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LETTER TO THE EDITOR

Phase transition in the double-exchange model: a Schwinger boson approach

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Abstract. Local alignment of a conduction electron's spin with core spins caused by strong ferromagnetic coupling imposes a severe restriction on the Hilbert space. This is incorporated in a representation in which the electron is a composite object. Within a mean-field approximation we find a transition from a ferromagnetic metal to a paramagnetic state at a temperature $T_c \ll T_F$, the Fermi temperature, i.e., there is a separation of energy scales. The electron Green function exhibits a two-fluid character: a Fermi liquid component associated with the ordered spins which disappears above T_c, and an incoherent component with disordered spins which breaks particle-hole symmetry. Implications for manganites, which exhibit very large magnetoresistance, are discussed.

Recent discovery of very large magnetoresistance in $La_{1-x}Ca_xMnO_3$ (and other manganites) [1, 2, 3] has revived interest in the double-exchange model [4–7]. Approximately in the range $0.2 < x < 0.4$, the low-temperature phase of the manganites is a ferromagnetic metal. At a critical temperature T_c, there is a transition to a paramagnetic phase which appears to be insulating. The large increase in resistivity at T_c and the enormous magnetoresistance are linked to the transition and implies extreme sensitivity to external magnetic fields. The important physical effects are believed to originate from the d orbitals of the manganese ions which occupy the cubic sites of the perovskite structure. The E_g orbitals form a conduction band containing $1 - x$ electrons per site. The electron strongly interacts ferromagnetically via the Hund's rule mechanism with the $S = 3/2$ core spin formed from the T_g orbitals. We thus consider the ferromagnetic Kondo lattice Hamiltonian given by

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} - J_H \sum_i \boldsymbol{S}_i \cdot \boldsymbol{s}_i. \tag{1}$$

Here $c_{i\sigma}$ destroys an E_g electron at site i and the first term is the usual nearest-neighbour hopping Hamiltonian with $t_{ij} = t$. The second term describes the Hund's rule coupling between the core spin $\boldsymbol{S}_i$ and the conduction electron spin density $\boldsymbol{s}_i$. The nominal two-fold degeneracy of the E_g orbitals could in fact be lifted by a coupling to the lattice. For the most part we ignore the degeneracy, its effect will be discussed later.

In the large J_H limit, the conduction-electron spin adiabatically follows the core spins. As elucidated by Anderson and Hasegawa [5], this induces a ferromagnetic correlation between neighbouring spins in order to facilitate coherent propagation. However, the forced alignment also removes a large part of the Hilbert space since at each site, doubly-occupied and the *antiparallel* singly-occupied states are both projected out. More precisely, an electron combines with the core spin to form two manifolds of total spin $S \pm \frac{1}{2}$ with

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energies $-\frac{1}{2}J_H S$ and $+\frac{1}{2}J_H(S+1)$, respectively. As $J_H \to \infty$, the $S-\frac{1}{2}$ and the doubly occupied sectors are projected out. This restriction is far more stringent than that in the infinite U Hubbard model where only double occupancy is forbidden, and dominates the physics.

We derive an exact representation in which spins are treated as Bose fields that are coupled to spinless charge fermions so that the physical electron is a composite object. Within a mean-field (MF) approximation we find a transition from a ferromagnetic metallic state to a paramagnetic state with reasonable values for $T_c \ll T_F$, i.e., there is a separation of energy scales. We show, analytically, that the MF electron Green function exhibits a two-fluid character: a Fermi liquid component associated with the ferromagnetically ordered spin configuration, and an incoherent component associated with the disordered spin configurations which breaks particle-hole symmetry. With increasing temperature (T), there is a transfer of spectral weight to the latter, until at T_c the Fermi liquid component disappears.

Functional integral representation. Consider first the on-site problem with a classical $\boldsymbol{S}_i$, pointing along some arbitrary direction. Let f_i and g_i be operators that destroy single electrons with spins parallel and antiparallel to $\boldsymbol{S}_i$, respectively. Then $c_{i\sigma}$ are given by linear combinations:

$$c_{i\sigma} = \frac{1}{\sqrt{2S}}[b_{i\sigma} f_i + \mathrm{sgn}(\sigma) b^*_{i,-\sigma} g_i]$$

where $b_{i\sigma} = r_{i\sigma}\mathrm{e}^{\mathrm{i}\phi_{i\sigma}}$ are complex numbers with $\sum_\sigma b^*_{i\sigma} b_{i\sigma} = 2S$. If $\boldsymbol{S}_i$ is expressed as (S, θ, ϕ) in spherical coordinates, then we can choose

$$r_{i\uparrow} = \sqrt{2S}\cos\frac{\theta_i}{2} \qquad r_{i\downarrow} = \sqrt{2S}\sin\frac{\theta_i}{2} \qquad \phi_i = \phi_{i\downarrow} - \phi_{i\uparrow}.$$

