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Spin-charge separation in the two-dimensional Hubbard and t-J models at low electronic density

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The spin- and density-correlation functions of the two-dimensional Hubbard model at low electronic density $\langle n \rangle$ are calculated in the ground state by using the power method, and at finite temperatures by using the quantum Monte Carlo technique. Both approaches produce similar results, which are in close agreement with numerical and high-temperature-expansion results for the two-dimensional t-J model. Using perturbative approximations, we show that the examination of the density-correlation function alone is not enough to support recent claims in the literature that suggested spin and charge separation in the low electronic density regime of the t-J model.

The normal state of the high-temperature superconductors does not behave as an ordinary Fermi liquid (FL).[1] For the last several years, Anderson[2] has strongly supported the idea that instead it may be described as a Tomonaga-Luttinger liquid (TLL).[3] The TLL state has been shown by exact theories[4] and numerical studies[5,6] to be the ground state of the Hubbard model, and also the t-J model, in one dimension. A special property of the TLL state is the separation of spin and charge degrees of freedom.

For these ideas to be applicable to the cuprates, the crucial question is whether phenomenologically realistic two-dimensional (2D) models of correlated electrons present features in the ground state similar to those of their one-dimensional counterparts. Recently, several numerical studies have addressed this important issue, namely, the possibility of spin-charge separation in the two-dimensional t-J model. Using a ground-state projection technique ("power" method) to study the low electronic density region, two of us[7] have found indications that spin, charge, and pairing correlations behave in a similar manner as in 1D. Qualitatively the TLL state seems to provide a consistent *phenomenological* interpretation of the numerical data. In parallel, based on the results of high-temperature expansions, Putikka *et al.*[8] have argued that spin-charge separation occurs in the 2D t-J model at low and high electronic densities (particularly at high electronic density). The gauge theory[9] approach also predicts a non-Fermi liquid (NFL) behavior, although it may not necessarily correspond to a TLL state. On the other hand, for the 2D Hubbard model, analytical studies[10] based upon diagrammatic methods suggest the presence of a Fermi liquid at low electronic density.

Since it is well known that the t-J model is equivalent to the Hubbard model in the strong-coupling limit, the results described above are apparently inconsistent. However, the nonperturbative constraint of no double occupancy in the t-J model may produce subtle differences with the Hubbard model. Precisely, one of the purposes of this paper is to study numerically the possible variation of physical properties between these two models as the constraint of no double occupancy is relaxed. Our analysis shows that the density- and spin-correlation functions in the ground state of the 2D Hubbard and t-J models are qualitatively similar at least at low electronic density. To examine the question of spin-charge separation we compare our results for the density correlations obtained by the power method at zero temperature on 8×8 and 16×16 clusters, and by the Quantum Monte Carlo (QMC) method[11] at finite temperature, with that of the high-temperature expansions.[8] Excellent agreement between the results of these three methods is obtained. However, from our analysis we cannot identify the spinless fermions (SF) Fermi wave vector $2\mathbf{k}_F^{SF}$ as the characteristic wave vector of the t-J and Hubbard models at low electronic density as suggested by Putikka *et al.*[8] Both the density and spin correlations can be understood qualitatively in terms of perturbative approaches such as a random-phase approximation (RPA)[12] with a renormalized Hubbard coupling $\tilde{U}$. In addition, the correlations in real space at low electronic density are shown to decay so rapidly with distance that the subtle issue of spin-charge separation in these models is difficult to address unless these small correlations are accurately evaluated on a finite cluster, or the functional form of the correla-

tions at large distance is obtained with some reliable technique.

The Hamiltonian for the 2D t-J model considered here has the form

$$H_{tJ}=-t\sum_{\langle ij\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j), \tag{1}$$

with the constraint of no double occupancy. The Hamiltonian for the 2D Hubbard model is well known and will not be reproduced here. For very large U/t the Hubbard model is equivalent to the t-J model with $J=4t^2/U$, up to two-particle hopping terms. The good agreement between results for the t-J and Hubbard models reported below justifies the omission of these three-site terms.[13] Two numerical methods are used to calculate the equal-time density- and spin-correlation functions, $N(\mathbf{q})$ and $S(\mathbf{q})$, defined by the relations

