Superconductivity in the Two-Dimensional t-J Model

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(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.

DOI: 10.1103/PhysRevLett.88.117002 PACS numbers: 74.20.Mn, 71.10.Fd, 71.10.Pm, 71.27.+a

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 antiferromagnetic (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 nonsuperconducting (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 2D t-J model ground state must be fully understood, to distinguish it among the many proposals.

In this paper, using N-site clusters we investigate the properties of the t-J model,

$$H = J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) - t \sum_{\langle i,j \rangle \sigma} \tilde{c}^{\dagger}_{i,\sigma} \tilde{c}_{j,\sigma} + \text{H.c.}, \tag{1}$$

where $\tilde{c}_{i,\sigma} = c_{i,\sigma}\ (1 - n_{i,\bar{\sigma}})$, $\langle \ldots \rangle$ stands for nearest-neighbor sites, and n_i and $\mathbf{S}_i$ are the electron density and spin at site i, respectively. Our study focuses on the low hole-doping region of chains, two-leg ladders, and square clusters, using different numerical techniques: quantum Monte Carlo (QMC) [pure variational and fixed-node (FN) approximations], DMRG, and Lanczos. Within our QMC approach, it is possible to further improve the variational and FN accuracy by applying a few ($p \leq 2$) Lanczos steps to the variational (VMC, $p = 0$) wave function $|\Psi_V\rangle$, $|\Psi_p\rangle = (1 + \sum_{k=1}^{p} \alpha_k H^k)|\Psi_V\rangle$ [6]. Accurate estimates of energy and correlation functions can also be extracted, by extrapolating a sequence ($p = 0, 1, 2$) of Lanczos calculations to the exact large-p limit, where the variance $\sigma^2 = \langle \Psi_p | H^2 | \Psi_p \rangle - \langle \Psi_p | H | \Psi_p \rangle^2$ vanishes exactly [6].

Our BCS variational wave function is defined as

$$|\Psi_V\rangle = \mathcal{P}_N \mathcal{P}_G J \exp\left(\sum_{i,j} f_{i,j} c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} \right) |0\rangle, \tag{2}$$

where $\mathcal{P}_N$ is the projector onto the subspace of N particles, $\mathcal{P}_G$ is the Gutzwiller projector, which forbids doubly occupied sites, and $J = \exp(\sum_{i,j} v_{i,j} h_i h_j)$ is a Jastrow factor, defined in terms of the hole density at site i, with $h_i = (1 - n_{i\uparrow})(1 - n_{i\downarrow})$, and $v_{i,j}$ being the variational parameters. The Fourier transform f_k of the pairing amplitude, $f_{i,j}$, satisfies [3] $f_k = \Delta_k / [\epsilon_k - \mu + \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2}]$, where ϵ_k is the free electron dispersion, μ is the chemical potential, and Δ_k is the BCS SC gap function. For square lattices and periodic boundary conditions (PBC), in the low-doping region, the most relevant contribution to Δ_k has $d_{x^2-y^2}$ symmetry, namely, $\Delta_k = \Delta(\cos k_x - \cos k_y)$ [3,7]. For ladders, $\Delta_k = \Delta_x \cos k_x + \Delta_y \cos k_y$ was used, whereas in the 1D case $\Delta_k = \Delta_1 \cos k + \Delta_3 \cos 3k$. 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 are results obtained using the FN approximation with $|\Psi_V\rangle$ and $|\Psi_p\rangle$ as guiding wave functions, respectively. Finally, 0 variance indicates results obtained with the variance extrapolation method.

The central point we wish to make in this Letter is that, by using Eq. (2) as a variational wave function, the physics is not crucially dependent on the level of the subsequent approximations, i.e., Eq. (2) is already a qualitatively accurate representation of the true ground state. By using

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 Δ, 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 Δ decreases with increasing hole doping [9], suggesting a relation of this quantity with the pseudogap of underdoped cuprates [10]. In hole-pair based theories, a similar result is obtained with the hole-binding energy, finite even at half-filling, playing the role of Δ [4].

To show that the wave function [Eq. (2)] 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 [11]. The spin structure factor $S_z(q) = 1/N \sum_{i,j} e^{iq(R_i - R_j)} \langle S_i^z S_j^z \rangle$ 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 (Figs. 1a and 1b), which generates robust AF correlations 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].

