gg \Gamma$. Calculations below report the results for the case of a single *spinless* screening channel $l = 1$.

For $\varepsilon_d \gg \varepsilon_{dc}$ ($\to 0$ for $\Gamma \to 0$), the $n_d = 0$ state is favored in the low-energy regime. For $V_l = 0$, the Hamiltonian flows directly from the high-temperature fixed point to the "frozen impurity" fixed point [9] at $T \to 0$, around which properties are those of a local Fermi liquid. For $V_l \gg |\varepsilon_d|, \Gamma$, the NRG calculations also lead to a local Fermi-liquid state, with charge in the screening channel $\langle Q_1 \rangle = \frac{1}{2}$ (phase shift $\sim -\pi/2$ in the screening channel), as may be deduced from Eq. (9). Lack of particle-hole symmetry leads to potential scattering terms in the hybridizing and screening channels at the fixed point:

$$w_5 \left(\sum_\sigma f^\dagger_{0\sigma 0} f_{0\sigma 0} - 1\right) + w_6 (f^\dagger_{01} f_{01} - 1/2). \qquad (10)$$

Low-energy properties are determined by an effective Hamiltonian of the form of Eq. (6).

The opposite case, $\varepsilon_d \ll \varepsilon_{dc}$, favors $n_d = 1$ in the low-energy regime. For $V_l = 0$, the Hamiltonian flows from the high-temperature fixed point to a local moment fixed point characterized by a doubly degenerate set of states, which is in turn (marginally) unstable to a non-degenerate Fermi-liquid fixed point [9]. When $V_l \gg \Gamma$, a Fermi-liquid fixed point is again found at $T \to 0$, but now with $Q_1 = -1/2$ (phase shift $\sim \pi/2$ in the screening channel) and correspondingly, w_6 has the opposite sign from the previous case. The symmetry of the ground state for $\varepsilon_d > \varepsilon_{dc}$ is therefore different from that at $\varepsilon_d < \varepsilon_{dc}$, so we might anticipate a quantum critical point at $\varepsilon_d = \varepsilon_{dc}$ in the mixed-valence regime $\Gamma > |\varepsilon_d|$, where n_d fluctuates between 0 and 1.

The mixed-valence regime is characterized by a high-temperature magnetic susceptibility $\chi = \frac{1}{6} T^{-1}$ and, for $V_l = 0$, a local Fermi-liquid low-temperature state indistinguishable from that found in the conventional Anderson model [9]. On the other hand, for V_1 above a critical value we find an unstable critical point. This critical point is signaled by the vanishing of the potential scattering parameter w_6 of Eq. (10) and simultaneously a divergence of the hopping parameter in the screening channel, w_3, and the interaction coefficient w_4 of Eq. (5), as $\varepsilon_d \to \varepsilon_{dc}$. These coincide with $\langle Q_1 \rangle \to 0$ and a diverging charge susceptibility χ'_ρ. Asymptotically near the critical point, the low-energy spectrum is doubly degenerate with $Q_1 = \pm 1/2$ (and the hybridizing channel has the $\pi/4$ phase shift of the mixed-valence configuration). Scattering between these two manifolds of eigenstates scales to zero at zero energy separation due to orthogonality, leading to the divergence of χ'_ρ of the form $\chi'_\rho \sim |\varepsilon_d - \varepsilon_{dc}|^{-\nu}$, with $\nu = 1.8 \pm 0.2$. This behavior is illustrated in Fig. 1 which also shows that $\langle Q_1 \rangle \sim |\varepsilon_d - \varepsilon_{dc}|^{1/\delta}$, with $\delta \approx 2.7$. We expect that, as in the particle-hole symmetric model, the transverse charge (i.e., pairing) susceptibility is equally singular.

Actually, for $|\epsilon_d - \epsilon_{dc}| \lesssim 10^{-5}$, χ_ρ saturates in our calculation due, we believe, to the truncations in the NRG procedure. For $\epsilon_d \gtrsim \epsilon_{dc}$, the spin susceptibility, χ_σ, has the same form as χ_ρ, with a similar saturation. However, by contrast with χ_ρ, χ_σ grows for $\epsilon_d \lesssim \epsilon_{dc}$ (i.e., on the $n_d = 1$ side), as a result of the sharp decrease in the Kondo temperature with decreasing ϵ_d.

