Superconductivity in the Two-Dimensional $t$-$J$ Model at Low Hole Doping.

E. S. HEEB and T. M. RICE

Theoretische Physik, ETH Hönggerberg, CH-8093 Zürich, Switzerland

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Abstract. - By combining a generalized Lanczos scheme with the variational Monte Carlo method, we can optimize the short- and long-range properties of the ground state separately. This allows us to measure the long-range order of the ground state of the $t$-$J$ model as a function of the coupling constant $J/t$, and identify a region of finite $d$-wave superconducting long-range order. With a lattice size of 50 sites we can reliably examine hole densities down to 0.16.

Presently one of the most interesting questions in the study of strongly correlated electron systems is to determine the region of superconductivity in the phase diagram of the two-dimensional $t$-$J$ model [1,2]. Despite considerable effort, high-temperature expansion [3,4] and Quantum Monte Carlo calculations [5,6] are unable to provide conclusive evidence for or against superconductivity. Although variational calculations [7] are in favour of superconductivity, they are not able to establish independent evidence in a region of the phase diagram where magnetically ordered phases are competing with superconductivity and have almost the same energy. To date the strongest unbiased indication for superconducting order in the ground state comes from exact diagonalization of a $4 \times 4$ cluster [8]. With such a small cluster only a few filling fractions are available and it remains open how much the finite-size effects contribute to the results. In this letter we will present results on $\sqrt{50} \times \sqrt{50}$ cluster, which allows us to reach smaller hole dopings and reduce the finite-size effects. By varying the long-range and short-range correlations separately we can go beyond a standard variational approach and we are able to measure the long-range pair-pair correlation function. This enables us to identify a region of a $d$-wave superconducting ground state in the phase diagram.

The $t$-$J$ model has attracted considerable attention, because it is the simplest model to describe strongly correlated electrons. The perturbative approaches are not possible since there is no exact solution that could be used as a starting point. In contrast, many of the numerical methods that have been used for strongly correlated electrons do not rely on a small parameter in the Hamiltonian. Exact diagonalization provides reliable results of a variety of properties. However, for the two-dimensional $t$-$J$ model only systems up to a size of $4 \times 4$ have been investigated for all fillings [9]. The results for bigger systems are
restricted to certain fillings only, e.g., 2 holes on 26 sites [10]. The limited number of systems and fillings makes it difficult, if not impossible, to obtain reliable information about the thermodynamic limit. Properties that are related to the short-range behavior like the energy are more reliable than those involving long-range behavior. Indeed, the evidence for the presence or absence of superconducting long-range order from exact diagonalization is very limited [8,11]. High-temperature expansions directly lead to results which are valid in the thermodynamic limit [3], but the extrapolation from finite temperatures to $T = 0$ is difficult. So far, only the equal-time behaviour of the spin and charge degrees of freedom have been successfully analysed [4], while the question of superconducting order remains open. The Quantum Monte Carlo methods [12] which are very powerful for weakly interacting systems show severe restrictions due to the fermion sign problem especially in the strong-coupling limit. The available results cover mainly the intermediate coupling regime of the Hubbard model [5], whereas for the inherently strong coupling $t$-$J$ model only the cases of one and two holes have been considered [6].

With variational approaches no fermion sign problem occurs and the systems are big enough to show only small finite-size effects. If enough information about the symmetry of the ground state is known, a variational wave function can be constructed to model this ground state. Typically, such a variational wave function is given analytically from a mean field ansatz, so that even for fermions expectation values can be readily evaluated by Monte Carlo sampling [13]. It is well known that in the $t$-$J$ model various phases with different broken symmetries compete with each other. The energies of these phases will be close to each other at small dopings so that the energy differences are comparable to the error introduced by using modified mean field forms for the variational wave functions. The results of these variational studies remain therefore inconclusive to some extent, and the regions of stability of the various phases in the phase diagram can only be estimated qualitatively [7].

Systematic iterative improvements have been used to remove the bias in the choice of the wave function. These methods range from the power method [14] to Lanczos iterations [15]. While they do remove the bias, these methods are restricted to a few iterations only. The computing time needed to reduce the statistical error increases rapidly with the number of iterations. In this letter we will use a generalized Lanczos approach which optimizes the short- and long-range correlations separately and extract the relevant information from one iteration.