In the quantum case, $b_{i\sigma}$ becomes a time-dependent Bose field. Then it is convenient to use functional integral techniques [7]. Note that the core spin variables can be expressed as: $S_i^+ = b^*_{i\uparrow} b_{i\downarrow}$, $S_i^z = \frac{1}{2}(b^*_{i\uparrow} b_{i\uparrow} - b^*_{i\downarrow} b_{i\downarrow})$. This is nothing but the exact Schwinger boson representation of the core spin [8, 9].

Clearly, the representation is valid for all J_H. Here we focus on the $J_H \to \infty$ limit. Then we can ignore the upper (antiparallel) level (i.e. terms containing g) so that: $c_{i\sigma} = \frac{1}{\sqrt{2S}} b_{i\sigma} f_i$ where $c_{i\sigma}$ and f_i are Grassman fields. The partition function can be written as a functional integral with an action given by

$$\mathcal{A} = \int_0^\beta \mathrm{d}\tau \left[\sum_{i\sigma} \left(1 + \frac{f_i^* f_i}{2S}\right) b^*_{i\sigma} \frac{\partial b_{i\sigma}}{\partial \tau} + \left(f_i^* \frac{\partial f_i}{\partial \tau} + \mu_f f_i^* f_i \right) + \frac{1}{2S} \sum_{ij\sigma} t_{ij} b^*_{i\sigma} b_{j\sigma} f_i^* f_j \right] \quad (2)$$

where μ_f is the chemical potential and the integrals over the Bose fields are to be done subject to constraints $\sum_\sigma b^*_{i\sigma} b_{i\sigma} = 2S$. The action is invariant under the gauge transformation: $f_j \to f_j \mathrm{e}^{\mathrm{i}\psi_j}$; $b_{j\sigma} \to b_{j\sigma}\mathrm{e}^{-\mathrm{i}\psi_j}$. Hence, one of the Bose fields, say $b_{j\uparrow}$, can be chosen to be real. Then, written in terms of the polar variables (S, θ, ϕ), the action becomes identical to the one derived by Millis *et al* [7].

In essence, the electron has become a composite object. Its charge (density $n_i = f_i^* f_i$) is carried by a *spinless* fermion field f, and its spin (density $\boldsymbol{s}_i = (f_i^* f_i / 2S)\boldsymbol{S}_i$) is wedded to the core spin and is carried by the Bose fields. The double-exchange mechanism is explicit in the last term in the action (2) which describes hopping of a spinless charge characterized by a fluctuating hopping parameter tB_{ij}/S, where $B_{ij} \equiv \frac{1}{2}\sum_\sigma b^*_{i\sigma} b_{j\sigma}$ essentially measures the nearest-neighbour ferromagnetic correlation and has a magnitude

$$|B_{ij}| = S\left[\cos^2\left(\frac{\theta_i - \theta_j}{2}\right) - \sin\theta_i \sin\theta_j \sin^2\left(\frac{\phi_i - \phi_j}{2}\right)\right]^{\frac{1}{2}}.$$

This is maximum (= S) for ferromagnetic alignment: $\theta_i = \theta_j$; $\phi_i = \phi_j$. Note the similarity with the infinite U Hubbard model. Physics is quite different, however [10]. In the present case, *the charge field is free*, i.e., not enslaved to the spin-field by a projective constraint. The representation is therefore natural since there is no freedom of choice of statistics (i.e., no slave boson).