The structure of our problem appears related to that of the two-channel single-impurity [13] and the two-impurity [14] Kondo problems. In each case two stable Fermi-liquid fixed points of different symmetries are separated by a non-Fermi-liquid critical point. In fact, in the two-channel problem conformal field theory yields $\nu = 2$ [15].

As near any quantum critical point the nature of the fluctuations in the critical regime of the mixed-valence

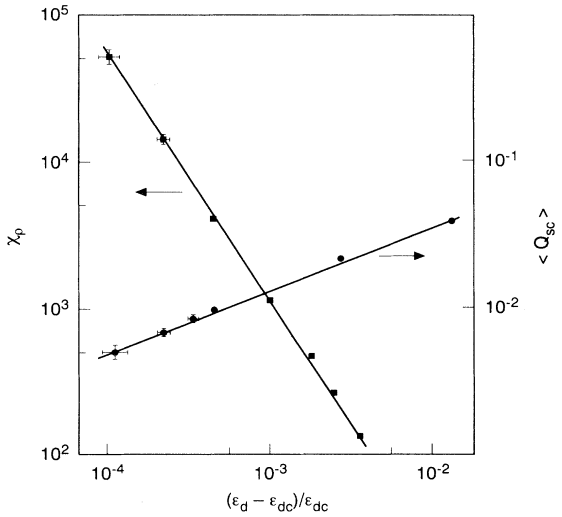

FIG. 1. The charge susceptibility and the charge in the screening channel as a function of $\varepsilon_d - \varepsilon_{dc}$.

quantum critical point is characterized by "lengths" $\xi \sim (\varepsilon_d - \varepsilon_{dc})^{-\nu}$ and $\xi_T \sim T^{1/z}$. By general finite size scaling arguments [16], in the critical regime $\xi_T \ll \xi$, i.e., $T >> |\varepsilon_d - \varepsilon_{dc}|^{\nu z}$, the local fluctuation spectra must take the form

$$\chi''_{\rho,\sigma}(\omega) \sim |\omega|^{\mu_{\rho,\sigma}} F_{\rho,\sigma}(\omega/T)\mathrm{sgn}(\omega). \quad (11)$$

Quite generally, for $\omega \ll T$ one expects $\chi'' \sim \omega$, implying that $F \sim (|\omega|/T)^{1-\mu}$; in turn, this leads to a static susceptibility, $\chi'_{\rho,\sigma}(0) \sim T^{\mu_{\rho,\sigma}}$. In the regime $|\varepsilon_d - \varepsilon_{dc}| >> T^{1/z\nu}$, Fermi-liquid behavior, $\chi'_{\rho,\sigma}(0) \sim$ const, is expected, consistent with our findings. On the other hand, at the highest temperatures, $\chi_{\rho,\sigma} \sim T^{-1}$. We are unable to demarcate in our numerical results the quantum critical region intermediate between the local-moment and the Fermi-liquid regime, and thus are unable to determine the value of μ. However, by a simple scaling argument [17] $\nu = 2$ corresponds to $\chi'(\omega) \sim \log[\max(|\omega|, T)]\mathrm{sgn}\omega$ (i.e., $\mu = 0$). This is the marginal-Fermi-liquid spectrum [18], in terms of which the anomalous normal state properties of the high-T_c metals have been discussed.

Finally, we briefly discuss the relevance of the present calculation to the Cu-O lattice problem. This raises two important questions: First, are there further singularities introduced by the lattice or effects which otherwise remove the singularities discovered in the single-impurity problem? Second, what is the range of parameters over which the properties of the lattice are controlled by the single-impurity critical point?