The Hamiltonian for the $t$-$J$ model is defined in the subspace with no doubly occupied sites as

$$H = -t \sum_{\langle i,j \rangle, \tau} \langle \bar{c}_{i,\tau}^\dagger c_{j,\tau} \rangle + \text{h.c.} + J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - \frac{1}{4} n_i n_j \right),$$

(1)

where $\bar{c}_{i,\tau}^\dagger = c_{i,\tau}(1 - n_{i,\tau})$ prevent doubly occupied sites and the rest of the notation is standard. We perform our calculations on a 50-site cluster with periodic boundary conditions and periods $(7,1)$ and $(-1,7)$. Exact diagonalization [8] has found that at the largest distance available in the $4 \times 4$ cluster the pair-pair correlation function $C(R) = (1/N) \sum \langle J_{\perp} \rangle$ corresponding to a nearest-neighbor singlet $d$-wave pairing operator $J_{\perp} = (1/2) \sum_{\tau} c_{i,\tau} c_{i,\tau}^\dagger$ is dominant. This long-range order is realized in a mean-field wave function as follows:

$$| \Psi(D, \mu) \rangle = \mathcal{L}_G \mathcal{L}_N \prod_k (u_k + v_k c_{-k,\dagger} c_{k,\dagger}) | 0 \rangle,$$

(2)

where $\mathcal{L}_G$ and $\mathcal{L}_N$ are the Gutzwiller- and N-particle projectors, respectively. The ratio $v_k/u_k = \sqrt{\xi_k} / (\sqrt{\xi_k} + \sqrt{\xi_k^2 + \Delta_k^2})$ with $\xi_k = -2(\cos(k_x) + \cos(k_y)) - \mu$ has the standard BCS
form. With \( J_k = D(\cos(k_x) - \cos(k_y)) \) this wave function has by construction a finite long-range \( d \)-wave order in the thermodynamic limit for a finite \( D \)-parameter, whereas for \( D = 0 \) it reduces to the Gutzwiller-projected Fermi sea. For the \( k \) points where \( J_k \) has a node, the ratio \( v_k / u_k \) is not well defined when \( \xi_k < 0 \). In the thermodynamic limit the nodes of \( J_k \) in the Brillouin zone are negligible. The effect of these nodes on the wave function accounts for much of the finite-size effects. Due to the tilted periodic boundary conditions the 50 sites lattice has only one point with \( J_k = 0 \) (at \( k = 0 \)) and is thus an optimal choice to reduce the finite-size effects. Since \( k = 0 \) is deep inside the Fermi sea, we set \( v_k = v_0 \rightarrow 1 \) and \( u_k = u_0 \rightarrow 0 \) which leads to a ratio \( v_k / u_k \rightarrow \infty \). In an actual calculation we choose a large but finite ratio. For \( D \rightarrow 0 \) the choice of this ratio has a bigger influence on the wave function and the Fermi sea will be defined as the extrapolation from small but finite values of \( D \). It is important to note that this wave function is constructed to display a specific long-range behavior and that there is no direct control over the short-range part. The Hamiltonian with its nearest-neighbour terms may, therefore, well favour a gap parameter \( D \) which is shifted away from the value that would correspond to the correct long-range behaviour of the ground state. Standard variational calculations provide no control that would allow one to find out whether \( D \), which determines the long-range correlations, is over- or under-estimated. This is one of the main disadvantages of the standard variational calculations.

We remedy this situation by optimizing the short-range correlations independently of the variational wave function. Since the Hamiltonian only contains nearest-neighbour terms, we construct the most general nearest-neighbour operator, which conserves the quantum numbers for the spin and space symmetries:

\[
\psi = \psi_0 + \sum_{\langle i, j \rangle} \left( \bar{c}_i \bar{c}_j + \text{h.c.} \right) + \sum_{\langle i, j \rangle} S_i \cdot S_j + \sum_{\langle i, j \rangle} \frac{1}{4} n_i n_j.
\]

In the combined wave function \( \psi(D) \) we can adjust for the best short-range correlations through the choice of the parameters \( x_i \). The parameter \( D \) now only controls the long-range behavior for which it was designed. By using an operator \( \psi \) with the same length scale as the Hamiltonian \( \mathcal{H} \), we arrive at a scheme, which is similar to a Lanczos iteration. However, we allow the parameters \( x_i \) to be adjusted independently of the coupling strengths in the Hamiltonian. Our approach can, therefore, be regarded as a generalization of the Lanczos scheme.

In standard variational calculations the Rayleigh-Ritz principle (RR) is used to find the best variational parameters. The expectation value \( E_{RR} = \min \langle \psi | \mathcal{H} | \psi \rangle / \langle \psi | \psi \rangle \) is the lowest upper bound for the ground-state energy that can be achieved with a given set of variational wave functions \( | \psi \rangle \). Additionally, the variance \( \sigma_{\mathcal{H}}^2 = \langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 \) is small if a wave function is close to an eigenstate of the Hamiltonian. When approaching the ground state, both of these values should become smaller. Although, this is a necessary condition, it is not sufficient to distinguish from the case where one approaches an excited eigenstate.

