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Absence of static stripes in the two-dimensional $t-J$ model determined using an accurate and systematic quantum Monte Carlo approach

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We examine the two-dimensional $t-J$ model by using variational approach combined with well established quantum Monte Carlo techniques [S. Sorella *et al.*, Phys. Rev. Lett. **88**, 117002 (2002)] that are used to improve systematically the accuracy of the variational ansatz. Contrary to recent density-matrix renormalization group and projected entangled-pair state calculations [P. Corboz *et al.*, Phys. Rev. B **84**, 041108(R) (2011)], a uniform phase is found for $J/t = 0.4$, even when the calculation is biased with an ansatz that explicitly contains stripe order. Moreover, in the small hole doping regime, that is, $\delta \lesssim 0.1$, our results support the coexistence of antiferromagnetism and superconductivity.

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Introduction. The comprehension of the low-energy properties of strongly correlated systems remains one of the biggest challenges in modern condensed matter physics. Indeed, although a fairly good understanding has been achieved in some limiting cases (especially for large spatial dimensions, thanks to dynamical mean-field theory[1,2]), many important questions remain wide open in the two-dimensional case, where the competition between charge/spin ordering and superconductivity is very strong. Unfortunately, in this case, there are not unbiased techniques that may be used to obtain accurate results for low temperatures and large system sizes. Therefore, several approximate methods have been developed and applied in the last few years, like for example variational (VMC)[3] and fixed-node (FN) Monte Carlo,[4] density-matrix renormalization group (DMRG)[5] or its developments based upon the so-called tensor network states, including multiscale entanglement renormalization ansatz (MERA)[6] and projected entangled-pair states (PEPS),[7] which has been recently generalized to fermionic systems[8] and infinite lattices (iPEPS).[9]

Different calculations on the $t-J$ model have shown contradicting outcomes,[10–18] and the whole phase diagram of this model is still highly debated. One important issue, related to the mechanism of pairing in the cuprate materials, is whether some charge instability may take place (at $q = 0$, leading to phase separation, or at finite q, leading to the so-called stripes) or instead the homogeneous ground state is stable.[19] In the latter case, the residual attraction among quasiparticles may lead to a superconducting state. Previous FN calculations emphasized the existence of a stable superconducting ground state,[20] while DMRG and iPEPS results suggested a stripe order.[21]

The competition between superconductivity and stripes have been studied in several papers and different aspects have been addressed in the recent past.[22–24] For example, two of us showed that a relatively small anisotropy in the superexchange (and hopping) parameters may lead to a striped order.[25] In this regard it is crucial to have a controlled method that may give variational results in order to make a direct comparison of energies (and other correlation functions) among different methods and reach a final consensus.

In this Rapid Communication we adopt the same method used in Ref. 20 by applying a few Lanczos steps to the variational wave function and by filtering out its high-energy components (by means of the Green's function Monte Carlo with the FN approximation), the accuracy of the calculations may be highly improved. This approach is particularly effective at low doping and is actually unbiased at half-filling. Moreover, an estimation of the exact energy may be given by the variance extrapolation: besides the energy, the variance of the state can also be calculated, and the energy with zero variance can be extracted. From our finding, the existence of a striped phase for $\delta \approx 1/8$ is rather unlikely: even the best approximation to the ground state does not show any evidence toward charge inhomogeneity. Although the present calculations cannot rule out the possibility of having small static stripes, our Monte Carlo approach is expected to reproduce qualitatively correct ground-state properties; in particular, it is reliable for determining the spatial dependent hole density. Whenever an external modulated potential is added to the $t-J$ Hamiltonian, the FN approximation gives rise to stripes, even when the initial state is chosen to be homogeneous.

Model and methods. The $t-J$ model on the two-dimensional square lattice is defined by

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

where $\langle \cdots \rangle$ indicates nearest-neighbor sites, $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) creates (destroys) an electron with spin σ on the site i; $\mathbf{S}_i$ and n_i are the spin and density operators on the site i, respectively. The $t-J$ Hamiltonian is defined in the subspace without doubly occupied sites. In the following, we will take the amplitude for nearest-neighbor hopping $t = 1$, and consider the superexchange $J/t = 0.4$. The hole doping will be denoted by $\delta = 1 - N/L$, where N and L are the number of electrons and sites, respectively. Periodic boundary conditions are taken in both directions and $L \times L$ or 45-degree tilted lattices (with $L = 2l^2$, l being an odd integer, so that the noninteracting ground state is nondegenerate at half-filling) are considered.

