Deviations from Fermi-Liquid Behavior above T_c in 2D Short Coherence Length Superconductors

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We show that there are qualitative differences between the temperature dependence of the spin and charge correlations in the normal state of the 2D attractive Hubbard model using quantum Monte Carlo simulations. The one-particle density of states shows a pseudogap above T_c with a depleted $N(0)$ with decreasing T. The susceptibility χ_s and the low frequency spin spectral weight track $N(0)$, which explains the spin-gap scaling: $1/T_1T \sim \chi_s(T)$. However, collective excitations contribute to the charge channel, and the compressibility $dn/d\mu$ is T independent. This anomalous "spin-charge separation" is shown to exist even at intermediate $|U|$ where the momentum distribution $n(\mathbf{k})$ gives evidence for a degenerate Fermi system.

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The unusual normal state properties of high T_c superconductors (SC) have led to many studies exploring possible scenarios for the breakdown of Fermi liquid theory (FLT) [1]. Much of this effort has been in one of two directions: search for genuinely new non-Fermi-liquid ground states arising from strong correlations in the proximity of an insulating state, or search for a low energy scale such that for temperatures above it one would see deviations from FLT. In this paper we take a different point of view and ask the question: Is the normal state of a short coherence length SC necessarily a Fermi liquid? More specifically, if the ground state is a condensate of fermion pairs, and the phase transition leads to a degenerate Fermi system above T_c, do the correlations in that normal state have to be described by Landau's FLT? If not, what are the characteristic deviations from FLT?

For weak coupling SC, with the coherence length $\xi_0 \gg a$, the lattice spacing, the normal state is a FL and both amplitude and phase coherence are established at T_c. As ξ_0/a decreases, the temperature scale T^* at which the amplitude builds up separates from T_c at which phase coherence is established [2,3]. In the extreme limit of tightly bound pairs, the system is a normal Bose liquid above T_c. The question then is if there is a broad intermediate coupling regime, especially in 2D, where the normal state $T_c < T < T^*$ has a "Fermi surface" and yet exhibits non-Fermi-liquid correlations.

The simplest lattice model within which this problem can be studied is the attractive Hubbard model where the pair size can be tuned by varying the strength of the interaction. In the absence of a small parameter we use quantum Monte Carlo (MC) simulations [4,5] to gain insight into the intermediate coupling regime above T_c. While the $U < 0$ Hubbard model is not a realistic microscopic model for the high T_c materials, it has two merits: its simplicity (fewest parameters) and the reliability of low temperature MC simulations, since it is one of the few interacting fermion models which is free of the "sign problem" at all densities [6].

We begin by summarizing our main results which are obtained in the normal state ($T > T_c$): (1) The momentum distribution $n(\mathbf{k})$ shows a structure reminiscent of a Fermi surface, though broadened by both thermal and interaction effects. (2) A pseudogap opens up in the one-particle density of states (DOS) well above T_c. The DOS is strongly T dependent—hence the notation $N_T(0)$—with $dN_T(0)/dT > 0$. We obtain $N_T(0)$ using a new method that avoids numerical analytic continuation. (3) At low T, the spin susceptibility $\chi_s(T) = N_T(0)$, while the compressibility $(dn/d\mu)$ is T independent. The spin and charge responses are thus qualitatively different. (4) The low frequency spin spectral weight has the form $K(\mathbf{q}) = \mathrm{Im}\chi(\mathbf{q},\omega)/\omega \sim N_T(0)/\Gamma_0(\mathbf{q})$ where the T dependence is largely in the DOS and $\Gamma_0(\mathbf{q})$ is essentially the same as in a noninteracting system. This naturally explains the spin-gap scaling $1/T_1T \equiv \sum_q K(\mathbf{q}) \sim \chi_x(T)$, noted in our previous work [5], and observed in the underdoped high T_c cuprates [7].

These results show that the normal state of a short coherence length 2D SC exhibits marked deviations from usual Fermi liquid behavior. One obtains a kind of "spin-charge separation" with the spin correlations determined by one-particle excitations, while collective excitations also contribute to the charge channel.