$$N(\mathbf{q})=\sum_{\mathbf{r}}e^{i\mathbf{q}\cdot\mathbf{r}}\langle\delta n_0\delta n_{\mathbf{r}}\rangle, \tag{2}$$

$$S(\mathbf{q})=\sum_{\mathbf{r}}e^{i\mathbf{q}\cdot\mathbf{r}}\langle S^z_0S^z_{\mathbf{r}}\rangle, \tag{3}$$

where $S^z_{\mathbf{r}}=\frac{1}{2}\Sigma_{\alpha\beta}c^{\dagger}_{\mathbf{r}\alpha}\sigma^z_{\alpha\beta}c_{\mathbf{r}\beta}$, and $\delta n_{\mathbf{r}}=\Sigma_{\sigma}c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}\sigma}-\langle n\rangle$. Here $\langle n\rangle$ is the average density of electrons. The brackets in Eqs. (2) and (3) refer to thermal averaging in the grand canonical ensemble when the QMC method is used. At zero temperature, the ground-state wave function obtained by the power method in the canonical ensemble is used to calculate the average. We have observed that the well-known fermion determinantal sign problem does not pose a difficulty in the low-electronic-density region considered in this paper in any of the techniques. However, this problem becomes more severe with increasing density, and thus we restrict our analysis to the low density region.

The power method has been proven to be very effective in calculating ground-state correlation functions of the t-J model in 1D (Ref. 6) and 2D.[7] The ground-state wave function is projected out by applying a large power of the Hamiltonian, $(-H)^p$, to a trial wave function. The power p required to reach convergence depends on the choice of the trial functions. For the case of the Hubbard model we use the well-known Gutzwiller wave function,[14] i.e., $|\text{GW}\rangle=g^D|\text{FG}\rangle$, where $|\text{FG}\rangle$ is the ideal Fermi gas wave function on a lattice and D is the total number of doubly occupied sites. Here, g is the only variational parameter. At $g=0$, the factor g^D becomes the well-known projection operator P_d that projects out states with doubly occupied sites. For the t-J model we use the wave function proposed by Hellberg and Mele[15] in 1D and later generalized by Valenti and Gros[16] to 2D. This function, which we shall call Ψ_{HMVG}, is basically of the same form as $|\text{GW}(g=0)\rangle$, i.e., a Slater determinant for up-spin electrons and one for down-spin electrons. In addition to these two determinants, it contains a long-range correlation part between all the particles, $\Pi_{i<j}|\mathbf{r}_i-\mathbf{r}_j|^{\nu}$ (while for nearest-neighbor particles we chose $\nu=0$). It was shown in Ref. 7 that this wave function is very close to the ground state for $J/t\leq 2$ in the low-electronic-density region.

$S(\mathbf{q})$ and $N(\mathbf{q})$ are plotted in Figs. 1(a) and 1(b), respectively, against momenta along the Γ-X-M-Γ directions for an 8×8 cluster. The open circles represent the QMC results obtained at temperature $T=t/10$, $U=4t$, and $\langle n\rangle=0.159$. The open squares are for $U=8t$ and $\langle n\rangle=0.155$, at $T=t/8$. The $U=8t$ results deviate further from the ideal Fermi gas shown by the dashed line than the $U=4t$ data. The open triangles represent ground-state results for $U=8t$ obtained for the same lattice with 10 particles ($\langle n\rangle=10/64\approx 0.156$), by applying $p=12$ powers of the Hubbard Hamiltonian to the $|\text{GW}\rangle$ wave function with $g=0.5$. In most regions of $\mathbf{q}$ space the open triangles and squares take the same values. It is gratifying to find out this excellent agreement between two very different numerical techniques, namely, the power method and QMC. To gauge the effect of the constraint of no double occupancy, in the same figures we also present results for the t-J model[7] at $J=0.1t$. These results, which are represented by the solid triangles in Figs. 1(a) and 1(b), are obtained from the trial wave function Ψ_{HMVG}—$\nu=0.1$ with

