Spin and Charge Dynamics of the t-J Model

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We investigate the dynamical spin and charge correlation functions, $S(\mathbf{Q},\omega)$ and $N(\mathbf{Q},\omega)$, for the two-dimensional (2D) t-J model by using the exact diagonalization technique. Both quantities are compared with the 1D t-J model. At high electron density ($n > 0.7$), a remarkable feature emerges: $S(\mathbf{Q},\omega)$ shows a pronounced peak at low energy of order J which is consistent with $2k_F$ low-energy excitations, whereas low-energy $2k_F$-backscattering processes are strongly suppressed in the charge-density response. $N(\mathbf{Q},\omega)$ consists of a dense and broad continuum, qualitatively different from the 1D charge response, implying strong interactions between charge and spin degrees of freedom.

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One of the fundamental questions about two-dimensional (2D) strongly correlated electron systems is whether their spin and charge response shares some similarity with the one-dimensional (1D) correlated systems [1]. It is well known that the 1D systems show non-Fermi liquid behavior, i.e., they are Tomonaga-Luttinger (TL) liquids [2]. One of the characteristic features is the asymptotic power-law decay of the equal-time charge-charge correlation function with $2k_F^{\mathrm{SF}}$ oscillations, where $k_F^{\mathrm{SF}} = 2k_F$ is the Fermi momentum of spinless fermions (SF's). In a recent high temperature series expansion study (HTSE) Putikka *et al.* [3] investigated the equal-time charge correlation function and observed in the corresponding structure factor $N(\mathbf{Q})$ a change of slope at $2\mathbf{k}_F^{\mathrm{SF}}$, which they considered as a fingerprint for charge-spin separation in 2D. Also other studies show similar trends for $N(\mathbf{Q})$ [4–6]. Yet the observation of this feature does not necessarily imply an asymptotic behavior of the charge correlations similar to 1D and the existence of related low-energy charge excitations with $\mathbf{Q} = 2\mathbf{k}_F^{\mathrm{SF}}$. For example the increased value of $\mathbf{Q}$ where the change of slope in $N(\mathbf{Q})$ occurs may simply reflect an increase of the average distance of particles as a consequence of the double occupancy constraint, as was argued by Chen *et al.* [5]. Moreover conclusions based on the static structure factor are highly indirect, and the investigation of the dynamical charge reponse is necessary. Surprisingly there is not much known about the dynamical charge structure factor $N(\mathbf{Q},\omega)$. Even in 1D where the exact Bethe ansatz solution for the Hubbard model exists, $N(Q,\omega)$ is not known except for certain limiting cases [7].

To fill this gap at least partially we investigate in this Letter the dynamical spin and charge correlation functions, $S(\mathbf{Q},\omega)$ and $N(\mathbf{Q},\omega)$, of the 1D and 2D t-J models as a function of electron density n, by using a standard exact diagonalization technique. As far as we know, this is the first work which reports a systematic study of $N(\mathbf{Q},\omega)$ for the 1D and 2D t-J models. A remarkable difference between the 1D and 2D systems appears in $N(\mathbf{Q},\omega)$ at high electron density in spite of the similar behavior of the static structure factor $N(\mathbf{Q})$. While $N(Q,\omega)$ in 1D shows pronounced peaks corresponding to the excitations of SF's, $N(\mathbf{Q},\omega)$ in 2D consists of a dense and broad continuum. The difference demonstrates strong interaction between spin and charge degrees of freedom in the 2D system. An interesting crossover from low to high electron density also occurs in the dynamical response functions for the 2D t-J model. At low electron density, the characteristic excitation energies of $S(\mathbf{Q},\omega)$ and $N(\mathbf{Q},\omega)$ are unrenormalized, i.e., similar to those of noninteracting electrons. At high density, $S(\mathbf{Q},\omega)$ shows low-energy $2k_F$ excitations with energy of order J, whereas the low-energy $2k_F$-scattering processes are strongly suppressed in the charge channel, the suppression of which is similar to the 1D model.