Consider the attractive Hubbard Hamiltonian $H = -t\sum_{i,j;\sigma} c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.} - |U|\sum_i n_{i\uparrow}n_{i\downarrow} + \mu\sum_{i;\sigma} n_{i\sigma}$, where the hopping is between nearest neighbor sites. All energies are measured in units of t, and the lattice spacing $a = 1$. We shall focus here on $|U| = 4$ and $\langle n\rangle = 0.5$. Qualitatively similar results were obtained at $|U| = 8$ and at other fillings [8]; details will be published separately.

To establish that we are above T_c in our *finite system,* we estimate the correlation length $\xi(T)$ from the spatial decay of the SC order parameter correlation function on systems of size up to $L = 16$. We find that for $|U| = 4$ we have $\xi \sim 3$–4 at $T = 1/6$; thus $\xi(T) \ll L$ and the system is normal. Earlier finite size scaling estimates [4] gave $T_c \simeq 0.05$ for $|U| = 4$, $\langle n\rangle = 0.5$. The crossover

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scale T^* is estimated [5] to be $T^* \simeq 1$ based on the deviation of $\chi_s(T)$ from the random phase approximation (RPA) result at high T.

Single-particle properties.—To ascertain that the system is degenerate at moderate $|U|$, we study the momentum distribution $n(\mathbf{k}) = \sum_\sigma \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle$ on large lattices of size up to $N = L^2 = 16^2$; see Fig. 1. It is clear that $n(\mathbf{k})$ shows a rapid variation with $\mathbf{k}$—a "Fermi surface"—even though it is broadened by the temperature and also affected by the interactions. We emphasize that we are *not* in the large-$|U|$ preformed boson limit, where the constituent fermions (tightly bound into singlet pairs) and nondegenerate and their $n(\mathbf{k})$ is independent of $\mathbf{k}$.

We now turn to the single-particle density of states (DOS) $N(\omega)$ with ω measured from μ. This is given by $N(\omega) = \frac{1}{N}\sum_{\mathbf{k}} \mathcal{A}(\mathbf{k},\omega)$. Here $\mathcal{A}$ is the spectral function, which is related to the imaginary time Green function $G(\mathbf{k},\tau) = -\langle T[c_{\mathbf{k}\sigma}(\tau)c^\dagger_{\mathbf{k}\sigma}(0)]\rangle$ via

$$G(\mathbf{k},\tau) = -\int_{-\infty}^{\infty} d\omega\, \frac{\exp(-\omega\tau)}{1+\exp(-\beta\omega)}\, \mathcal{A}(\mathbf{k},\omega) \quad (1)$$

for $0 < \tau < \beta = 1/T$. To estimate $\mathcal{A}$ and from it the DOS, given MC data for $G(\mathbf{k},\tau)$, involves inverting this Laplace transform. We avoid the numerical complications inherent in such an analytic continuation by deriving a general expression for $N(0)$ in terms of $G(\mathbf{k},\tau)$, which is valid *provided there is no low energy scale in the problem.* Fourier transforming to real space and looking at the local Green function at $\tau = \beta/2$, we get $G(\mathbf{r} = 0, \beta/2) = -\int d\omega\, \mathrm{sech}(\beta\omega/2)N(\omega)/2$. Let Ω be the frequency scale on which there is structure in the DOS; for $T \ll \Omega$ we obtain [9]

$$N(0) \simeq -\beta G(\mathbf{r} = 0, \tau = \beta/2)/\pi\,. \quad (2)$$

The one-particle DOS obtained from (2) is plotted in Fig. 2 as a function of temperature. We see that for $T > T_c$ a pseudogap develops at the chemical potential and the DOS $N_T(0)$ is depleted as T is reduced. This behavior should be compared with that in weak coupling where the DOS remains featureless above T_c, except for a small fluctuation dip [10]. The pseudogap at intermediate coupling may be thought of as the evolution of the weak coupling fluctuation dip into a regime where a/ξ_0 is no longer a small parameter.