Mean-field theory. We treat the constraints on the Bose fields on the average via a Lagrange multiplier Λ. A Hartree–Fock decomposition then yields actions that are quadratic in the charge and spin-fields: $\mathcal{A}_{MF} = \mathcal{A}_f + \mathcal{A}_b + \text{const}$. The factor $(1 + (f_i^* f_i/2S))$ can be absorbed by shifting μ_f and rescaling the Bose fields so that they correspond to a spin of renormalized magnitude: $S \to S_R = S\zeta = S + (1 - x/2)$. This is just the average total spin at a site with $1 - x$ electrons. The mean-field actions are then given by

$$\mathcal{A}_b = \int_0^\beta \mathrm{d}\tau\left[\sum_{i\sigma}\left(b_{i\sigma}^*\frac{\partial b_{i\sigma}}{\partial\tau} - \Lambda b_{i\sigma}^* b_{i\sigma}\right) + \frac{D}{2S_R}\sum_{ij\sigma} t_{ij} b_{i\sigma}^* b_{j\sigma}\right] \tag{3}$$

$$\mathcal{A}_f = \int_0^\beta \mathrm{d}\tau\left[\sum_{i}\left(f_i^*\frac{\partial f_i}{\partial\tau} + \mu_f f_i^* f_i\right) + \frac{B}{S_R}\sum_{ij\sigma} t_{ij} f_i^* f_j\right] \tag{4}$$

where $D = \langle f_i^* f_j\rangle$ is the average 'kinetic energy' of charge and $B = \langle B_{ij}\rangle$ is the average value of short-range ferromagnetic correlation. Thus, although the bare problem has a single energy scale (the bare bandwidth $W = 12t$), the propagation of charge and spin is governed by distinct energy scales as characterized by the hopping parameters $t_f = tB/S_R$ and $t_b = tD/2S_R$, respectively. These scales depend on T, and their determination is important from an experimental standpoint since W can be in the eV range, the experimental T_c is only a few hundred degrees [1–3].

The fermion spectrum is simply a cosine band $\epsilon_f(k) = -2t_f(\cos k_x + \cos k_y + \cos k_z)$. The parameter B is maximum (= S_R) in the ferromagnetic state and decreases with increasing T, but must remain finite at T_c since it measures only *short-range* magnetic correlations. Hence, we conclude that (1) charge fermions are itinerant both below and above the ferromagnetic transition and (2) the charge bandwidth, $W_f = WB/S_R$, equals the bare bandwidth W at $T = 0$, but decreases with increasing T as B decreases. (3) For fixed S_R, there is a symmetry about $x = 0.5$ (quarter filling), so we can restrict our attention to $x < 0.5$. In this regime the Fermi surface is hole-like. To determine T_c, we need to compute D which determines the Bose parameter t_b. For x not too large, we use a quadratic approximation for the hole spectrum to obtain

$$D = x - \frac{x(6\pi^2 x)^{2/3}}{10}\left\{1 + \frac{5\pi^2}{12}\left(\frac{kT}{t_f\epsilon_F}\right)^2\right\}$$

where $\epsilon_F = (6\pi^2 x)^{2/3}$ is the hole Fermi energy for a band with $t_f = 1$. Thus D is quite small, depends only on x at $T = 0$. For $x = 0.2$, $D \sim 0.1$ at $T = 0$, and decreases with increasing T. Therefore, $t_b/t_f = D/(2B) \sim D/(2S_R) \ll 1$. Hence, T_c must be much smaller than the fermion bandwidth.

The Bose Hartree–Fock problem is identical to that for a spin-S_R Heisenberg ferromagnet, characterized by a *temperature-dependent* exchange constant $J = tD/(2BS_R)$. The Bose spectrum is $\omega_k = 6t_b\gamma_k$, with $\gamma_k = 1 - \frac{1}{3}(\cos k_x + \cos k_y + \cos k_z)$. Long-range ferromagnetic order (along the x direction) appears through a Bose condensation in the $\boldsymbol{k} = 0$ mode, with the magnetization (condensate density) given by

$$m = S_R - \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\omega_k + \Lambda)} - 1}. \tag{5}$$

To obtain B we only need to replace 1 by γ_k in the numerator. The equations have been discussed in detail in [9]. Briefly, in the ordered regime, $\Lambda = 0$ and $m > 0$. The ground-state is ferromagnetic since at $T = 0$ both integrals vanish giving $m = S_R$ and $B = S_R$. By expanding the Bose spectrum we obtain the correct spin-wave theory results at low temperatures: $m = S_R - \text{const } T^{\frac{3}{2}}$ and $B = S_R - \text{const } T^{\frac{5}{2}}$. Above T_c, $m = 0$, and $\Lambda \propto \xi^{-2} > 0$, where ξ is the correlation length over which spins are ordered. These results depend only on the spin-wave spectrum and dimensionality, and are thus expected to be valid.

