Spin-charge separation at small lengthscales in the 2D $t - J$ model

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We consider projected wavefunctions for the 2D $t - J$ model. For various wavefunctions, including correlated Fermi-liquid and Luttinger-type wavefunctions we present the static charge-charge and spin-spin structure factors. Comparison with recent results from a high-temperature expansion by Putikka et al. indicates spin-charge separation at small lengthscales.

71.45.Gm,77.70.Dm,74.70.Vy

INTRODUCTION

The properties of correlated electrons in two-dimensions (2D) are controversially discussed. Anderson [1] has proposed that the well established Luttinger-liquid properties of one dimensional electron systems [2] might occur, to a certain extend, also in 2D. In 1D the spin and the charge excitations move independently at small frequencies [3], a phenomena called spin-charge separation. Separation of the spin and the charge degrees of freedom has some interesting consequences on the properties of the ground-state wavefunction. In the framework of the $t - J$ model the charge carriers are given by the holes which form in 1D, since they move independently with respect to the spin background, a hole Fermi-surface distinct from the Fermi-surface of the spins. This notion has been shown to be rigorous in the $U/t \to \infty$ limit of the 1D Hubbard model [4].

A huge amount of studies have been devoted, in the last years, to the enlargement of our knowledge upon 2D correlated electron systems. It is probably fair to say, that at the moment there is no method in sight capable of establishing rigorously the properties of 2D correlated electron systems at large lengthscales, or, what is equivalent, at small differential wavevectors as it would be necessary for the determination of true spin-charge separation in 2D. It is, on the other hand, an interesting question to ask, whether at small to intermediate lengthscales spin and charge excitations can move independently or not.

Considering a variational wavefunction originally introduced by Hellberg and Mele in the context of the 1D $t - J$ model [5], it has been shown [6] that (i) it is possible to define Luttinger liquids in two dimensions variationally and (ii) that the projected kinetic energy favours Luttinger-liquid type correlations in 2D, as it does in 1D [5]. Chen and Lee [7] have shown that the static spin-spin structure factor, $S_q$, of this Luttinger-liquid wavefunction compares favourably with the $S_q$ of the numerically obtained exact ground state of a $10 \times 10$ cluster. Also, the recent high-temperature expansion study by Putikka et al. [8] has provided reliable data on $S_q$ and the static charge-charge structure factor, $N_q$, of the 2D $t - J$ model. An unexpected result has been the observation of a prominent enhancement of $N_q$ near $(\pi, \pi)$ at quarter filling. Putikka et al. found additionally that $N_q$ could be fitted very closely at all densities with the curve appropriate for spinless Fermions, i.e. assuming an independent hole Fermi-surface. These results for $N_q$ have been confirmed at small densities by a study using the power method, Quantum Monte Carlo and a perturbation expansion [9].

The high-temperature expansion [8] and the numerical studies [5] can, of course, not determine the properties of the 2D $t - J$ model at long lengthscales and therefore address the question of true spin-charge separation. They do,
on the other hand, provide reliable data on $S_q$ and $N_q$ at short to intermediate lengthscales. Here we will interpret these data for the correlation functions of the 2D $t - J$ model within the context of projected wavefunctions. For a class of variational wavefunctions with both short- and long-ranged correlations we calculate $S_q$ and $N_q$ and find that short-ranged charge-charge repulsion can explain the data by Putikka et al. and by Chen et al. [8,9]. Furthermore we show that it is the projected kinetic energy which gives rise to the prominent peak in $N_q$. Interpreting these results we come to the conclusion that the strength of the short-ranged correlations can only be explained when the spin and the charge degrees of freedom move independently at small lengthscales. These results may partially support Anderson’s concept [10] of incoherent one-particle tunneling in between the different CuO-layers of the high-temperature superconductors.

