Superconductivity in the two-dimensional $t$-$J$ model

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Using computational techniques, it is shown that pairing is a robust property of hole doped antiferromagnetic (AF) insulators. In one dimension (1D) and for two-leg ladder systems, a BCS-like variational wave function with long-bond spin-singlets and a Jastrow factor provides an accurate representation of the ground state of the $t$-$J$ model, even though strong quantum fluctuations destroy the off-diagonal superconducting (SC) long-range order in this case. However, in two dimensions (2D) it is argued – and numerically confirmed using several techniques, especially quantum Monte Carlo (QMC) – that quantum fluctuations are not strong enough to suppress superconductivity.

The nature of high temperature superconductors remains an important unsolved problem in condensed matter physics. Strong electronic correlations are widely believed to be crucial for the understanding of these materials. Among the several proposed theories are those where antiferromagnetism induces pairing in the $d_{x^2-y^2}$ channel [1]. These approaches include the following two classes: (i) theories based on Resonant Valence Bond (RVB) wave functions, with electrons paired in long spin singlets in all possible arrangements [2,3], and (ii) theories based on two-hole $d_{x^2-y^2}$ bound states at infinitesimal doping, formed to minimize the damage of individual holes to the AF order parameter, which condense at finite pair density into a superconductor [4]. However, recent density matrix renormalization group (DMRG) calculations have seriously questioned these approaches since non-SC striped ground states were reported for realistic couplings and densities in the $t$-$J$ model [5]. Clearly to make progress in the understanding of copper oxides, the most relevant contribution to $\Delta_k$ has $d_{x^2-y^2}$ symmetry, namely $\Delta_k = \Delta \cos k_x - \cos k_y$ [4]. For ladders, $\Delta_k = \Delta_x \cos k_x + \Delta_y \cos k_y$ was used (the optimized $\Delta_x$ and $\Delta_y$ have opposite signs), whereas in the 1D case $\Delta_k = \Delta_1 \cos k + \Delta_2 \cos 3k$. In the following, VMC denotes results obtained with $|\Psi_V\rangle$, VMC+PLS (with $p = 1, 2$) those obtained with $|\Psi_p\rangle$, and FN and FN+PLS results obtained using the FN approximation with $|\Psi_V\rangle$ and $|\Psi_p\rangle$ as guiding wave function, respectively. Finally, 0 variance indicates results obtained with the variance extrapolation method.

Using computational techniques, it is shown that pairing is a robust property of hole doped antiferromagnetic (AF) insulators. In one dimension (1D) and for two-leg ladder systems, a BCS-like variational wave function with long-bond spin-singlets and a Jastrow factor provides an accurate representation of the ground state of the $t$-$J$ model, even though strong quantum fluctuations destroy the off-diagonal superconducting (SC) long-range order in this case. However, in two dimensions (2D) it is argued – and numerically confirmed using several techniques, especially quantum Monte Carlo (QMC) – that quantum fluctuations are not strong enough to suppress superconductivity.

The wave function Eq. (2) describes preformed electron pairs, expected to become SC within the RVB scenario [4]. An important component of Eq. (3) is the Gutzwiller projector, which at half-filling freezes the charge dynamics, establishing quasi-long-range AF or-
der [3]. This shows that the projected BCS wave function describes magnetic regimes as well. In addition, the SC order parameter is not simply related to the pair amplitude $\Delta$, as in weak-coupling BCS. In fact, at low hole-doping, it is proportional to the number of holes, and not to the number of electrons. This result is natural in hole-pairing theories [4], where superconductivity at half-filling is not possible, suggesting that such theories may be similar to the RVB approach if the latter incorporates long-range singlets, and no-double occupancy is enforced. Moreover, it was observed that the variational parameter $\Delta$ decreases with increasing hole doping [3], suggesting a relation of this quantity with the pseudogap of underdoped cuprates [5]. In hole-pair based theories, a similar result is obtained with the hole binding energy, finite even at half-filling, playing the role of $\Delta$ [3].

Since undoped systems with short-range AF correlations appear properly described by the wave function Eq. (3), consider now hole-doped AF systems where superconductivity should emerge according to some theories [3]. For this purpose the pairing correlation function $\Delta_{\mu,\nu}(r)=S_{i+r,\mu}S_{i,\nu}$ was studied. Here $S_{i,\nu}^\dagger=S_{i,\dagger\nu}S_{i,\mu}$ creates an electron singlet pair in the neighboring sites $(i, i + \mu)$. Off-diagonal long-range order (ODLRO) is implied if $\rho_d=2\lim_{r \to \infty} \sqrt{\Delta_{\mu,\nu}(r)^2}$ remains finite in the thermodynamic limit. In 1D, ODLRO is suppressed by quantum fluctuations, but $\Delta_{\mu,\nu}(r)$ is finite at short distances and the accuracy of the wave function Eq. (3) can be assessed, the FN providing exact results in 1D. As shown in Fig. 1, the 1D pairing correlations are indeed non-zero, although rapidly decaying with distance. Our variational wave function reproduces accurately the pairing correlations, but only when a long-range Jastrow factor is included, otherwise the tendency to pairing is overemphasized. The accuracy of the variational wave function is excellent also for small 2D clusters, where the exact solution can be obtained by Lanczos. In this case the quantum fluctuations appear not strong enough to destroy superconductivity, see Fig. 2.