Spin and charge correlations.—In Fig. 2 we also plot the uniform, static spin susceptibility χ_s. The T dependence of χ_s was already noted in Ref. [5]; what we see here is that this T dependence comes entirely from that of the one-particle DOS, so that $\chi_s(T) = N_T(0)$ (to within the errors inherent in extracting the latter).

It is interesting to ask whether the charge channel also exhibits the same pseudogap. The compressibility $(dn/d\mu)$ was obtained by numerically differentiating [11] the average density $\langle n\rangle$ determined as a function of μ. We found that $dn/d\mu$ shows significant system size dependence (much more than, e.g., χ_s); small system data show (finite size) upturns that are pushed down to lower T with increasing L. The results on the largest lattice ($L = 16$) plotted in Fig. 3 show that the system becomes more compressible with increasing $|U|$ (see below). More significantly, in sharp contrast to the one-particle DOS, $dn/d\mu$ is very weakly T dependent.

Within a simple RPA (particle-hole bubbles), we obtain $(dn/d\mu)^{\mathrm{RPA}} = 2N_0(0)/[1 - |U|N_0(0)]$. This is valid

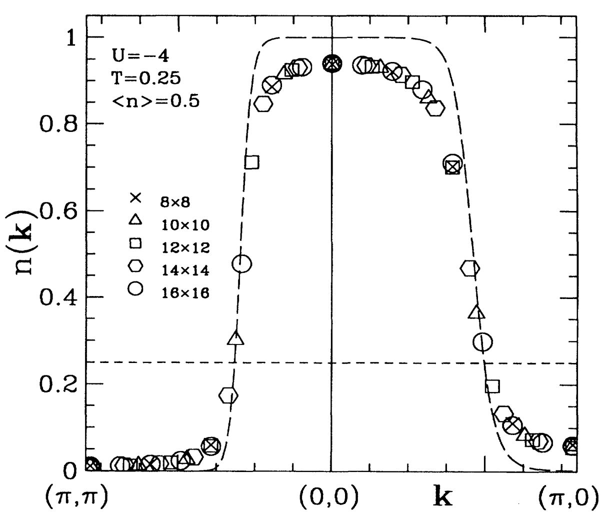

FIG. 1. The momentum distribution $n(\mathbf{k})$ vs $|\mathbf{k}|$ along [1,0] and [1,1] for $|U| = 4$, $\langle n\rangle = 0.5$, and $T = 0.25$. The Fermi function ($U = 0$) is shown as the long dashed curve, and the $U = -\infty$ Bose limit result is plotted as the short dashed curve. The statistical error bars on all the MC data, unless explicitly shown, are less than the size of the symbols in this and other figures.

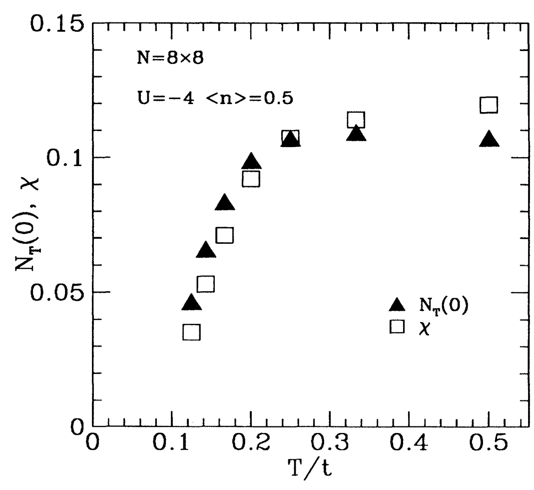

FIG. 2. The one-particle density of states $N_T(0)$ at the chemical potential (full triangles) and the spin susceptibility χ_s (open squares) as a function of temperature for $|U| = 4$, $\langle n\rangle = 0.5$, and $L^2 = 8^2$.

