Superconductivity in the Two-Dimensional $t$-$J$ Model


1Istituto Nazionale per la Fisica della Materia, and SISSA, I-34014 Trieste, Italy
2National High Magnetic Field Lab and Department of Physics, Florida State University, Tallahassee, Florida 32306
3Institut de Physique Théorique, Université de Lausanne, CH-1015 Lausanne, Switzerland
4Instituto de Fisica Rosario (CONICET) and Universidad Nacional de Rosario, 2000 Rosario, Argentina
5Istituto Nazionale per la Fisica della Materia, Unità di Ricerca di Firenze, I-50125 Firenze, Italy
6Istituto Nazionale per la Fisica della Materia and Dipartimento di Scienze, Università dell’Insubria, I-22100 Como, Italy

(Received 18 September 2001; published 28 February 2002)

Using computational techniques, it is shown that pairing is a robust property of hole-doped antiferromagnetic insulators. In one dimension 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—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 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—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 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—that quantum fluctuations are not strong enough to suppress superconductivity.

Using computational techniques, it is shown that pairing is a robust property of hole-doped antiferromagnetic insulators. In one dimension 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—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 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—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 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—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 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 long-range order in this case. However, in two dimensions it is argued—and numerically confirmed using several techniques, especially quantum Monte Carlo—that quantum fluctuations are not strong enough to suppress superconductivity.
Eq. (2) we show that a $d$-wave superconductor exists in the 2D $t$-$J$, a result that recently has been very controversial.

The wave function [Eq. (2)] describes preformed electron pairs, expected to become SC within the RVB scenario [2,3]. An important component of Eq. (2) is the Gutzwiller projector, which at half-filling freezes the charge dynamics, establishing quasi-long-range AF order [8]. 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 short distances. It seems that the Gutzwiller projection of the BCS wave function allows for a quantitative description of AF correlations in low-dimensional systems [12].

Since undoped systems with short-range AF correlations appear properly described by the wave function [Eq. (2)], consider now the hole-doped AF systems where superconductivity should emerge according to some theories [1–4]. For this purpose the pairing correlation function $\Delta_{\mu\nu}^{p}(r) = \langle \hat{c}_{i\mu}^{\dagger} \hat{c}_{i+\mu,\nu} \rangle$ was studied. Here $S_{i,\mu} = (\hat{c}_{i,\mu}^{\dagger} \hat{c}_{i,\mu} - \hat{c}_{i,\mu} \hat{c}_{i,\mu}^{\dagger})$ creates an electron singlet pair in the neighboring sites ($i, i + \mu$). Off-diagonal long-range order (ODLRO) is implied if $P_{d} = 2 \lim_{r \to \infty} \sqrt{\Delta_{\mu\nu}^{p} (r)}$ remains finite in the thermodynamic limit. In 1D, ODLRO is suppressed by quantum fluctuations, but $\Delta_{\mu\nu}^{p} (r)$ is finite at short distances and the accuracy of the wave function [Eq. (2)] can be assessed, with the FN providing exact results in 1D. As shown in Fig. 1c, the 1D pairing correlations are indeed nonzero, 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 also excellent for small 2D clusters, where the exact solution is known (Fig. 1d).

Now we consider doped two-leg ladders. In Fig. 2, the results on a 30 \times 2 ladder with open boundary conditions (OBC) and $J = t$ are presented. It is known [13] that for two-leg ladders the pairing correlations are the dominant ones, i.e., they decay the slowest, but there is no true long-range order since the system is quasi-1D. We reproduced the results of Ref. [13], and our results show that also in this case the ground state is well described by a projected BCS wave function with a density Jastrow term, although charge oscillations induced by hole-pair formation are strong in DMRG (here considered as exact), but considerably weaker with VMC. However, it is remarkable that the
FN approach gives the correct rung density profile, showing that, even in a nontrivial 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 [14]. Therefore, this QMC approach combining VMC and FN methods represents a novel powerful tool to assess the reliability of a variational state [14], and to obtain accurate properties of $t$-$J$ models [15].