To show that the wave function Eq. (3) accurately describes not just a SC state but several magnetic systems as well, consider the half-filled model on chains and ladders. In the first case, the ground state is quasi-antiferromagnetically ordered, with zero staggered magnetization and power-law spin correlations, while in the second case there is a finite spin gap in the spectrum, and exponentially decreasing spin correlations [10]. The spin structure factor $S_z(q) = 1/L \sum_{i,j} e^{iq(R_i-R_j)}(S_i^z S_j^z)$ shows a cusp at $q = \pi$ in 1D, and a broad maximum at $q = (\pi, \pi)$ for two-leg ladders. These features are remarkably well reproduced by our variational wave function (Fig. 1b), which generates robust AF correlations at short distances. The state used is also surprisingly accurate in energy compared to work based on a pure Gutzwiller wave function [3], and on numerical exact studies. It seems that Gutzwiller projecting the BCS wave function allows for a quantitative description of AF correlations in low-dimensional systems [3].

FIG. 1. $S_z(q)$ and energies for (a) 1D and (b) two-leg ladders at zero hole doping. The numerically exact result (open circles) was obtained with the FN method. Pairing correlations for the $t$-$J$ model in (c) 1D (absolute value) and (d) on a tilted 2D cluster for parallel (upper points) and orthogonal (lower points) singlets.

Now we consider doped two-leg ladders. In Fig. 2, pairing correlations for a $30 \times 2$ ladder, with 12 holes, $J=t$ and OBC. In (b) the distance $r$ runs from the center of the ladder.

FIG. 2. (a) Average rung hole density and (b) pairing correlations for a $30 \times 2$ ladder, with 12 holes, $J=t$ and OBC. In (b) the distance $r$ runs from the center of the ladder.

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system such as a two-leg ladder with hole pairs, the correlation functions can be well-controlled by QMC methods. In general, it is observed that whenever the VMC method is not quantitatively accurate, the proper correlation functions are obtained by applying the FN approximation [13]. Therefore, this QMC approach combining VMC and FN methods represents a novel powerful tool to assess the reliability of a variational state [13], and to obtain accurate properties of t-J models for cuprates [14].

After testing the numerical methods, let us now address the main subject of the paper, i.e. the possibility of SC in the 2D t-J model. For this case no exact solution (analytical or numerical) is available and, therefore, it is crucial to perform a careful computational analysis, comparing the results of different techniques. While DMRG allows for an almost exact ground-state characterization for 1D systems and two-leg ladders, unfortunately in 2D the results appear to depend on the boundary conditions [13]. In order to compare the performances of QMC and DMRG (with \( m \) states kept), not only the standard PBC have been considered, for which reliable DMRG calculations on large 2D clusters presently are not possible, but also the cylindrical boundary conditions (CBC), open (periodic) in the \( x \) (\( y \)) direction, and OBC in both directions. To reduce the number of variational parameters with CBC and OBC, the Jastrow factor was restricted to depend only on the distance between sites, i.e., \( v_{i,j} = v_{n-i,j} \). Site dependent chemical potentials \( \mu_i \) were also used as additional variational parameters to consider possible non-uniform charge distributions. To test the stability of our variational wave function directly in 2D, a \( 6 \times 6 \) lattice with 6 holes was considered. In Fig. 3, a comparison among different numerical techniques for several boundary conditions is shown. The large-\( m \) extrapolated energies of DMRG are remarkably similar to those of QMC for CBC and OBC, but not for PBC where QMC produces substantially better energies. As in 1D, for the \( 6 \times 6 \) cluster FN does not provide qualitative changes in the pairing correlations with respect to the VMC outcome, and the FN+2LS and VMC+2LS correlations are close. In addition, the \( m=1200 \) DMRG results lead to similar correlations. The agreement among the many methods suggests that the QMC method correctly reproduces ground state properties also in 2D systems, where the Jastrow term does not suppress the ODLRO present in the VMC, providing sizable long-range pairing.

The most natural boundaries without spurious symmetry breaking are PBC, since the finite-cluster eigenstates have all the lattice symmetries. Therefore, here the subsequent effort building toward the main result of the paper focuses on PBC clusters. For these boundary conditions, our improved variational calculation is accurate and no sign of static stripes has been found at the couplings investigated, although dynamical effects are still possible (see below). For 8 holes on the \( 8 \times 8 \) lattice and \( J/t=0.4 \), our best variational energy per site (FN+2LS) is \( E=-0.66672(6)t \), close to the zero variance extrapolation \( E=-0.671171(1)t \), and much better than the pure variational calculation, \( E=-0.64266(8)t \).

The main result of our paper is in Fig. 4, where the SC order parameter \( P_\delta \) vs \( \delta \) at \( J/t=0.4 \), using the techniques and cluster sizes shown. Inset shows \( S_\delta (q) \) at optimal density.
incommensurability (SI) appears in the FN+2LS results at optimal density. At other densities $\delta$, such as 0.25, a similar mild tendency toward SI was also observed. Then, it is conceivable that the SC state may contain very weak dynamical stripe tendencies, as recently observed in the spin-fermion model \cite{13}. Alternatively, band effects or AF correlations across-holes \cite{14} could be responsible for the SI structure. In this doping region, the charge structure factor $N(q)$ is found to be basically featureless.

In addition, a low-density of 8 holes on a tilted 242-site cluster was also analyzed to investigate coexistent antiferromagnetism and superconductivity, as seen in recent experiments for underdoped YBCO \cite{17}. The pure variational approach shows a small SC order parameter, and a vanishing small AF order (Fig. 5). Indeed, at half-filling, the projected $d_{x^2-y^2}$ BCS state underestimates the magnetic order since it has zero magnetization with a logarithmically divergent $S_z(\pi, \pi)$ \cite{13}, and hole doping reduces further the AF correlations. Remarkably, the FN approach enhances both the SC and AF tendencies. In particular, the spin correlations show robust long-range order implying that antiferromagnetism survives a small hole density, in agreement with other techniques. The present effort substantially improves on previous calculations where $d$-wave superconductivity was predicted to exist at intermediate $J/t$ \cite{14}, and highlights the power of the recently developed QMC methods \cite{15}.

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