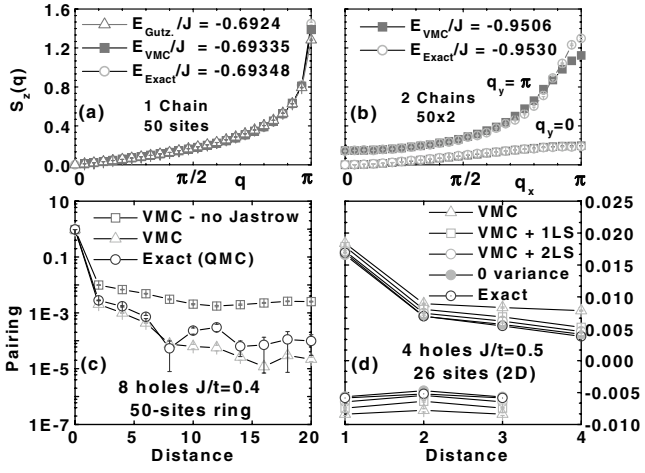

FIG. 1. $S_z(q)$ and energies for (a) 1D and (b) two-leg ladders at zero hole doping. The numerically exact result (open circles) was obtained with the FN method. Pairing correlations for the t-J model in (c) 1D (absolute value) and on (d) a tilted 2D cluster for parallel (upper points), i.e., $\mu =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

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 $\Delta_i^{\mu,\nu}(r) = \langle S_{i+r,\mu} S_{i,\nu}^\dagger \rangle$ was studied. Here $S_{i,\mu}^\dagger = (\tilde{c}_{i,\uparrow}^\dagger \tilde{c}_{i+\mu,\downarrow}^\dagger - \tilde{c}_{i,\downarrow}^\dagger \tilde{c}_{i+\mu,\uparrow}^\dagger)$ creates an electron singlet pair in the neighboring sites $(i, i + \mu)$. Off-diagonal long-range order (ODLRO) is implied if $P_d = 2 \lim_{r\to\infty} \sqrt{|\Delta_i^{\mu,\nu}(r)|}$ remains finite in the thermodynamic limit. In 1D, ODLRO is suppressed by quantum fluctuations, but $\Delta_i^{\mu,\nu}(r)$ 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 30×2 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

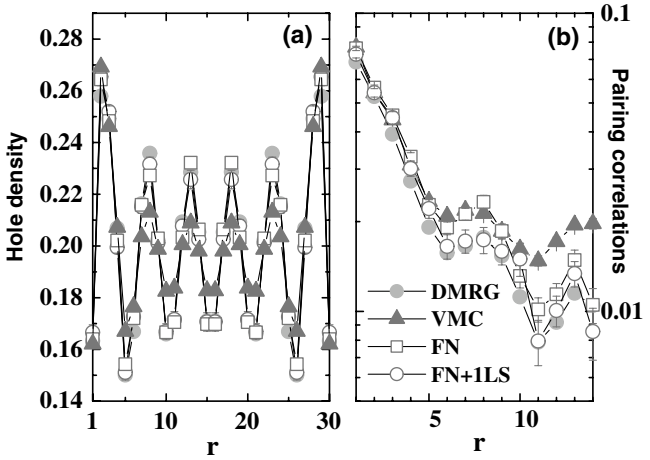

FIG. 2. (a) Average rung hole density and (b) pairing correlations for a 30×2 ladder (with 12 holes) with $J = t$ and OBC. In (b) the distance r runs from the center of the ladder.

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., $v_{i,j} = v_{i-j}$. Site dependent chemical potentials μ_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 6×6 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 6×6 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 8×8 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 sites 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 (π, π), concomitant with exponentially decaying AF correlations in real space. A slight tendency

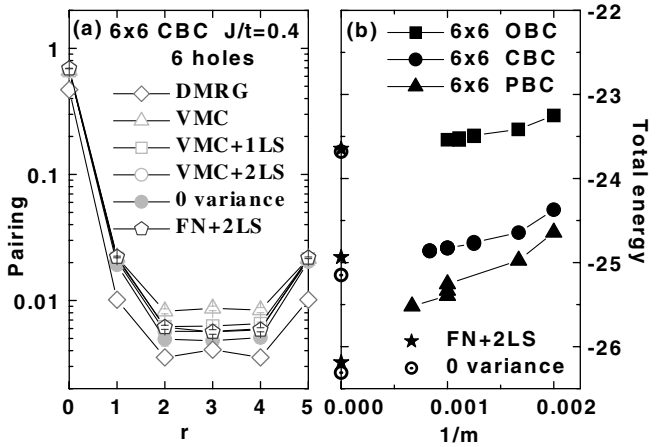

FIG. 3. Pairing correlations (a) and total energy (b) for various techniques on 6×6 lattices. m is the number of states in the DMRG approach. In (a) the distance r runs along the center of the cylinder in the periodic direction.