Our starting variational wave function is defined as

$$|\Psi_v\rangle = \mathcal{P}_N \mathcal{P}_G \mathcal{J}_d \mathcal{J}_s |\Phi_{\rm MF}\rangle, \tag{2}$$

where $\mathcal{P}_N$ is the projector onto the subspace with N electrons, $\mathcal{P}_G$ is the Gutzwiller projector, which enforces no double occupation on each site; and $\mathcal{J}_d = \exp(1/2 \sum_{i,j} u_{ij} n_i n_j)$ and $\mathcal{J}_s = \exp(1/2 \sum_{i,j} v_{ij} S_i^z S_j^z)$ are density-density and spin-spin Jastrow factors, respectively. Finally, $|\Phi_{\rm MF}\rangle$ is a mean-field state that may contain BCS pairing, antiferromagnetic order, or both. In our recent papers[17,18] we have shown that very good variational energies can be obtained by orienting the magnetic order parameter in the x-y plane, so that quantum fluctuations may be included thanks to the Jastrow term $\mathcal{J}_s$. In this case, however, the wave function takes the form of a Pfaffian.[17,18] Conversely, whenever the antiferromagnetic order is taken along the z direction, we deal with a determinant.[3] The variational parameters are the u_{ij} and v_{ij} (for all independent distances in the lattice) and few parameters that describe the mean-field state $|\Phi_{\rm MF}\rangle$ (i.e., the pairing amplitude $\Delta_{\rm BCS}$, the antiferromagnetic parameter $\Delta_{\rm AF}$, as well as the chemical potential and the next-nearest-neighbor hopping describing the variational electron dispersion). Due to the presence of strong correlations (i.e., the Gutzwiller projector and the Jastrow factors), a variational Monte Carlo approach is required to compute the energy and all physical observables.

The accuracy of the wave function (2) may be improved in different ways. The first one is by applying Lanczos steps:

$$|\Psi_p\rangle = \left(1 + \sum_{k=1}^{p} \alpha_k H^k\right) |\Psi_v\rangle, \tag{3}$$

where the α_k are additional variational parameters. Clearly, whenever $|\Psi_v\rangle$ is not orthogonal to the exact ground state, $|\Psi_p\rangle$ converges to it for large p. However, on large sizes, only a few steps can be efficiently performed: here we consider the case with $p = 1$ and $p = 2$ ($p = 0$ corresponds to the original variational wave function). Moreover, an estimation of the true ground-state energy may be achieved by the variance extrapolation: for sufficiently accurate states we have that $E \approx E_{\rm ex} + {\rm const} \times \sigma^2$, where $E = \langle \mathcal{H} \rangle / L$ and $\sigma^2 = (\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2)/L$ are the energy and variance per site, respectively. Therefore, the exact ground-state energy $E_{\rm ex}$ may be assessed by fitting E vs σ^2 for $p = 0$, 1, and 2.

Another way to improve the VMC calculations is through the FN approach,[4] where the ground state of an auxiliary FN Hamiltonian is obtained. In this case, the main approximation relies on the fact that the nodal surface is assigned *a priori*, by taking a given guiding function that is usually the best variational state. Most importantly, the resulting energies are still variational, so to have a totally controlled approximation of the original problem.[4]

In this paper the guiding function is obtained by optimizing the Jastrow and the mean-field state, with the method described in Ref. 26. Then, we find the best Lanczos parameters α_p for $|\Psi_p\rangle$; finally, we perform the FN calculations with $p = 0$, 1, and 2.

Results. Before showing the results on large systems, we would like to mention that a very good accuracy on small lattices (where Lanczos diagonalizations can be performed) is obtained. We compared our results with the exact ones on the 26-site lattice for two and four holes, and different values of J/t (see Supplementary Material[27]). Both the Lanczos and the FN techniques largely improve the variational wave function and the best FN calculations (with two Lanczos steps) reaches an accuracy of $(E_{\rm ex} - E)/E_{\rm ex} \approx 0.002$ and ≈ 0.003 for two and four holes, respectively (for $J/t = 0.4$).