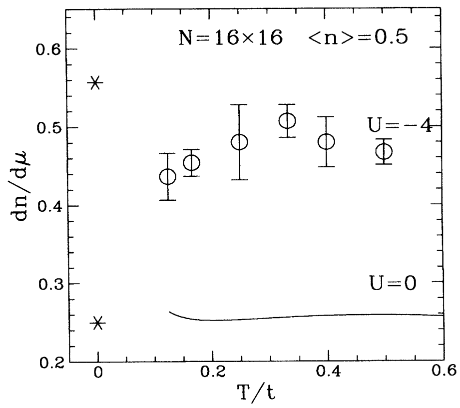

FIG. 3. The compressibility $(dn/d\mu)$ for $\langle n\rangle = 0.5$, $|U| = 0$ (full line), and $|U| = 4$ (open circles), as a function of T obtained on a 16^2 lattice. The $T = 0$ noninteracting and the $T = 0$ mean field result for $|U| = 4$ are also shown.

only when $|U|N_0(0) \ll 1$, where it correctly explains the trend that attractive interactions increase $dn/d\mu$; for large $|U|$ RPA fails in that it predicts an entirely spurious instability (phase separation) when $|U|N_0(0) = 1$. In fact, pairs form at large $|U|$ and their residual interactions are repulsive, so that the compressibility of the system remains finite for *all* $|U|$. It is simplest to see this in the broken symmetry state at $T = 0$ where we find [12] that, within mean field (MF) theory, $dn/d\mu$ decreases monotonically with $|U|$ from $dn/d\mu \simeq 2N_0(0)[1 + |U|N_0(0)]$ for small $|U|$ to $dn/d\mu \simeq |U|/4dt^2 - 2/|U|$ for $|U|/t \gg 1$. The $T = 0$ MF result [12] is also shown in Fig. 3 and is found to be of the right order of magnitude as the normal state MC result; note that we do not expect $dn/d\mu$ to change dramatically as T goes through T_c.

The difference between the spin and charge response functions could be characterized as a sort of spin charge separation [13]. In its mildest form this exists even in a Landau Fermi liquid where χ_s and $dn/d\mu$ are quantitatively different, the two being renormalized by different FL parameters: F_0^a and F_0^s. What we see here is much stronger: As a result of strong interactions, χ_s and $dn/d\mu$ acquire *qualitatively different* T dependences. As argued above, the spin response is dominated by incoherent single-particle excitations, which is T dependent because triplet excitations require breaking up the singlet pair correlations, while the pair excitations directly contribute to the charge channel.

Spin-gap scaling.—We next use our results for the T-dependent DOS $N_T(0)$ to gain insight into the suppression of low frequency spectral weight in the spin channel as probed by $K(\mathbf{q}) = \lim_{\omega\to 0} \mathrm{Im}\chi(\mathbf{q},\omega)/\omega$. To contrast with our MC results, it may be useful to recall that for a Fermi liquid (all quantities denoted by a subscript 0) $K_0(\mathbf{q}) = N_0(0)/\Gamma_0(\mathbf{q})$ is T independent for $T \ll \epsilon_F$ with $\Gamma_0(\mathbf{q}) \sim v_F q$. Further $\sum_{\mathbf{q}} \Gamma_0^{-1}(\mathbf{q}) \simeq N_0(0)$ leads to the Korringa law $(1/T_1T)_0 = \sum_{\mathbf{q}} K_0(\mathbf{q}) \sim N_0^2(0)$.

In Fig. 4 we plot the MC results for $K(\mathbf{q})$ for $\mathbf{q} \neq 0$. The analytic continuation for K used the method of Ref. [5]. From Fig. 4(a) we see that $K(\mathbf{q})$ is more or less uniformly suppressed at all $\mathbf{q}$ with decreasing T. Further, this T dependence is similar to that of $\chi_s(T)$ (or the DOS) shown at $\mathbf{q} = 0$ in Fig. 4(a). For fixed T the $\mathbf{q}$ dependence of $K(\mathbf{q})$ resembles that of the noninteracting system; see Fig. 4(b). These results thus suggest that $K(\mathbf{q};T) = \alpha N_T(0)/\Gamma_0(\mathbf{q})$, with α independent of T and $\mathbf{q}$; i.e., the T dependence comes from a DOS with a pseudogap, while the $\mathbf{q}$ dependence is that of the noninteracting system. This form for $K(\mathbf{q};T)$ leads to $1/T_1T = \sum_{\mathbf{q}} K(\mathbf{q};T) \simeq \alpha N_0(0)N_T(0)$, thus providing a natural explanation for the spin-gap scaling $1/T_1T \sim \chi_s(T)$ found in our earlier MC studies [5].