The Hamiltonian describing the t-J model is

$$H = -t \sum_{\langle i,j\rangle\sigma} (\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{j\sigma} + \mathrm{H.c.}) + J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \quad (1)$$

where $\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i\bar{\sigma}})$ is the annihilation operator of an electron with spin σ at site i with the constraint of no double occupancy, $\mathbf{S}_i$ is the spin operator, and the summation $\langle i,j\rangle$ runs over nearest-neighbor (n-n) pairs. We take $t = 1$ as the unit of energy. A standard Lanczos algorithm for small clusters is applied to obtain the ground state and dynamical quantities. The continued fraction in the algorithm is truncated at 200 iterations. We use a 16-site chain and 4×4 and 18-site unit cells for the 1D and 2D t-J models, respectively.

The equal-time spin and charge correlation functions are defined as $S(\mathbf{Q}) = \langle 0|S_{-\mathbf{Q}}^z S_{\mathbf{Q}}^z|0\rangle/L$ and $N(\mathbf{Q}) = \langle 0|N_{-\mathbf{Q}}N_{\mathbf{Q}}|0\rangle/L$, with $S_{\mathbf{Q}}^z = \sum_i e^{i\mathbf{Q}\cdot\mathbf{R}_i} S_i^z$ and $N_{\mathbf{Q}} = \sum_i e^{i\mathbf{Q}\cdot\mathbf{R}_i}(n_i - n)$, where S_i^z is the z component of the spin operator and $n_i = n_{i\uparrow} + n_{i\downarrow}$. $|0\rangle$ denotes the ground state, and L is the total number of sites. The dynamical

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spin-spin and charge-charge correlation functions are given by

$$S(\mathbf{Q},\omega) = \frac{1}{L}\sum_{\nu} |\langle\nu|S^z_{\mathbf{Q}}|0\rangle|^2 \delta(\omega - E_\nu + E_0) \quad (2)$$

and

$$N(\mathbf{Q},\omega) = \frac{1}{L}\sum_{\nu} |\langle\nu|N_{\mathbf{Q}}|0\rangle|^2 \delta(\omega - E_\nu + E_0), \quad (3)$$

where $|\nu\rangle$ is the νth eigenvector with eigenvalue E_ν.

We begin with a discussion of $S(Q,\omega)$ and $N(Q,\omega)$ for the 1D case. The calculated results for $J = 0.4$ and electron density $n = 0.75$ (12 electrons in the 16-site chain) are shown in Fig. 1. A log-scale is taken to emphasize spectra with small weight. $N(Q,\omega)$ shows perfect SF behavior [filled peaks in Fig. 1(a), which are an order of magnitude larger than the background], as expected from the Bethe ansatz solution of the Hubbard model in the $U \to \infty$ ($J \to 0$) limit [7]. For example, at $Q = \pi$ there are two distinct excitations for the 16-site chain. The spectra nicely show the low-energy excitations at $2k_F$ ($3\pi/4$) and $4k_F$ ($2\pi - 4k_F = \pi/2$) in S and N, respectively. Similar features of $N(Q,\omega)$ have also been observed by Preuss *et al.* [8] in a recent Monte Carlo study of the 1D Hubbard model. Additional small structures appear due to spin and charge mixing. Among these faint features are the low-energy $2k_F$ excitations in $N(Q,\omega)$. These structures vanish in the $J \to 0$ limit.