Let us now address the main subject of this 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 its accuracy appears to depend on the boundary conditions [14]. 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., $v_{i,j} = v_{r-i,j}$. Site dependent chemical potentials $\mu_i$ were also used as additional variational parameters to consider possible nonuniform 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 consistent with 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 also correctly reproduces ground-state properties 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 this 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 $E = -0.671(1)t$, and much better than the pure variational calculation, $E = -0.64266(8)t$.

The main result of our paper is shown in Fig. 4, where the SC order parameter $P_d$ is shown for clusters of 64 states at several densities, and 242 sites close to optimal doping. These results, stable among the many methods used here and with weak size effects, are indicative of a robust SC ground state away from half-filling in the 2D $t$-$J$ model. In view of the success of the present QMC techniques to reproduce known results for chains, ladders, and OBC 2D clusters, it is reasonable to consider the data in Fig. 4 as accurate, implying a finite $P_d$ around optimal doping reduced by at most 30% with respect to VMC (see inset). In addition, the results are in good qualitative agreement with experimental tendencies, including an optimal doping at $\delta \sim 0.18$. The spin structure factor (not shown) has a broad peak at $(\pi, \pi)$, concomitant with exponentially decaying AF correlations in real space. A slight tendency

![FIG. 3. Pairing correlations (a) and total energy (b) for various techniques on $6 \times 6$ lattices. $m$ is the number of states in the DMRG approach. In (a) the distance $r$ runs along the center of the cylinder in the periodic direction.](image)
toward spin 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. Alternatively, band effects or AF correlations across holes [16] could be responsible for the SI structure. In this doping region, the charge structure factor $N(q)$ has a small bump at small $q$’s [14], which, however, is not related to static stripes. Our conclusion is that, if stripes are present, they have a very dynamical character.

In addition, we have investigated the possible coexistence between antiferromagnetism and superconductivity at low doping, as seen in recent experiments for underdoped YBCO [17]. The pure variational approach shows a small SC order parameter, and a vanishing small AF order at low doping, as seen in recent experiments for underdoped YBCO [17]. The FN energies (not shown) for 0, 8, 24, and 40 holes in 242 sites are clearly stable against phase separation, but are quite close to it [20].

Moreover, hole-hole correlations display sharp peaks at hole distance $\sqrt{2}$ (see Fig. 5), indicating the tendency to have short-range hole pairs in the low hole-density ground state [4]. These pairs were identified in previous studies [21,22], illustrating the good agreement among different techniques. Generally, at $J/t \sim 0.4$ a clear signal at distance $\sqrt{2}$ always emerges upon Jastrow and/or FN improvement from a two-hole RVB wave function, where electrons rather than holes naively appear to be paired. This result illustrates the flexibility of the QMC approach, and unveils unexpected similarities between the Jastrow corrected long-singlet RVB [2,3] and the hole-pair approaches [4], both yielding closely related results.

In conclusion, robust indications of superconductivity have been found in the 2D $t$-$J$ model. The results were obtained by substantially improving the RVB wave function with Jastrow factors [3,4,7], with recently developed QMC methods [6]. The RVB wave function was shown to reproduce essentially exact results for chains and ladders already at the variational level, strongly supporting the validity of our findings in 2D.

This work was partially supported by MURST (COFIN ‘01), NSF (DMR-0122523), the NHMFL In-House Research Program, Fundación Antorchas, and PICT Grant No. N03-03833 (ANPCYT).

FIG. 5. Spin-spin correlations (a) and pairing (b) versus distance for $J = 0.4t$. The clusters have 242 sites (8 holes) and 122 sites (4 holes). The inset of (b) shows the hole-hole correlations for 8 holes on 242 sites.

[12] Equation (2) is qualitatively different from spin-gapped short-range RVB states involving only nearest-neighbor singlets. This is evident from $f_{i,j}$, which is nonzero even at large distances, allowing for AF correlations.