An approximate treatment of the quantum critical point [19] and mean-field extensions to the lattice lead to the conclusion that the largest low-energy cutoff of the singularities discussed here occurs at the coherence temperature, T_{coh}, of the local pairing fluctuations between impurities, which determines the onset of superconducting order. For the purpose of discussing the normal state above T_{coh} we may then regard the lattice as a periodic arrangement of "impurities" in contact with a reservoir of electrons. (This is consistent with the marginal-Fermi-liquid hypothesis for the normal state of the high-T_c materials, which assumes that the singularities are q independent, i.e., local in space.) The chemical potential, μ, is then determined by using the self-consistent solution of $\langle Q_1 \rangle$ as a function of $\varepsilon_d - \mu$ as found here, in conjunction with the condition of a fixed average total charge for the lattice, Q_t:

$$\langle Q_1 \rangle_\mu + \langle Q_0 \rangle_\mu = Q_t. \quad (12)$$

The latter yields a family of smooth solutions for $\langle Q_1 \rangle$ as a function of $\varepsilon_d - \mu$ depending on Q_t. For a fixed ε_d and Q_t, due to the rapid change of $\langle Q_1 \rangle$ close to $\varepsilon_d - \mu = \varepsilon_{dc}$ in the single-impurity problem (recall $\langle Q_1 \rangle \sim |\varepsilon_d - \varepsilon_{dc}|^{\frac{1}{\delta}}$), a self-consistent lattice solution exists for a range of Q_t around a critical value, Q_{tc}. (This procedure is the same as used in determining the pressure-volume relation near the critical point of a gas-liquid transition.) The crossover temperature from the quantum critical regime to the Fermi-liquid regime in the lattice can then be estimated from $T_x \approx \Gamma[|Q_t - Q_{tc}|/Q_{tc}]^{\delta\nu z}$. With $z \geq 1$ and taking Γ as large as 10^4 K, $T_x < 1$ K for $|Q_t - Q_{tc}|/Q_{tc} \sim 0.1$. These ideas can be checked by using a recently developed RG method for embedding impurity models in an infinite dimensional lattice [20].

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[1] For a review, see for example, B. Batlogg, Physica (Amsterdam) **169B**, 7 (1990).
[2] J. Friedel, Can. J. Phys. **34**, 1190 (1956); A. Blandin and J. Friedel, J. Phys. Radium **20**, 160 (1959).
[3] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[4] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[5] P. Nozières, J. Low Temp. Phys. **17**, 31 (1974).
[6] C. M. Varma, E. Abrahams, and S. Schmitt-Rink, Solid State Commun. **62**, 681 (1987); in *Novel Mechanisms of Superconductivity*, edited by V. Krusin and S. Wolf (Plenum, New York, 1987).
[7] Such a model was first proposed by F. D. Haldane, Phys. Rev. B **13**, 281 (1976); **15**, 2477 (1977), in order to make the Anderson Hamiltonian away from particle-hole symmetry conform to Friedel's sum rule. Haldane also presented the Hartree-Fock phase diagram of this model.
[8] T. Giamarchi, C. M. Varma, A. E. Ruckenstein, and P. Nozières (to be published); I. E. Perakis (to be published).
[9] H. R. Krishna-murthy, J. W. Wilkins, and K. G Wilson, Phys. Rev. B **21**, 1008 (1980); **21**, 1044 (1980).
[10] P. W. Anderson, J. Phys. C **3**, 2436 (1970).
[11] See, for example, P. Nozières and C. De Dominicis, Phys. Rev. **178**, 1097 (1969).
[12] See, for example, C. M. Varma, in *Moment Formation in Solids*, edited by W. J. L. Buyers (Plenum, New York, 1984).
[13] P. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980).
[14] B. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988); B. Jones and C. M. Varma, Phys. Rev. B **40**, 324 (1989).
[15] A. Ludwig (private communication).
[16] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989); S. Sachdev and J. Ye, Phys. Rev. Lett. **69**, 2411 (1992).
[17] A. M. Tsvelick, J. Phys. Condens. Matter **2**, 2833 (1990); I. Affleck and A. Ludwig, Phys. Rev. Lett. **67**, 161 (1991); D. Cox (private communication).
[18] C. M. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. E. Ruckenstein, Phys. Rev. Lett. **63**, 1996 (1989).
[19] A. E. Ruckenstein and C. M. Varma (unpublished).
[20] Q. Si and G. Kotliar, Phys. Rev. Lett. **70**, 3143 (1993).