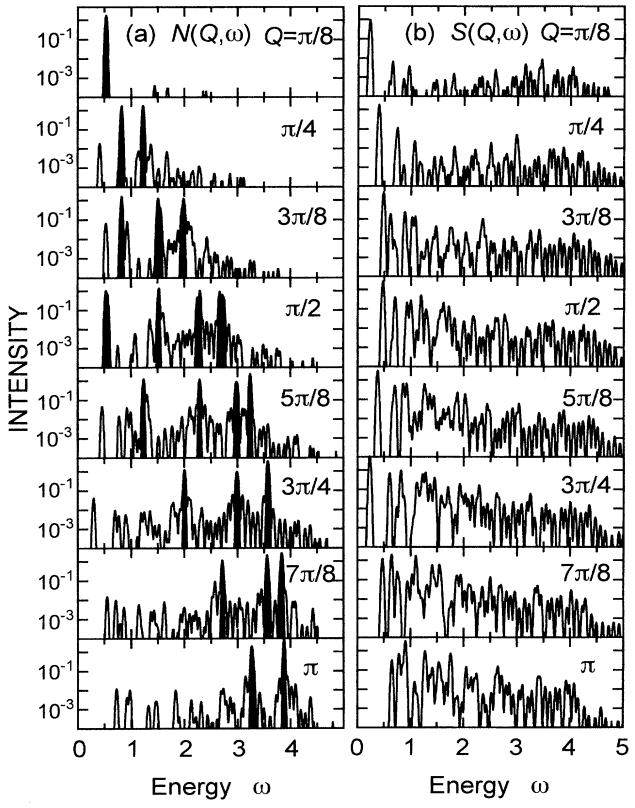

FIG. 1. Energy dependence of (a) $N(Q,\omega)$ and (b) $S(Q,\omega)$ for the 1D 16-site t-J model ($J = 0.4$) with antiperiodic BC at $n = 0.75$ (12 electrons). A log-scale is taken to emphasize spectra with small weight. The filled peaks in (a) correspond to peaks originated from excitations of the spinless fermions.

The energy of the lowest excitation in $S(Q,\omega)$ at $Q = \pi/8$ is the measure of spin velocity v_s and is lower than that of $N(Q,\omega)$ characterizing the charge velocity v_c. The difference of the velocities is a direct demonstration of the charge-spin separation characteristic for the 1D TL liquids [2,9]. It is interesting to notice that the small background in $S(Q,\omega)$ extends over the whole bandwidth of the noninteracting model $\omega = 4$.

In the 1D system there is no qualitative change with electron density n, except for a change of the characteristic momenta, $2k_F$ and $4k_F$, and the characteristic density dependence of the spinon energy [7,10] in the range $Q < 2k_F$, which we clearly see even at $n = 0.25$.

In the 2D t-J model, on the other hand, there is a dramatic change of the spectra between small and large electron concentration. At small electron density, for example, 4 electrons in a 4×4 unit cell, both spectra $S(\mathbf{Q},\omega)$ and $N(\mathbf{Q},\omega)$ are qualitatively consistent with the excitations of noninteracting electrons (not shown): The dominant excitations are unrenormalized and have the same energy scale as in the noninteracting case, although small energy shifts and splittings of the spectra exist due to strong correlations. Details for small n ($n < 0.5$) will be discussed elsewhere [11].

At large electron density ($n > 0.7$), however, the spectra $S(\mathbf{Q},\omega)$ and $N(\mathbf{Q},\omega)$ are strikingly different. Figure 2 shows results for the 4×4 unit cell and $J = 0.4$ at $n = 0.75$. In the calculation, we adopt a mixed boundary condition (BC), where periodic (antiperiodic) BC are chosen in y (x) directions, to form the closed shell structure in the noninteracting limit. This BC lifts the degeneracy of equivalent $\mathbf{Q}$ points except for $\mathbf{Q} = (\pi/2, \pi/2)$. It is clear that the distributions of the spectral weight are completely different between $S(\mathbf{Q},\omega)$ and $N(\mathbf{Q},\omega)$ in contrast to the low density case [12].

Similar to the 1D case, there is a clear separation of energy scales of charge and spin excitations. The spin excitations appear as a sharp dispersive peak with energy $\omega \sim 2.5J$ at (π,π) and $\sim 0.8J$ at $2\mathbf{k}_F \simeq (\pi, \pi/2)$ [13], which almost completely exhausts the sum rule given by $S(\mathbf{Q})$. The background at higher energy is smaller than expected from slave boson theories, probably due to an insufficient treatment of spin correlations in that approach [14]. The main spectral weight of the charge excitations is located at the energy region of order of several t. Very different from 1D is the dense and strongly broadened spectrum of $N(\mathbf{Q},\omega)$ in view of the small unit cell. We interpret this as a manifestation of a substantial charge-spin interaction which couples the charge excitations to the full Hilbert space. It is remarkable that the structure of $N(\mathbf{Q},\omega)$ remains almost unchanged if we vary J from