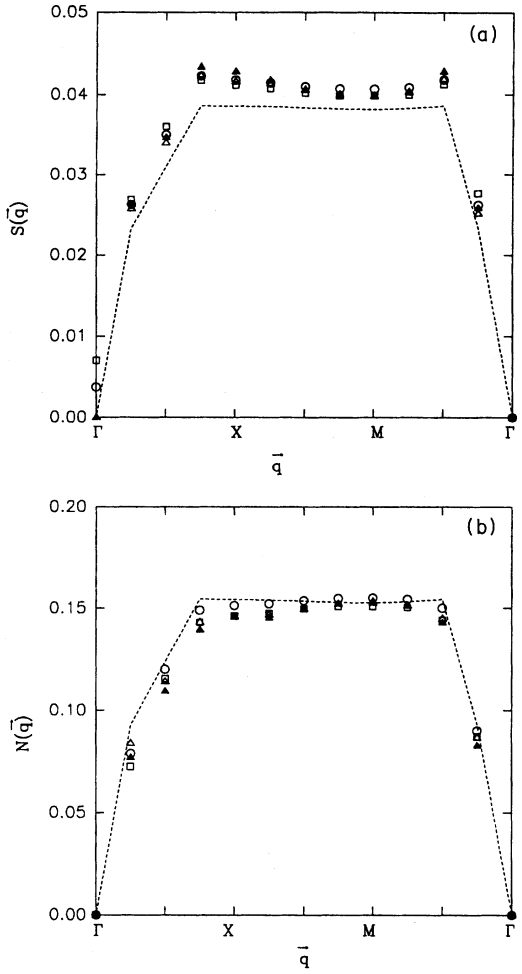

FIG. 1. (a) Spin-correlation function $S(\mathbf{q})$ and (b) density-correlation function $N(\mathbf{q})$ in momentum space along the Γ-X-M-Γ directions on a 8×8 square lattice. Open circles represent QMC results at $U=4t$, $\langle n\rangle=0.159$, and $T=t/10$. The open squares correspond to $U=8t$, $\langle n\rangle=0.155$, and $T=t/8$. The open triangles represent ground-state results for the Hubbard model at $U=8t$ with 10 electrons. The solid triangles denote ground-state results for the t-J model at $J=0.1t$. The dashed line is the result for an ideal Fermi gas.

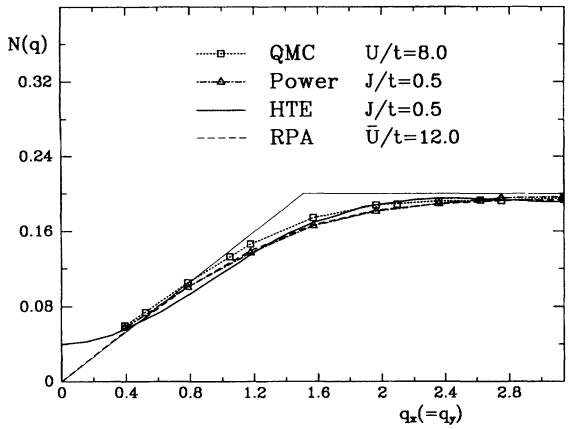

FIG. 2. The density correlation $N(\mathbf{q})$ along the diagonal direction $q_x=q_y$ on a 16×16 cluster. The open squares represent the QMC results obtained at $T=t/4$, $U=8t$, and $\langle n\rangle=0.2$ (results on 12×12 lattices are also shown). The open triangles are power method ground-state results for the t-J model at $J=t/2$. The solid line is the result obtained by the high-temperature expansion of Ref. 8. The dashed line denotes the RPA prediction. The result for an ideal Fermi gas is plotted as a thin continuous line.

power $p=16$. The t-J model results agree very well with the open triangles which correspond to the Hubbard model with $U=8t$ ($J=t/2$ in the t-J model language). Hence, there is little difference in the correlation functions between strong and intermediate couplings.

Let us now analyze the implications of Figs. 1(a) and 1(b). All the curves in Fig. 1(a) have peaks at the $2\mathbf{k}_F$ wave vectors, except the ideal Fermi gas which only presents a discontinuous derivative. The peak size increases with the value of U/t. The presence of these peaks[7] implies a stronger spin-density-wave correlation at finite coupling than the ideal gas. It is interesting to notice that a similar peak is observed[6] in 1D. Though the magnitude of the peak in 1D is much greater than in 2D, this large difference may be partly due to the dimensionality effect. Unlike 1D in which there is only one $2\mathbf{k}_F$ wave vector, in 2D there is a characteristic vector in each direction in the two-dimensional momentum space, each one carrying a peak in $S(\mathbf{q})$. In contrast to the spin correlations, $N(\mathbf{q})$ shown in Fig. 1(b) is reduced at $\mathbf{q}=2\mathbf{k}_F$ as compared to the values of the ideal Fermi gas shown by the dashed line. The reduction is larger as the coupling U/t is increased. The plateau observed for $k>2k_F$ for the ideal gas seems to have shifted to a larger value of k. Putikka *et al.*[8] have argued this wave vector to be $2\mathbf{k}_F^{\mathrm{SF}}$. The presence of the Fermi wave vector $\mathbf{k}_F^{\mathrm{SF}}$ for a spinless fermionic system would imply the separation of charge and spin degrees of freedom.