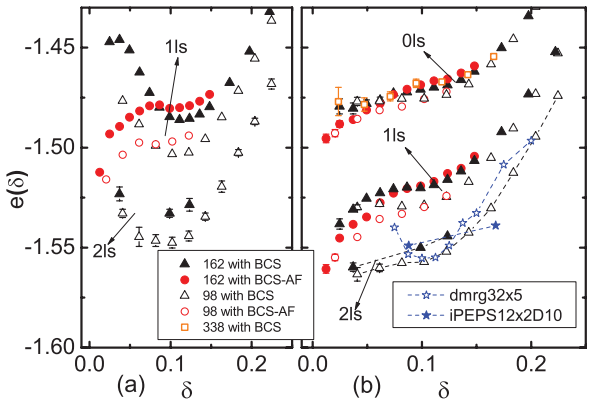

FIG. 1. (Color online) Energy per hole as a function of the doping for $J/t = 0.4$. Variational (left) and fixed-node (right) results are reported for $p = 0$ and 1 ($p = 0,1$ and 2) Lanczos steps for the wave function with (without) antiferromagnetism. The best variational DMRG and iPEPS energies[21] and the fixed-node with $p = 2$ are connected by dashed lines for a better comparison.

Let us now move to larger sizes and first analyze the tendency toward phase separation. In Fig. 1 we show our results of the energy per hole $e(\delta) = [E(\delta) - E(0)]/\delta$ for various cluster sizes.[28] $e(\delta)$ is a powerful detector for phase separation: a monotonic behavior of $e(\delta)$ vs δ indicates a finite compressibility and a stable uniform phase, while a minimum, on finite systems, or a flat behavior in the thermodynamic limit, indicate an instability.[10] Close to half-filling, the Pfaffian wave function is considerably better than the simple superconducting state, clearly indicating a coexistence of pairing and antiferromagnetic order.[17,18] As the doping increases, the antiferromagnetic parameter decreases and eventually vanishes for $\delta \approx 0.1$. The general trend is clear: the increased accuracy of the calculation favors the homogeneous state, marked by a monotonic behavior of the energy per hole vs the doping. In particular, one Lanczos step strongly improves the quality of the results, the gain in the FN energy being approximately $0.05t$, independently of δ. Even the second Lanczos step is efficient for these large sizes, providing a further energy gain of about $0.02t$. We also mention that the results obtained with the variance extrapolation are consistent with the DMRG and iPEPS ones[21]; indeed, we have that $e(\delta) = -1.61(1)$ for $0.03 \lesssim \delta \lesssim 0.12$. Remarkably, we have obtained the same extrapolated values (within three error bars) by using the two wave functions with or without antiferromagnetic order, see Fig. 2. However, the extrapolated values have too large error bars and cannot be used to study the issue of phase separation.

The application of few Lanczos steps on a given wave function is not size consistent; nevertheless, an estimation of the thermodynamic limit can be attempted by considering the largest size, where the $p = 0$ calculations do not show significant size effects. Therefore we have considered $p = 2$

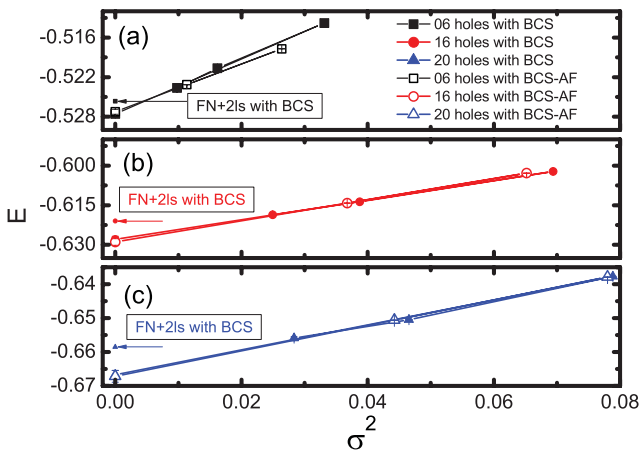

FIG. 2. (Color online) Variational results for the variance extrapolation on a 162-site cluster for different numbers of holes: $p = 0$ and 1 ($p = 0,1$ and 2) Lanczos steps have been performed on the wave function with (without) antiferromagnetism. The best fixed-node results are also marked by arrows.