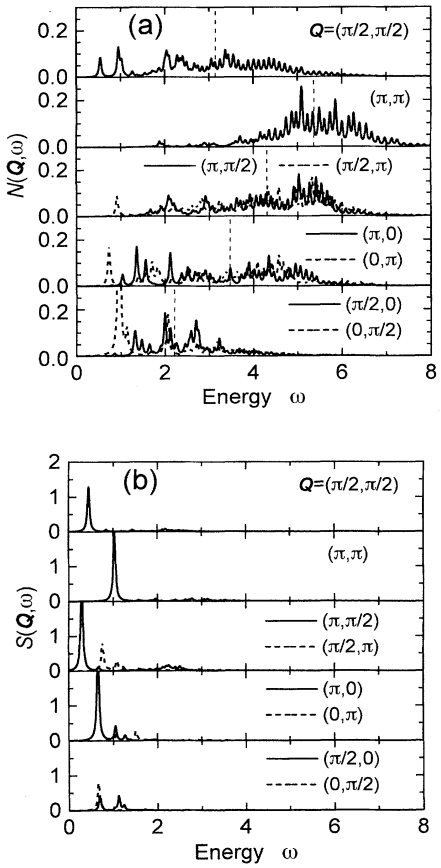

FIG. 2. Energy dependence of (a) $N(\mathbf{Q}, \omega)$ and (b) $S(\mathbf{Q}, \omega)$ for the 2D 4×4 t-J model ($J = 0.4$) at $n = 0.75$ (12 electrons). A mixed BC is taken to form a closed shell structure. The vertical solid line in (a) denotes the position of the first moment of the spectra for each panel.

0.05 to 1, contrary to 1D where $N(Q, \omega)$ turns into a pure SF-like spectrum in the small J limit. The only exception is the spectrum at $\mathbf{Q} = (0, \pi/2)$, where a pronounced low-energy peak is growing with increasing J. We interpret this as the precursor of an exchange-driven charge-density wave instability.

The momentum, $\mathbf{Q} = (0, \pi/2)$, however, is probably favored by the form of the 4×4 unit cell and the mixed BC chosen here. It is also remarkable that $N(\mathbf{Q}, \omega)$ does not show any clear low-energy excitations at $2\mathbf{k}_F \simeq (\pi, \pi/2)$.

The reduction of low-energy $2\mathbf{k}_F$-backward scattering in the charge channel is characteristic for a number of calculations we have performed for other system sizes and hole concentrations. Figure 3, for example, shows $N(\mathbf{Q}, \omega)$ for an 18-site unit cell with 16 electrons. In this case $2\mathbf{k}_F \sim (2\pi/3, 2\pi/3)$ or (π, π) [15], and there are again no clear low-energy $2k_F$ excitations. It is also remarkable that there is intensity at very low energy at $\mathbf{Q} = (\pi/3, \pi/3)$ and $(2\pi/3, 0)$ compared to the lowest

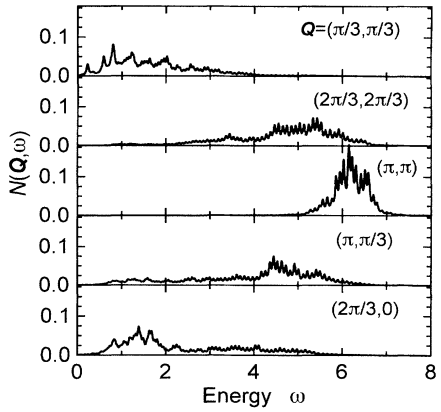

FIG. 3. Energy dependence of $N(\mathbf{Q}, \omega)$ for the 2D 18-site t-J model ($J = 0.1$) with periodic BC at $n = 0.889$ (16 electrons).

structures for noninteracting SF's which are at $\omega \sim 2t$ for this unit cell. On the other hand, there is no pronounced peak in $S(\mathbf{Q}, \omega)$ at these $\mathbf{Q}$ values. It is tempting to identify these wave vectors with $2\mathbf{k}_F^{\mathrm{SF}}$. Yet a definite conclusion requires simulations for much larger systems.

Our zero-temperature results for the structure factor $N(\mathbf{Q})$ are fully consistent with the HTSE results of Putikka *et al.* [3]. However, as our momentum resolution is not fine enough we cannot decide whether the subtle SF features in $N(\mathbf{Q})$ exist.