We have solved the fermion–boson self-consistency problem numerically. The relevant temperature scale is T_c. Figure 1 shows, $2kT_c/W$, as a function of doping. Also shown are the charge fermion bandwidth $W_f/W = t_f/t$, and $2\mu/W$, evaluated at T_c, where μ is the chemical potential for holes. Two aspects need to be stressed. (1) T_c is smaller than the fermion bandwidth by an order of magnitude. Hence, the charge fermions remain degenerate with a well defined Fermi surface across the magnetic transition. (2) The magnitude of T_c is quite reasonable. Thus for a bare bandwidth of 2 eV, T_c ranges from 20 to 40 meV for $0.14 < x < 0.5$. Of course, fluctuations would bring down T_c somewhat.

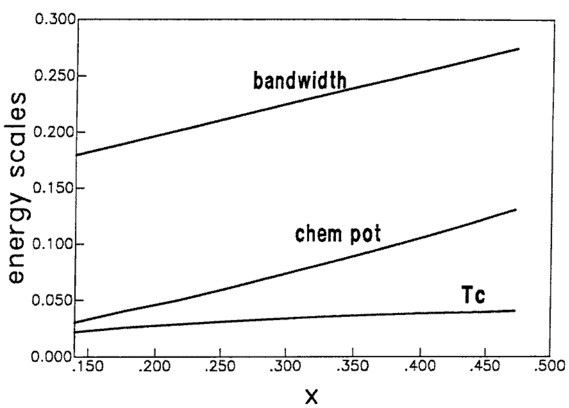

Figure 1. Energy scales: plot of $2kT_c/W$, $2\mu_h/W$ and the W_f/W as a function of doping x. Here $W = 12t =$ bare bandwidth, $W_f = 12t_f =$ fermion bandwidth at T_c and $\mu_h =$ is the hole Fermi energy.

Recently, Millis *et al* [7] estimated a much larger value for T_c although essentially the same mean-field decomposition is implicit in their treatment [11]. The origin of the discrepancy is easily understood. First, instead of solving the problem self-consistently, they estimate T_c from the *Heisenberg* model which has the same magnon spectrum. This is not quite accurate since their is no exact equivalence between the two models. Secondly, they use a two-fold degenerate level (two spinless charge fermions at each site). Now the Fermi surface is *electron-like*. Then $T_c \propto D \sim (1 - x)$, whereas $T_c \propto D \sim x$ for the non-degenerate case. For $x = 0.2$, this alone gives a four-fold increase in T_c for the doubly-degenerate case. The issue of degeneracy is yet to be settled. The high-field Hall effect seems to be consistent with a hole-like Fermi surface [12].

Spectral function. The physical electron is a composite object, and is thus a superposition of pairs of charge fermions and spin bosons subject to momentum and energy conservation:

$c_{k\omega\sigma} = (2S_R N\beta)^{-\frac{1}{2}} \sum_{q\nu} b_{q\nu\sigma} f_{k-q,\omega-\nu}$, where ω and ν are the odd and even Matsubara frequencies. The mean-field Green function is simply a convolution of the fermion and boson Green functions [13]. For ($x < 0.5$) we can work with charge 'holons'. Then the spectral function is given by

$$A(k\omega) = \frac{m\pi}{S_R}\delta(\omega + \epsilon_k - \mu) + \frac{1}{8\pi^2 S_R}\int \mathrm{d}^3q[f(\epsilon_{q-k} - \mu) + n(\omega_q + \Lambda)]\delta(\omega - \omega_q - \Lambda + \epsilon_{q-k} - \mu) \quad (6)$$

where $n(x)$ and $f(x)$ are Bose and Fermi functions, and $\epsilon_k = -\epsilon_f(k)$. Physically, each term in the integral (sum) describes the propagation of a charge riding on a particular mode of the core spins. The first term is associated with the condensate (spin-ordered) component and clearly constitutes a coherent Fermi liquid. However, this is no ordinary Fermi liquid. It represents spinless fermions with a spectral weight proportional to the *magnetization m(T)*, and thus weakens with increasing T and disappears at T_c, as the spectral weight is continuously transferred to the second term which corresponds to spin-waves. Below we show that this term, which we call A_1, is incoherent and has a number of unusual properties.