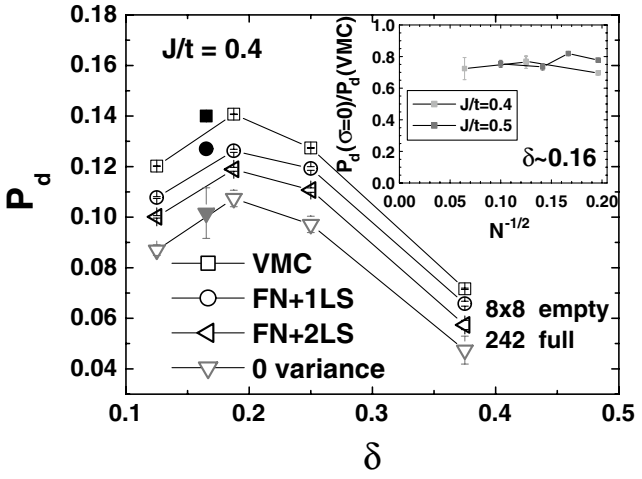

FIG. 4. Superconducting order parameter P_d vs δ at $J/t = 0.4$. The inset shows the size scaling of P_d for $\delta \sim 0.16$.

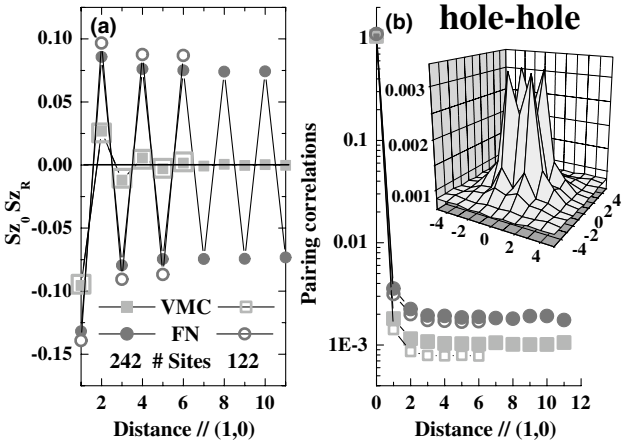

FIG. 5. Spin-spin correlations (a) and pairing (b) versus distance for $J = 0.4t$. The clusters have 242 sites (8 holes) and 122 sites (4 holes). The inset of (b) shows the hole-hole correlations for 8 holes on 242 sites.

toward spin incommensurability (SI) appears in the FN + $2LS$ results at optimal density. At other densities δ, 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* stipes. 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 (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 $S_z(\pi, \pi)$ [8], and hole doping further reduces 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 density range [18,19], as in experiments [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).

[1] D. J. Scalapino, Phys. Rep. **250**, 329 (1995).
[2] P. W. Anderson, Science **235**, 1196 (1987).
[3] C. Gros *et al.,* Z. Phys. B **68**, 425 (1987).
[4] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994), and references therein.
[5] S. R. White and D. J. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998).
[6] S. Sorella, Phys. Rev. B **64**, 024512 (2001); E. Dagotto and A. Moreo, Phys. Rev. D **31**, 865 (1985).
[7] H. Yokoyama and M. Ogata, J. Phys. Soc. Jpn. **65**, 3615 (1996); see also E. Dagotto and J. Riera, Phys. Rev. Lett. **70**, 682 (1993).
[8] L. Capriotti *et al.,* Phys. Rev. Lett. **87**, 097201 (2001).
[9] A. Paramekanti *et al.,* Phys. Rev. Lett. **87**, 217002 (2001).
[10] See, for example, T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999), and references therein.
[11] E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
[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.
[13] C. A. Hayward *et al.,* Phys. Rev. Lett. **75**, 926 (1995).
[14] F. Becca *et al.,* Phys. Rev. Lett. **87**, 167005 (2001).
[15] The FN wave function is not a simple variational state, but is the ground state of a realistic FN Hamiltonian [D. F. B. ten Haaf *et al.,* Phys. Rev. B **51**, 13 039 (1995)].
[16] G. B. Martins *et al.,* Phys. Rev. Lett. **84**, 5844 (2000).
[17] Y. Sidis *et al.,* Phys. Rev. Lett. **86**, 4100 (2001); see also S. Ono *et al.,* Phys. Rev. Lett. **85**, 638 (2000).
[18] M. Calandra and S. Sorella, Phys. Rev. B **61**, R11894 (2000).
[19] G. J. Chen *et al.,* Phys. Rev. B **42**, 2662 (1990).
[20] This result is in agreement with SO(5) predictions [S. C. Zhang *et al.,* Phys. Rev. B **60**, 13 070 (1999)].
[21] D. Poilblanc, Phys. Rev. B **48**, 3368 (1993); D. Poilblanc, Phys. Rev. B **49**, 1477 (1994).
[22] S. R. White and D. J. Scalapino, Phys. Rev. B **55**, 6504 (1997).