An important question concerns the statistics of the elementary charge excitations. Because of the constraint of no double occupancy at the same site, frequently electron creation operators are written as composite operators, where the charge is either associated with a SF or hard-core boson (HCB) operator. Therefore one may expect noninteracting SF or HCB charge response as a zeroth order approximation. For the 2D square lattice $N(\mathbf{Q})$ of HCB's and SF's do not differ much and both are close to the result for the t-J model [3]. The dynamical response functions of HCB's and SF's consist of one or a few peaks for small unit cells and are quite distinct from the typical $N(\mathbf{Q}, \omega)$ of the 2D t-J model. In particular, we note that the spectra of HCB's consist essentially of a single peak at an energy ω_{HCB} which closely agrees with the first moment $\omega_1 = \int d\omega N(\mathbf{Q}, \omega)/N(\mathbf{Q})$ of the spectra for the t-J model [see Fig. 2(a)].

To get further information about the statistics of the elementary charge excitations, we introduce next nearest neighbor hopping t' and examine the structure factor $N(\mathbf{Q})$. Let us consider the case of quarter filling ($n = 0.5$). For this density the noninteracting SF's form a half-filled band, and the Fermi surface for a certain t' agrees with that for $-t'$. $N(\mathbf{Q})$ of the SF model is, thus, independent of the sign of t'. On the other hand, $N(\mathbf{Q})$ of the HCB model depends on the sign of t'. Listed in Table I are the results of $N(\mathbf{Q})$ at $\mathbf{Q} = (\pi, \pi)$ for the t-J, SF, and HCB models. We find that the t' dependence

TABLE I. The t' dependence of $N(\mathbf{Q})$ at $\mathbf{Q} = (\pi, \pi)$ and $n = 0.5$ for a 4×4 unit cell with various boundary conditions (BC's). $J = 0.4$ for the t-J model.

Model	(BC)	t' −0.4	0.0	0.4
t-J	(peri.)	0.482	0.428	0.363
	(anti.)	0.583	0.430	0.339
HCB	(peri.)	0.644	0.412	0.326
SF	(peri.)	0.375	0.425	0.375
	(mixed)	0.5	0.5	0.5

for the t-J model is qualitatively similar to that for the HCB model; $N(\pi, \pi)$ of the t-J and HCB models decreases with increasing t', while the SF model exhibits the same value for $t' = -0.4$ and 0.4. We note that this is consistent with recent studies of different charge correlation functions in the ground state of the large-U Hubbard model, where similarity to HCB correlations was found [16,17].

It has been suggested that the model in 2D also behaves as a TL liquid [1], in the sense that as $\mathbf{Q} \to 0$ charge and spin excitations are described by single collective modes with, in general, different velocities v_c and v_s. Unfortunately, unlike 1D, the interesting small momentum regime cannot be reached with the present method.

In summary, we have investigated $S(\mathbf{Q}, \omega)$ and $N(\mathbf{Q}, \omega)$ for the 2D t-J model and compared them with the 1D t-J model. Our results for the 2D model show an interesting crossover from low to high electron concentration and characteristic differences to 1D. At low n, the dominant excitations of $S(\mathbf{Q}, \omega)$ and $N(\mathbf{Q}, \omega)$ are consistent with those of noninteracting electrons. At high n ($n > 0.7$) $S(\mathbf{Q}, \omega)$ shows a pronounced peak at low energy of order J and is consistent with $2k_F$ low-energy excitations, whereas $N(\mathbf{Q}, \omega)$ consists of a dense and broad continuum at high energy whose first frequency moment is found to agree with the HCB model. $N(\mathbf{Q}, \omega)$ is very different from the SF-type spectra of the 1D t-J model, which consist in small systems of only very few peaks. The dense continuum in 2D implies strong interactions between spin and charge degrees of freedom in 2D system. A remarkable similarity to the 1D model is the suppression of low-energy $2k_F$ scattering in the charge channel at large density. This is strikingly different from weakly correlated Fermi liquids and is probably the source of the unconventional transport properties of the copper oxides. We note that a recent $1/N$-expansion study for the 2D Hubbard model also shows a significant reduction of scattering processes with large momentum transfer [18].

Although the systems studied are quite small, we believe that our results for the charge dynamics provide new constraints important for the theoretical treatment and understanding of strongly correlated electron systems in two dimensions.

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