To examine the important issue of whether $2\mathbf{k}_F^{\mathrm{SF}}$ appears in the numerical results, and in order to reduce possible finite-size effects we have calculated $N(\mathbf{q})$ on a 16×16 lattice using both the QMC and power-method techniques. In Fig. 2, $N(\mathbf{q})$ is plotted as a function of $\mathbf{q}$ along the diagonal direction $q_x=q_y$. The open squares represent the QMC results obtained at temperature $T=t/4$, $U=8t$, and $\langle n\rangle=0.2$. The open triangles represent ground-state results obtained for the same cluster with 50 particles (i.e., $\langle n\rangle\approx0.195$) by applying twelve powers of the t-J Hamiltonian to the Ψ_{HMVG} variational wave function with $\nu=0.04$. The results of the high-temperature expansions[8] corresponding to $J=t/2$ and temperature $T=J/2$ are indicated by the solid line. There is very little difference between the results of these three numerical methods. This implies that the numerical accuracy of the data is not questionable, but only the interpretation needs to be analyzed carefully. For comparison, the result of the ideal Fermi gas is plotted as the thin continuous line in Fig. 2. It is obvious that the results of the interactive system deviate appreciably from the ideal gas results. However, these results do not unambiguously support the identification of a singularity at $2\mathbf{k}_F^{\mathrm{SF}}$. A more conservative interpretation is that they indicate a broad maximum of $N(\mathbf{q})$ at $\mathbf{q}=(\pi,\pi)$ which may just reflect the short-range effective repulsion between particles.

To explore further this assumption we compare $N(\mathbf{q})$ against the $T=0$ RPA results (dashed line in Fig. 2). The best fit is obtained by choosing the renormalized interaction $\bar{U}$ to be $12t$. Thus, the apparent shift of the characteristic wave vector can be mimicked very well by a simple perturbative (Fermi liquid based) approach. We have also calculated $S(\mathbf{q})$ using RPA.[12] The peaks at $2\mathbf{k}_F$ are also reproduced this time using a smaller effective coupling $\bar{U}=3t$. Such a qualitative description of spin- and density-correlation functions in terms of a simple RPA tends to support the point of view that the ground state of the Hubbard model is just a strongly correlated Fermi liquid. But this may also be misleading. It is also possible to reproduce the correlation functions of a *one*-dimensional Hubbard model by using the RPA approximation. Just like in two dimensions, a small effective interaction $\bar{U}$ is enough to produce a large peak in $S(\mathbf{q})$ at the proper wave vector $2\mathbf{k}_F$. To fit the density-correlation function, a larger $\bar{U}$ is needed, i.e., the systematic behavior is very similar in 1D and 2D (as emphasized in Ref. 7).

The excellent agreement between techniques that work at zero and finite temperature shown in Fig. 2 suggests that the shift in $N(\mathbf{q})$ cannot be due to subtle long distance correlation functions but to short distance effects. To study this hypothesis we analyzed in real space the density-density correlation, $C(\mathbf{r})$, for the case of the one-band Hubbard model. Figure 3(a) shows that this correlation decays rapidly with distance and it becomes negligible at four lattice spacings away from the origin [numerically the signal at this distance is approximately $5\times10^{-4}C(\mathbf{r}=\mathbf{0})$]. These 2D correlations are considerably smaller than those obtained in the case of the one-dimensional Hubbard model, which we know shows spin-charge separation. This analysis shows that it would be difficult to obtain reliable numerical information about the behavior of the correlation functions at distances larger than a few lattice spacings. Thus, a proper study of spin-charge separation seems beyond present day accuracy of computational and series expansion analysis at low electronic density.