In the ordered state, $\Lambda = 0$. Since ($\omega_q > 0$), it follows that, at $T = 0$, A_1 is non-zero only for $\omega > 0$. This is because we can only create an excited boson at $T = 0$. Therefore, the particle-hole symmetry near the Fermi surface, a property of ordinary Fermi liquids, is violated. This is a consequence of broken time-reversal invariance and would be observable in photoemission and tunnelling (density of states) measurements. The density of states is given by

$$D(\omega) = \frac{m}{2S_R}D_h(\mu - \omega) + \frac{1}{2S_R}\int \mathrm{d}z\, D_b(z) D_h(z + \Lambda + \mu - \omega)\Big[n(z + \Lambda) + f(z + \Lambda - \omega)\Big] \quad (7)$$

where ω is measured relative to the Fermi surface, and D_b and D_h are the boson and fermion densities of states. The first term is the condensate contribution. Since $D_b(z)$ is non-zero only for $z > 0$, we see immediately that, at $T = 0$, the integrand contributes only if $\omega > z > 0$, exhibiting the particle-hole asymmetry. In the region $kT, \omega \ll \mu$, the fermion density of states D_h varies slowly with frequency and can be replaced by its value at the Fermi level. Also $D_b(\omega) = \mathrm{const}\,\Theta(\omega)\omega^{1/2}$ at low frequencies. Then both above and below T_c we obtain,

$$D(\omega) = D_h(\mu + \Lambda - \omega)\left[\frac{1}{2} + \frac{1}{2S_R}\phi(\omega, T)\right] \quad (8)$$

where ϕ is the symmetry violating contribution and has the scaling form $\phi(\omega, T) = \omega^{3/2} g(\frac{\omega-\Lambda}{kT})$. At $T = 0$, $\phi = \Theta(\omega)(\omega/\omega_m)^{3/2}$, where ω_m is the maximum boson energy. For $T > 0$, ϕ has the same $\omega^{3/2}$ form for $\omega \gg kT$, but acquires a finite value for $\omega_{\leqslant} 0$, which vanishes exponentially as $T^{3/2}\mathrm{e}^{-\beta|\omega|}$ as $\omega \to -\infty$. Precisely on the Fermi surface ($\omega = 0$), ϕ is temperature dependent and scales as $T^{3/2}$. These results follow from the quadratic nature of the (ferromagnetic) spin-wave spectrum and spatial dimensionality of the system.

The spectral function itself can be calculated analytically by using the quadratic approximations for the fermion and boson spectra: $\epsilon_k \approx t_f(\boldsymbol{Q} - \boldsymbol{k})^2$, $\omega_q \approx t_b q^2$. Let $\Omega \equiv (1 - \frac{t_b}{t_f})(\omega - \Lambda + \epsilon_k - \mu)/\epsilon_k$. Then the non-condensate part of the spectral function

(A_1) is given by

$$A_1 = \frac{\Theta(1-\Omega)\Theta(\omega_m-\omega_-)}{16\pi S t_f t_b \beta |Q-k|}\left[\log\frac{1+\mathrm{e}^{-\beta(\omega_1+\Lambda-\omega)}}{1+\mathrm{e}^{-\beta(\omega_2+\Lambda-\omega)}} + \log\frac{1-\mathrm{e}^{-\beta(\omega_2+\Lambda)}}{1-\mathrm{e}^{-\beta(\omega_1+\Lambda)}}\right] \tag{9}$$

where $\omega_1 = \omega_-$, $\omega_2 = \min(\omega_m, \omega_+)$, ω_m is the maximum boson energy and

$$\omega_\pm = \frac{2t_b t_f \epsilon_k}{(t_f-t_b)^2}\left[1-\frac{1}{2}\Omega \pm (1-\Omega)^{\frac{1}{2}}\right].$$

Note that $\omega_+ > \omega_- \geqslant 0$. The quasiparticle peak, if it exists, would occur at $\Omega = 0$. At $T = 0$ only the first term in (9) contributes. It has no singularity and exists only for $\omega > \omega_- \geqslant 0$, exhibiting the lack of p–h symmetry. For $T > 0$, this term just broadens out. The second term in (9) contributes only for $T > 0$ and also has a non-Fermi liquid character. In the ordered region ($\Lambda = 0$) it has a logarithmic singularity $\sim -\log\omega_- \sim -\log\Omega^2$. But as shown in figure 2, even this weak singularity disappears for $T > T_c$ i.e., for a finite Λ as small as $0.0025W$. Hence, above T_c, the charge of the electron is itinerant and has a Fermi surface. But the spin is localized, and the electron itself does not exist as a well defined quasiparticle nor does it have a well defined Fermi surface. In other words, associated with the magnetic transition there is a transition from a Fermi liquid to an incoherent state.