In our approach we use the same Rayleigh-Ritz principle but with the addition of the generalized Lanczos operators (RRGL). We arrive at the expectation value \( E_{RRGL} = \min \langle \psi | \mathcal{H} | \psi \rangle / \langle \psi | \psi \rangle \) which is still a lowest upper bound for the ground-state energy. Also the variance is again used to estimate the width of the energy spectrum of the wave function. Additionally to the standard variational approach we can now compare the RR to the RRGL wave function. This allows us to judge whether the mean-field parameter \( D \) in RR is indeed shifted to adjust for the short-range behaviour or whether the long-range correlations are maintained in the ground state. Furthermore, we know from the Lanczos method used in exact diagonalization that when one starts from a state with an energy
spectrum which is centred around an excited eigenstate, the first iteration will already redistribute the weights towards lower energies, such that the variance will first increase. In this way we use the variance as an unbiased indicator to judge the quality of the RR wave function. Using these criteria the wave functions equations (2), with $d$-wave order parameter, prove to be a good choice consistent with the results from exact diagonalization [8]. In this work we will therefore concentrate on the set of wave functions equations (2) as our starting point.

Figure 1 shows the energy for the RR- and the improved RRGL wave function at quarter filling. For 16 sites this corresponds to 8 holes, whereas for 50 sites we use 24 holes. For the case of 8 holes on 16 sites we can compare our results to the exact ground-state energy and we find that the short-range correlations account for about 80\% of the missing correlation energy. Figure 2 shows $\sigma_\varepsilon$, i.e. the width of the energy spectrum. This value is considerably reduced for the RRGL wave function consistent with a wave function which is closer to the ground state. For the 50 sites lattice there are no results for the exact ground-state energy available and we have to estimate how the various quantities scale with system size. While the wave function scales with the size of the system, the generalized Lanczos operators always act on the same length scale as the Hamiltonian. The energy and $\sigma_\varepsilon$ will, therefore, scale with the system size. $\sigma_\varepsilon$ is also the energy scale for the improvement $\Delta E = E_{RR} - E_{RRGL}$. If the wave function has the right long-range behavior, then the operators need to improve the correlations only on the same length scale as the Hamiltonian and the ratio $\Delta E / \sigma_\varepsilon$ should remain constant. Indeed we find this value to be slightly bigger for the 50 sites lattice than for 16 sites. This again supports the observation that the wave function

![Fig. 1.](image1.png)  
![Fig. 2.](image2.png)

Fig. 1. – Energy per site in units of $t$ as a function of $J/t$ at quarter filling. $E_{RR}$ is the energy for the standard variational (Rayleigh-Ritz, RR) approach, $E_{RRGL}$ is the energy after a generalized Lanczos iteration. For 16 sites the values of the exact diagonalization from Dagotto et al. (dotted line) are shown for comparison. The statistical error is smaller than the line width. a) 8 holes on 16 sites, b) 24 holes on 50 sites.

Fig. 2. – Standard deviation $\sigma_\varepsilon$ per site in units of $t$ as a function of $J/t$. This value measures the width of the energy spectrum and is a measure for the quality of the wave function. RR and RRGL correspond to the same wave functions as in fig. 1. a) 8 holes on 16 sites, b) 24 holes on 50 sites.
Fig. 3. – a) $d$-wave pair-pair correlation function $C(R)$ as a function of distance for $\varepsilon = 0.16$ and $D = 0.4t$. The solid line is the RR result. The dashed lines show the long-range correlation for the RRGL improvement for a value of $J > J_0$ and $J < J_0$, respectively. At the critical value $J_0$ the long-range correlation is unchanged from the RR ansatz. b) Long-range $d$-wave correlation $C_\infty$ as a function of the coupling constant $J/t$. The solid and dashed lines show $C_\infty$ for the same gap parameter as in a). For other variational parameters only the points $C_\infty(J/t)$, where $C_\infty$ is unchanged, are shown.

Equation (2) describes the correct long-range behavior of the ground state. For the 50 sites lattice we investigated several fillings, which all showed analogous results to the ones described above. Specifically, we looked at the closed-shell configurations of 8, 16, and 24 holes.