FN calculations for $L = 162$ (or even 98 for $\delta \gtrsim 0.17$), which compare well with the best energies obtained by DMRG and iPEPS. The latter ones provide slightly more accurate energies for $\delta \simeq 0.1$. However, considering that all these methods are significantly away from the estimated exact energy per hole obtained by DMRG and variance extrapolations [i.e., $e(\delta) \simeq -1.61$], this difference looks essentially irrelevant. In contrast with DMRG and iPEPS that find a minimum in the energy per hole,[21] our best FN approximations do not show any tendency to phase separation for any doping, and, therefore, represent a thermodynamically stable phase corresponding to a well defined variational state.

Let us now consider the more subtle issue of stripes. Recently, DMRG and iPEPS calculations suggested that the ground state has charge (and spin) modulations, at least close to $\delta = 1/8$.[21] Up to now we have considered a uniform mean-field state $|\Phi_{\rm MF}\rangle$, clearly biasing the VMC results towards a homogeneous state. Despite the fact that the FN method can in principle remove this bias and give rise to nonuniform results, we have not found any evidence in favor of stripes with this variational ansatz.

In order to gain some evidence that a charge inhomogeneity is not stabilized in the low-doping regime, we add a site-dependent chemical potential in the mean-field Hamiltonian

$$\mu_{R_i} = \mu_0 + \delta\mu \cos\left(\frac{4\pi}{l_s} x_i\right), \tag{4}$$

where $R_i = (x_i, y_i)$ is the coordinate of the site i and l_s is equal to 8 or 12. By starting from a finite $\delta\mu$, the VMC optimization leads to a perfectly uniform state with $\delta\mu = 0$; moreover, FN calculation strongly reduces the density modulation present in the original variational wave function, see Fig. 3. Although a small inhomogeneity remains in the density profile, the FN energy is always higher than the one with $\delta\mu = 0$. For these calculations we considered 12×12, 16×16, and 24×24 lattices and $\delta = 1/8$. Similar results have been obtained also for $\delta = 1/12$ on a 12×12 lattice (not shown).

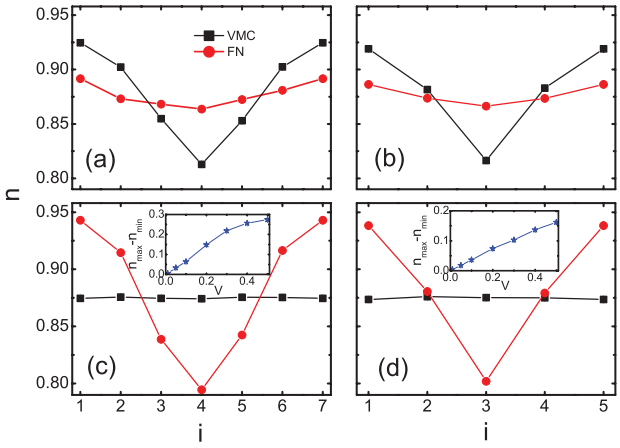

FIG. 3. (Color online) Upper panels: local density n_i when a site-dependent chemical potential with $\delta\mu = 1.6$ [see Eq. (4)] is added to the variational wave function; the cases with $l_s = 12$ (a) and 8 (b) are reported. Lower panels: local density n_i when a site-dependent potential [see Eq. (5)] is added to the $t-J$ Hamiltonian, with $l_s = 12$ and $V = 0.2$ (c) and $l_s = 8$ and $V = 0.4$ (d). Variational and fixed-node results are reported for a 12×12 cluster and $\delta = 1/8$. Insets: the difference between the largest and the smallest local density (at the fixed-node level) as a function of V.

In order to show the effectiveness and the reliability of the FN method to detect charge inhomogeneities, we add a modulated potential directly in the $t-J$ Hamiltonian:

$$V_{R_i} = V \cos\left(\frac{4\pi}{l_s} x_i\right). \tag{5}$$

Then we consider a uniform mean-field wave function and compute the local density for 12×12 and 24×24 lattices and $\delta = 1/8$. The results are also reported in Fig. 3. Clearly the VMC results show a completely flat behavior of the density in different sites; by contrast, the FN simulations are able to recover a strongly modulated density. This fact demonstrates that the presence of charge order could be detected by using this approach, even when a uniform guiding function is used in the FN technique.