**WAVEFUNCTION**

We consider variational wavefunctions for the 2D $t - J$ model, which is given by

$$H_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} + \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}) + J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j,$$

(1)

where the $\hat{c}_{i,\sigma}^\dagger (\hat{c}_{i,\sigma})$ are the creation (anihilation) operators on site $i$ of electrons with spin $\sigma = \uparrow, \downarrow$, in the subspace of no double occupancy. The $\hat{S}_i$ are the spin operators on site $i$ and $\langle i,j \rangle$ denotes pairs of n.n. on the square lattice. The Jastrow-Luttinger wavefunction is given by

$$|\Psi(T,S)\rangle = \exp \left[ \frac{-1}{2T} \sum_{i<j} f(r_i - r_j) \hat{n}_i \hat{n}_j \right] P_0 |\psi_0\rangle,$$

(2)

where $|\psi_0\rangle$ denotes the filled Fermi sea of electrons, $P_0$ the projection operator on the subspace of no double occupancy. $\hat{n}_i = \hat{c}_{i,\uparrow}^\dagger \hat{c}_{i,\uparrow} + \hat{c}_{i,\downarrow}^\dagger \hat{c}_{i,\downarrow}$ is the density operator on site $i$ and

$$f(r_i - r_j) = -(1-S)(1-\delta_{(i,j)}) \ln |r_i - r_j| + S \delta_{(i,j)}.$$

(3)

In the limit $T \to \infty$ the wavefunction defined by Eq. (2) reduces to the Gutzwiller wavefunction, $P_0 |\psi_0\rangle$. A finite $1/(2T) > 0$ controls then the strength of the repulsive density-density Jastrow factor, given by Eq. (3). The second variational parameter, $S$, controls the details of the Jastrow factor. For $0 \leq S < 1$ the density-density correlation is long-ranged and it has been shown that this logarithmic correlator leads to an algebraic singularity in the momentum distribution function at the Fermi-edge and therefore to a Luttinger-liquid state. For $S = 1$, on the other side, the Jastrow correlator is short-ranged, with only nearest neighbor repulsion (for $T > 0$), and the resulting state is a correlated Fermi-liquid state.

The Jastrow-Gutzwiller wavefunction, as defined by Eq. (3), cannot be evaluated analytically. One then considers large but finite clusters and calculates properties of $|\Psi(T,S)\rangle$ numerically by the variational Monte-Carlo method. Here we are interested in the static spin-spin structure factor,

$$S_q = 1/L \sum_{i,j} e^{i q (r_i - r_j)} \langle \hat{S}_i^z \hat{S}_j^z \rangle,$$

(4)

and the static charge-charge structure factor,
\[ N_q = \frac{1}{L} \sum_{i,j} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} < \Delta \hat{n}_i \Delta \hat{n}_j >, \]  

(5)

where \( L \) is the number of sites of the lattice considered and \( \Delta \hat{n}_i \equiv \hat{n}_i - n \), with \( n \) being the particle density. In order to minimize finite-size effects in cluster calculations it is advantageous to consider closed shell configurations \[ \text{[13]}. \] Here we consider clusters with antiperiodic boundary conditions which tile the square lattice in \( \mathbf{L}_1 = (2m, 2m - 2) \) and \( \mathbf{L}_2 = (-2m + 2, 2m) \) directions (with \( m \) an integer). In Fig. (1) we illustrate the first Brillouin zone for a lattice with \( m = 6 \), which has \( L = 12^2 + 10^2 = 244 \) sites. Also shown in Fig. (1) are the electron Fermi-sea (filled circles) and the hole Fermi-sea (filled squares) for \( N_h = 124 \) holes. This type of lattices has the property that, whenever the number of holes is a multiple of four, but not of eight, both the electron Fermi-sea and the hole Fermi-sea are closed-shell configurations, as illustrated in Fig. (1). The dashed lines in Fig. (1) denote the locations of the Fermi surfaces for the same nominal densities \( n = (L - N_h)/L \) of electrons and of \( N_h/L \) holes respectively, in the thermodynamic limit. Here the Fermi surfaces in the thermodynamic limit are consistent with the respective Fermi surfaces of the finite cluster (this is not necessarily always the case \[ \text{[13]}. \])

RESULTS

In Fig. (2) we present for various \( \mathbf{q} \) in the first Brillouin zone the static charge-charge structure factor, \( N_q \), as defined by Eq. (3), for correlated Fermi-liquid wavefunctions, \( |\Psi(T, S = 1)\rangle \) as defined by Eq. (2), for the lattice illustrated in Fig. (1) with \( L = 244 \) sites and \( N_h = 124 \) corresponding to a particle density \( n = (L - N_h)/L \approx 0.49 \).