Can the results of our analysis be extended to higher densities? In Fig. 3(b), $N(\mathbf{q})$ is shown at quarter-filling using the Hubbard model with $U/t=8$ and the QMC technique. The results deviate considerably from the noninteracting Fermi gas, but they can be accurately reproduced by a simple perturbative calculation (first order) with an effective coupling $\bar{U}=4t$ (see also Ref. 17). Then, we believe that our conclusions for the Hubbard model can be extended to the domain $0.0\leq\langle n\rangle\leq0.5$. At higher densities the perturbative ap-

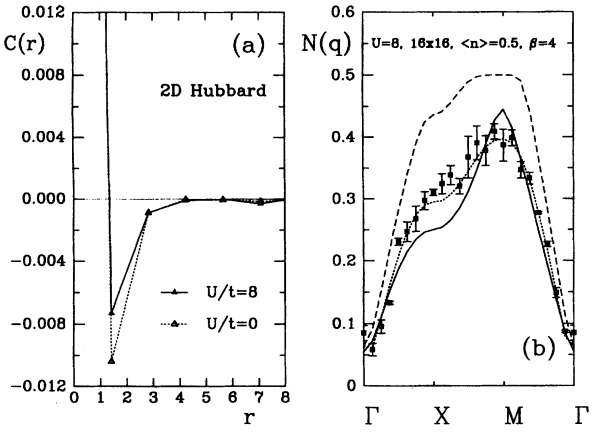

FIG. 3. (a) Density-density correlation $C(\mathbf{r})=\langle n_0 n_\mathbf{r}\rangle-\langle n\rangle^2$ as a function of the distance $\mathbf{r}$. The solid line is the power method result obtained at $J/t=0.5$ (i.e., $U/t=8$ in the Hubbard model) on a 16×16 cluster and density $\langle n\rangle\approx0.20$. The dashed line denotes the result for a tight-binding noninteracting system $U/t=0$ of the same size. The correlations are considered along the diagonal of the lattice (the lattice spacing is equal to one). (b) The density correlation $N(\mathbf{q})$ along the direction Γ-X-M-Γ using the QMC technique (full squares) on a 16×16 cluster, at $T=t/4$, $U/t=8$, and density $\langle n\rangle=0.5$. The dashed line indicates the result for an ideal Fermi gas, while the dotted line corresponds to a perturbative calculation using an effective coupling $\tilde{U}=4t$. The continuous line corresponds to noninteracting spinless fermions at the same density and temperature.

proach breaks down at intermediate and large couplings, due to antiferromagnetism. On the other hand, the results for the t-J model at the density are very similar to those of noninteracting spinless fermions, as remarked in Ref. 8 using the high-temperature expansions. The possible origin of this discrepancy is currently under study.

In summary, we have presented spin- and density-correlation functions for the one-band Hubbard model at low electronic density. The ground-state results obtained by the power method agree well with the finite-temperature results obtained by QMC. Measurements at intermediate U/t couplings for the Hubbard model are consistent with strong-coupling data for the t-J model. Compared against the ideal gas results, we confirm that $N(\mathbf{q})$ is appreciably reduced at $\mathbf{q}=2\mathbf{k}_F$ as claimed by Putikka *et al.*[8] This difference increases with the strength of the Hubbard interaction. The enhancement of spin-density-wave correlation as shown by the appearance of peaks at the $2\mathbf{k}_F$ wave vectors for $S(\mathbf{q})$ also increases with U/t. This result, observed in Ref. 7, is confirmed by the present study on larger clusters and thus finite-size effects seem small. On the other hand, the RPA approximation can provide a rough qualitative understanding of all these results. In addition, examining $N(\mathbf{q})$ on a 16×16 lattice we did not find evidence for the presence of the characteristic wave vector of a spinless fermion model. Actually, the density correlations in real space decay so rapidly that making any statement about their asymptotic behavior based on numerical techniques at finite temperature is risky. Thus, based on the current available information it is *not* possible to conclude that spin-charge separation takes place in the low electronic density of the 2D Hubbard and t-J models. However, we cannot rule out this possibility either. The complete separation of spin and charge as in the infinite U limit of the 1D Hubbard model may not be a proper guidance for 2D studies. A possible scenario is that although charge and spin are separated, they interact strongly as in the finite U/t Hubbard model in 1D. This question is currently being studied.

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