Finally, we can also add a spin structure to the charge modulation, so as to have

$$\langle n_{R_i} \rangle = (1 - \delta) - \delta n \cos\left(\frac{4\pi}{l_s} x_i\right), \tag{6}$$

$$\langle S^z_{R_i} \rangle = \delta s (-1)^{R_i} \sin\left(\frac{2\pi}{l_s} x_i\right). \tag{7}$$

The above structure implies a $2 \times l_s$ unit cell and contains the so-called π shift, namely antiparallel spins across the hole-rich sites at $x_i = 0$ and $l_s/2$. In the following we consider suitable variational parameters inside the mean-field Hamiltonian that defines the uncorrelated state (i.e., local chemical potentials and local magnetic fields), such to reproduce a stripe with $l_s = 8$ and take $\delta = 1/8$ on a 16×16 lattice. Then we optimize *all* parameters (for each site independently) and observe that the initial stripe melts and a perfect uniform state is finally recovered. Moreover, by performing the FN approach starting from a variational state with stripe order, we always obtain that the charge and spin modulations are reduced and a much more

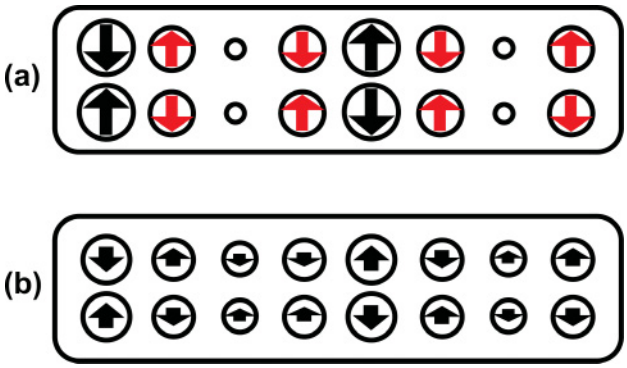

FIG. 4. (Color online) Initial variational ansatz with stripe order (a) and fixed-node calculation (b) for charge and spin distributions in the 2×8 unit cell of a 16×16 lattice. The size of the circles and arrows is proportional to the electron density and spin along z, respectively. Largest symbols in the variational calculations: $\langle n_{R_i} \rangle = 0.92$, $\langle S^z_{R_i} \rangle = \pm 0.09$.

uniform state is found (see Fig. 4); we also notice that the π shift is replaced by a small defect in a weak antiferromagnetic background.

Conclusions. In this work we have shown that the FN approach is particularly reliable, not only to improve the energy of a given variational ansatz, but also to determine the density profile of the ground state, in a way that is rather independent of the original ansatz. Indeed, the approximate FN ground state $|\Psi_{\rm FN}\rangle$ is not a "brute force" variational ansatz, but it represents the ground state of a physical Hamiltonian that is different from the exact one only in the region where the variational wave function is close to zero (namely within the so-called *nodal region*). Operators $\mathcal{O}$ that are diagonal in configuration space $|x\rangle$ (e.g., related to stripes or antiferromagnetic order) are weakly affected by this nodal error. Indeed, in the expectation value of $\mathcal{O}$, which takes the form of $\sum_x \Psi^2_{\rm FN}(x)\mathcal{O}_x$, the nodal region, where $\Psi_{\rm FN}(x) \simeq 0$, provides a very little contribution, thus explaining the reliability of the FN approach.

We have shown that the FN Monte Carlo, when combined with few Lanczos steps, is competitive with recent DMRG and iPEPS calculations, as far as the variational energy is concerned. The main outcome is that the ground state is homogeneous. No evidence of stripes are detected around $\delta = 1/8$: at low doping, a uniform state is stabilized, containing both superconductivity and antiferromagnetism. Despite our findings, we have to conclude honestly that the low-doping phase diagram of the $t-J$ model is not settled yet since very accurate methods provide very different phases with almost comparable energies. We believe that future calculations that employ the FN approach on top of iPEPS or DMRG may be helpful for the final understanding.[29]

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[27] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.85.081110 for we present the results for 2 and 4 holes on the 26-site cluster. Pure variational (VMC) and fixed-node (FN) results are shown, with 0, 1 and 2 Lanczos steps. We only considered BCS pairing and not antiferromagnetic order.
[28] The energy at half-filling has been computed for each cluster independently. We have seen that this choice minimizes finite size effects, that become negligible for $L \simeq 162$ sites.
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