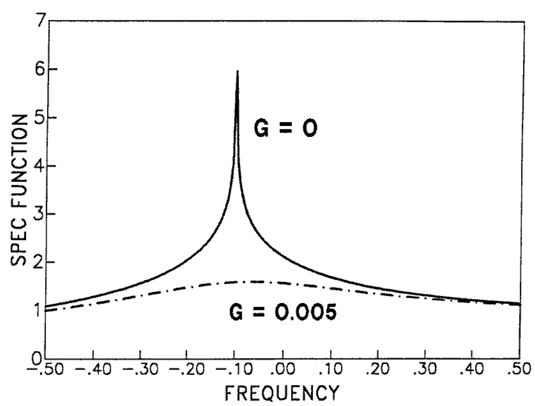

Figure 2. The incoherent part of the spectral function A_1 close to the Fermi surface. Below the transition (solid line) it has a weak logarithmic singularity which disappears above T_c for $\Lambda = 0.0025W$ (dotted line). The parameter $G \equiv 2\Lambda/W$. Energies are in units of $W/2$.

The spectral function clearly shows a two-fluid character: electrons are transferred to the incoherent component with increasing T. Obviously, an external uniform magnetic field would have the opposite effect since it forces core spins to line up (even above T_c). Hence the spectral function is expected to show extreme sensitivity as a function of a magnetic field.

Further work is needed in order to determine whether fluctuations (e.g., those that restore the broken gauge symmetry) would remove the lack of coherence and restore a Fermi liquid state above T_c. Similarly, in order to address the question of metal-insulator transition, a proper transport theory needs to be developed, which may involve inclusion of several scattering processes, and possibly localization effects.

The Schwinger-boson technique can also be extended to the finite J_H case. In particular, for large but finite J_H an antiferromagnetic ‘superexchange’ interaction between neighbouring spins is obtained (by integrating out the antiparallel spins) with $J_{AF} = 2t^2/(S^2 J_H)$. Based on our extensive analyses of the analogous t–J model, we expect an insulating Neel state at $x = 0$ and a ferromagnetic metallic state at intermediate x, with properties similar to the ones found here. We will discuss these issues further in a future paper.

Although, a microscopic transport theory is lacking, it is interesting to examine whether the observed transport anomalies are compatible with a two-fluid model from a purely phenomenological standpoint. Suppose, there are two parallel channels with densities n_c and n_{inc}, and mobilities μ_c and μ_{inc}, respectively. The conductivity is of the form $\sigma = \sigma_c + \sigma_{inc}$ where $\sigma_c = n_c e \mu_c$ and $\sigma_{inc} = n_{inc} e \mu_{inc}$. It is assumed that (i) n_c decreases with increasing T, but increases with increasing magnetic field, and (ii) μ_c is metallic, but $\mu_{inc} \ll \mu_c$, such that σ_{inc} is non-metallic and is descriptive of the experiments above T_c. (1) Below T_c, σ_c dominates even if $n_c \sim n_{inc}$ since $\mu_{inc} \ll \mu_c$. Thus the resistivity $\rho \sim 1/\sigma_c$ remains metallic. But close to T_c, it rapidly goes over to $1/\sigma_{inc}$, as observed, simply because n_c vanishes as $T \to T_c$. (2) Also, a reduction in n_c (rather than an increase in the scattering rate) allows ρ to acquire very large values in the metallic state (below T_c) without violating unitarity [14]. (3) Even a small magnetic field (a few tesla) causes a precipitous drop in the observed ρ, *and* shifts the resistivity peak by tens of degrees, an amount much larger than the Zeeman energy. This behaviour is hard to reconcile with a one-component model, but occurs naturally in a two-fluid system, since a magnetic field increases n_c. In the insulating regime, introduction of even a small number of coherent electrons would cause a large drop in ρ since $\mu_c \gg \mu_{inc}$. It would also cause a large shift in the resistivity peak which arises because σ_c decreases and σ_{inc} increases with T. (4) The model is consistent with the reported anomalous transfer of spectral weight in optical conductivity with increasing temperature, from a a metallic (Drude) to an incoherent component [15]. Finally, we note that extreme sensitivity to temperature and magnetic field has also been seen in the Hall effect [12].

We stress that the preceding discussion is only suggestive. The author is grateful to C Jayaprakash, T L Ho, P W Anderson and N P Ong for many useful discussions. Work at Princeton was supported by a grant from NSF (DMR 9104873).

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[11] Although the authors claim that there is only one energy scale, the theory of Millis *et al* is also characterized by the same two energy scales as our theory: the parameters $K \sim t_b$ and $\bar{t} \sim t_f$ (see the discussion following equation (6) in [7]).

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