To investigate the superconductivity, we measure the pair-pair correlation function $C(R)$. We find that for the 50 sites lattice $C(R)$ is flat for the larger distances indicating that the finite-size effects are small. We can, therefore, take $C_\infty = C(R_{\text{max}})$ as a measure for long-range order. In the standard variational approach $C_\infty$ is a monotonic function of $D$ and contains no additional information. With our new method we can now test how the introduction of the operators $\mathcal{O}$ in the wave function affects $C_\infty$. If we start with too much long-range order the operators $\mathcal{O}$ will redistribute the weight in the correlation function and suppress $C_\infty$. On the other hand, too small a value for $C_\infty$ will be enhanced. If we start with the correct long-range order that corresponds to the ground state, the operators $\mathcal{O}$ will only affect the short-range part of $C(R)$ and $C_\infty$ will be unaffected. In that case we have effectively separated the short- and long-range parts of the wave function.

We illustrate this for 8 holes on 50 sites corresponding to a hole density of 0.16. In fig. 3a) we show $C(R)$ for one value of $D = 0.4t$ and $\mu = -0.8t$. The solid line corresponds to the RR wave function. We can see that the long-range tail is well saturated. For $J < J_c$, the long-range correlations are suppressed, while for $J > J_c$ they are enhanced. This is shown by the dashed lines. For $D = 0.4t$, we find $J_c \approx 1.0t$. In fig. 3b) we show $C_\infty$ as a function of the coupling constant $J/t$. The solid line again corresponds to the RR-value, while the dashed line shows the suppression and enhancement for the RRGL-values. The point where the solid and dashed lines cross is the value $C_\infty(J/t)$ which remains unchanged under iteration and we take this as the long-range order $C_\infty$ of the ground state. For other values of the variational parameter $D$ we repeat the same procedure and obtain the points shown in fig. 3b). The error bars in $J/t$ indicate the region where the suppression or enhancement is within one standard deviation. There are no rigorous bounds for the deviation from the true value. However, the suppression or enhancement is stronger when the starting value is further away from $C_\infty$, indicating that the results are reliable. Indeed we find that our method can reproduce the exact values for 16 sites very well. We can thus map out $C_\infty(J/t)$ for the ground state and determine the critical value $J_c = (0.44 \pm 0.04)t$ for the onset of superconducting long-range order. For the other closed-shell configurations of 16 and 24 holes we obtain analogously the critical values $J_c = (0.62 \pm 0.08)t$ and $J_c = (0.78 \pm 0.11)t$, respectively. Using these points we construct the phase diagram fig. 4. Ohta et al. [11] observe a finite superconducting gap also at lower values of $J/t$ for 16- and 18-site systems. However, they only report results on open shells, in
order to have \( k \) points at the Fermi surface. For open shells the Fermi sea is degenerate and the \( d \)-wave condensate might be favoured in order to remove this degeneracy. Such finite-size effects are reduced for the closed-shell configurations used in this work.

The wave functions used in this work describe a homogeneous electron distribution for all variational parameters. For large values of \( J \), the \( t-J \) model exhibits phase separation [16,3]. In that region of the phase diagram, the ground state is not well represented by the homogeneous wave functions. However, since the phase-separated state is a mixture of two homogeneous states—the half-filled Heisenberg antiferromagnet (hole doping \( \varepsilon = 0 \)) and a state with finite hole doping—we can use the Maxwell construction to obtain its energy. For any fixed value of \( J \) the energy of the homogeneous wave functions will be a smooth function of the hole density \( \varepsilon \), which we can describe by a polynomial in \( \varepsilon \). In the region of phase separation this polynomial will be curved downwards, so that a combination of two homogeneous states (represented by a straight line) will lower the energy. The maximal hole density \( \varepsilon_c(J) \), which lowers the energy between 0 and \( \varepsilon_c \) determines the phase separation line as a function of \( J \). This line is also shown in fig. 4. For the Maxwell construction we only use the energies of the closed-shell configurations (8, 16, and 24 holes), for which we can expect the finite-size effects to be minimal. We can then identify the region of \( d \)-wave superconducting long-range order from close to quarter filling (\( \varepsilon = 0.48 \)) down to a hole density of \( \varepsilon = 0.16 \). This is shown by the shaded region in the phase diagram of fig. 4.

In conclusion we have presented a method which allows us to measure the long-range behaviour of the ground state by separating the long-range from the short-range contributions. This allows us to calculate the long-range \( d \)-wave pair-pair correlation function, which is a direct measure for the superconducting order parameter. We identify the region of \( d \)-wave superconducting long-range order down to a hole density of \( \varepsilon = 0.16 \). For smaller hole densities the calculations will have to be extended to larger lattice sizes. Our method extends the results from the exact diagonalization, as it can be applied to larger systems.

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