In Fig. (2) we have included for comparison the curve for \( N_q \) for spinless Fermions, i.e. assuming a well defined hole Fermi-sea as illustrated in Fig. (1). We observe that data for the Gutzwiller state, realized for \( 1/(2T) = 0 \), is qualitatively different from the curve for spinless Fermions. The data for \( |\Psi(1/(2T) = 0.2, S = 1)\rangle \) is, on the other hand very close to the curve for spinless Fermions and agree remarkable well with the results of Putikka et al. and Chen et al. \[ \text{[8,9]}. \] Noting that the correlated Fermi-liquid wavefunction \( |\Psi(1/(2T) = 0.2, S = 1)\rangle \) contains explicitly only nearest neighbour correlations we conclude that the static density-density correlation factor of the 2D \( t-J \) model is dominated by short-distance effects. This does, of course, not exclude the possibility of long-range correlations to be present in the paramagnetic state of the 2D \( t-J \) model, as these correlations cannot be calculated rigorously with present-day methods.

The energetics behind the results for \( N_q \) is dominated by the projected kinetic energy for small \( J/t \). The exchange hole between parallel spins in the Gutzwiller wavefunction is consequence of the Fermi statistics. In the \( t-J \) model the motion of electrons with spin \( \sigma \) is blocked also by the electrons with spin \(-\sigma \). A favourable kinetic energy is then obtained in a state in which an additional exchange hole in between electrons with opposite spins is simulated. This is exactly what the Jastrow factor defined by Eq. (3) does, as it does contain short-ranged repulsion between all electrons, regardless of their relative spin orientation. Consequently the probability of finding two n.n. sites both occupied decreases with increasing \( 1/(2T) \) (for \( S = 1 \)) and so does \( N_{(\pi,0)} \) as evidenced in Fig. (2). At quarter filling there is one particle for every second site, which leads to a large increase of the probability of finding two n.n.n. sites both occupied and consequently \( N_{(\pi,\pi)} \) increases with increasing \( 1/(2T) \). The extreme limit \( 1/(2T) \to \infty \) is energetically not advantageous, as it corresponds to a charge-density wave with a delta function at \( (\pi, \pi) \) and zero kinetic energy. Variationally we find the optimal value for \( 1/(2T) \approx 0.15 \) (within the constraint \( S \equiv 1 \)) for values of \( J \leq 0.25t \). Within the accuracy of the variational calculations this agrees fairly well with the \( 1/(2T) \approx 0.2 \) which
would give the best result for \( N_q \).

The fact that the system wants to simulate an exchange hole between all electrons, regardless of the relative spin orientation has a natural explanation within the spinless Fermion model. In the case the holes would form a distinct Fermi-sea, as illustrated in Fig. (1), a exchange hole in between electrons of both spin orientations would be one of the consequences. Even a partial formation of a hole Fermi-sea, i.e. with a washed-out Fermi-surface, would also result in an effective, short-ranged charge-charge repulsion, as observed in the data for \( N_q \). Note that at quarter filling \( \pi/k_F \approx 1 \). We therefore interpret the data presented in Fig. (2) as evidence for spin-charge separation at small lengthscales.

In Fig. (3) we present the results at quarter filling for \( N_q \) for the state with the best kinetic energy, allowing for any value of \( S \). The optimal state is given by \( 1/(2T) \approx 0.15, \ S \approx 0.6 \), which is a Luttinger-liquid state \([8]\). It has qualitatively the same features as the states with n.n. correlations only, shown in Fig. (2), but more washed out.

In Fig. (4) we present the results for \( N_q \) for the Gutzwiller state for the cluster with \( L = 244 \) sites and \( N_h = 124 \) and \( N_h = 52 \) holes, corresponding to electron densities \( n \approx 0.49 \) and \( \approx 0.79 \) respectively. The solid lines are the corresponding curves for spinless Fermions. We see that near half-filling the magnitude of \( N_q \), which again is very close to that of the spinless fermions \([8]\), is reproduced by the Gutzwiller wavefunction. The data points for states \( 1/(2T) > 0 \) do not differ much from the data of the Gutzwiller state at these fillings, as density fluctuations are reduced by the projection operator.