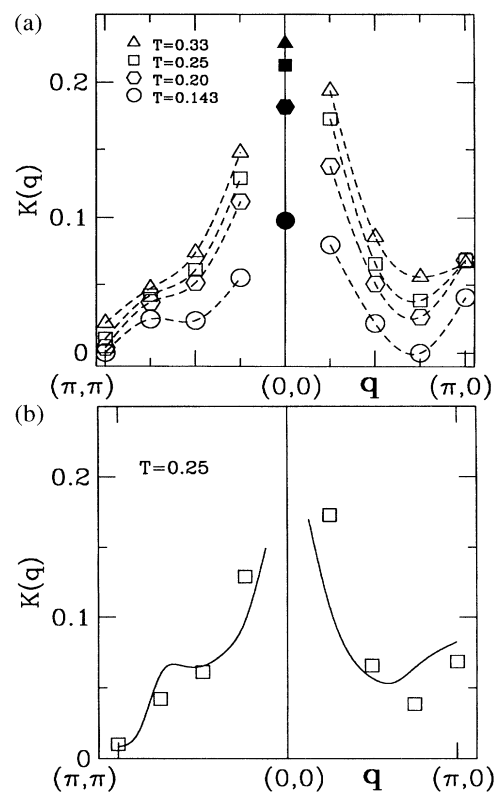

FIG. 4. (a) Low frequency spectral weight in the spin channel $K(\mathbf{q};T) = \lim_{\omega\to 0} \mathrm{Im}\chi(\mathbf{q},\omega)/\omega$ for $\mathbf{q} \neq 0$ (open symbols) plotted along [1,0] and [1,1] for various T. The dashed lines are guides to the eye. The filled symbols plotted at $\mathbf{q} = 0$ show $2.0\chi_s(T)$ with T corresponding to that of the open symbols. Note that the T dependence of $K(\mathbf{q})$ is similar to that of the susceptibility $\chi_s(T)$. All of the data are for $|U| = 4$, $\langle n\rangle = 0.5$, and $L^2 = 8^2$. (b) At a fixed T the $\mathbf{q}$ dependence of $K(\mathbf{q})$ is qualitatively similar to that of the noninteracting case. To show this we compare the $K(\mathbf{q})$ at $T = 0.25$ (open squares) with the full curve given by $2\chi_s(T)K^0(\mathbf{q})$, where $K^0(\mathbf{q})$ is the essentially T-independent spectral weight for the noninteracting system.

We note that $1/T_1T \sim \chi_s(T)$ is observed in the (planar) O and Y NMR in a large number of (usually underdoped) cuprates [7]. What distinguishes the results presented here from spin-gap theories [14] based on spin models is that the anomalies exist in a single layer 2D system with itinerant carriers with a large Fermi surface. Secondly, in the present approach these anomalies are directly related to the T dependence of the one-particle DOS. On the other hand, since we work with a "coarse-grained" model, rather than a realistic microscopic one, we cannot discuss the $\mathbf{q}$ structure of the spin response leading to differences in the Cu and O NMR, or the doping dependences. It is also an important open problem to study the normal state precursors of short coherence length SC with nodes in the gap.

In conclusion, we have shown that the normal state of a 2D short coherence length SC exhibits characteristic deviations from Fermi liquid behavior: While the momentum distribution gives clear evidence for a degenerate Fermi system, the one-particle DOS shows a pseudogap [15], and the spin and charge correlations show qualitatively different temperature dependences.

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