It is of interest to compare the variational Monte Carlo data for the Gutzwiller wavefunction with the predictions of the Gutzwiller approximation formula (GAF), which relates, by simple counting arguments \([14]\), the \( N_q \) in the projected state, as defined by Eq. (5), with the \( N_q^{(0)} \) in the unprojected state, defined by

\[
N_q^{(0)} = \frac{1}{L} \sum_{i,j} e^{iq(r_i-r_j)} \langle \psi_0 | \Delta \hat{n}_i \Delta \hat{n}_j | \psi_0 \rangle / \langle \psi_0 | \psi_0 \rangle
\]

via the approximative formula

\[
N_q \approx \frac{1}{1-n/2} N_q^{(0)}. \tag{7}
\]

We have included in Fig. (4) the predictions of the GAF, as given by Eq. (7) (dashed lines). The overall magnitude of \( N_q \) is well captured by the GAF, thought the variational Monte Carlo data has the tendency to be smoother at small dopings. The deviation of the data for the Gutzwiller state at \( n \approx 0.79 \) from the corresponding curve for spinless Fermions for small \( \mathbf{q} \)-vectors is open to interpretation. Note, that no reliable results do exist for \( N_q \) in this region \([8,9]\).

For the static spin-spin structure factor the Gutzwiller approximative fromula reads as

\[
S_q \approx \frac{1}{1-n/2} S_q^{(0)}. \tag{8}
\]

In Fig. (5) we present Eq. (8) at quarter filling together with the variational Monte Carlo data for \( S_q \) for the Gutzwiller wavefunction (filled triangles), the best Luttinger liquid wavefunction (filled circles) and the Fermi-liquid wavefunction with n.n. correlations only (filled squares). The overall magnitude is well reproduced by the GAF. Note that the Luttinger liquid state would have in the thermodynamic limit a cusp at \( 2k_F, \) with an algebraic singularity (at quarter filling \( 2k_F = (\pi,\pi) \) along the \((1,1)\) direction).

In conclusion we have shown that the known features of the static charge-charge structure factor of the 2D \( t-J \) model are dominated by short-ranged correlations. We interpret the results as evidence for spin-charge separation at small lengthscales.
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**FIG. 1.** An illustration of the Brillouin zone of the $12^2 + 10^2 = 244$ lattice with antiperiodic boundary conditions. The dashed lines indicate the location of the particle and the hole fermi surface at a filling $n = (244 - 124)/244 \approx 0.49$. The full circles/squares denote the k-states occupied by particles/holes on the finite lattice. Note that both the particle and the hole fermi-surfaces are closed-shell configurations.

**FIG. 2.** The charge-charge structure factor, $N_q$ for various $q$-directions in the 2D Brillouin zone at quarter filling ($n = 120/244$). The filled circles are the results for the Fermi-liquid wavefunction with n.n. density-density correlation in the Jastrow prefactor of strenght $1/(2T) = 0.0$, 0.15 0.2 and 0.25 respectively. The full line is the $N_q$ of spinless fermions, the dotted lines are guides to the eye.

**FIG. 3.** The charge-charge structure factor, $N_q$ for various $q$-directions in the 2D Brillouin zone at quarter filling. The filled circles are the results of the optimal Luttinger-liquid wavefunction and the full line is the $N_q$ of spinless fermions, the dotted lines are guides to the eye.

**FIG. 4.** The charge-charge structure factor, $N_q$ for various $q$-directions in the 2D Brillouin zone for fillings $n = (244 - 124)/244 \approx 0.49$ and $n = (244 - 52)/244 \approx 0.79$. The filled circles are the results for the Gutzwiller wavefunction, the dashed line the predictions of the Gutzwiller approximation formula (GAF) and the full lines the respective $N_q$ of spinless fermions. The dotted lines are guides to the eye.

**FIG. 5.** The spin-spin structure factor, $S_q$, for various $q$-directions in the 2D Brillouin zone at quarter filling. The results for the Gutzwiller wavefunction (triangles), for the optimal Luttinger-liquid wavefunction (circles) and for the correlated Fermi-liquid wavefunctions (squares) are compared with the Gutzwiller approximative formula (GAF), given by the dashed line. The dotted lines are guides to the eye.