PHYSICAL REVIEW B VOLUME 61, NUMBER 18 1 MAY 2000-II

From antiferromagnetism to *d*-wave superconductivity in the two-dimensional *t-J* model

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(Received 3 March 2000)

We have found that the two dimensional t-J model, for the physical parameter range $J/t=0.4$ reproduces the main experimental qualitative features of high-T_c copper oxide superconductors: *d*-wave superconducting correlations are strongly enhanced upon small doping and clear evidence of off-diagonal long-range order is found at the optimal doping $\delta\approx 0.15$. On the other hand, antiferromagnetic long-range order, clearly present at zero hole doping, is suppressed at small hole density with clear absence of antiferromagnetism at $\delta > \sim 0.1$.

The interplay between antiferromagnetism and superconductivity in the CuO_2 layers of the high T_c compounds is one of the most important effects where strong electron correlation may play the main role.[1,2] However, after many years of theoretical studies and experimental efforts[3] the most obvious question is still unclear: whether the occurrence of high T_c superconductivity is determined by the proximity of the compound to a perfect antiferromagnetic insulator.

In case strong correlation is the dominant force driving from antiferromagnetism to superconductivity a well accepted model is the two-dimensional (2D) t-J model:[2]

$$H=J\sum_{\langle i,j\rangle}\left(S_i\cdot S_j-\frac{1}{4}n_in_j\right)-t\sum_{\langle i,j\rangle}(c^\dagger_{i\sigma}c_{j\sigma}+\text{H.c.}), \quad (1)$$

where $c^\dagger_{i\sigma}$ creates an electron of spin σ on the site i, n_i, and S_i being the electron number and spin operators, respectively. Double occupations are forbidden and $\langle i,j\rangle$ denotes nearest-neighbor summation over the L lattice sites with periodic boundary conditions.

In the last decade the investigation of the properties of the 2D t-J model (and of the parent Hubbard model) has been a challenge for numerical calculations. Exact diagonalization (ED) (Ref. 4) shows that antiferromagnetic correlations are resistant up to $\delta\sim 0.15$ and superconductivity is present at intermediate doping but the lattice sizes considered were too small for being conclusive. On the contrary the quantum Monte Carlo (QMC) methods allow simulations on larger systems but suffer from the well known ''minus sign problem'' instability, which makes the simulation impossible at low enough temperatures.

At present, this instability can be controlled, only at the price of introducing some approximation, such as the fixed node (FN) approximation,[5] which is strictly variational on the ground-state energy, the constrained path quantum Monte Carlo[6] and the Green's-function Monte Carlo with stochastic reconfiguration (GFMCSR),[7] which has been developed to improve the accuracy of the FN. Both the FN and GFMCSR techniques will be extensively used in this work. Similar approximations on the ground-state wave function can be obtained by applying one (or more) Lanczos steps (LS) to the variational wave function,[8–10] or also using the density-matrix renormalization group (DMRG), which in 2D is also affected by a sizable error, and is not ''numerically exact'' as in 1D.

All these approximations allow to obtain a rather accurate value of the ground-state energy of the model, with an error typically less than 1% of the correlation energy even for large L. However, this kind of accuracy for the energy certainly does not allow us to draw reasonable conclusions on the interesting long-range properties of the model, see, e.g., Ref. 11. On the other hand, it is reasonable to expect that, by using approximate techniques that do not spoil the local character of the Hamiltonian, a similar good accuracy can be obtained on the ground-state expectation value of short-range operators such as, for instance, the kinetic energy and the exchange energies in Eq. (1). These operators O, acting only on nearest-neighbor sites, share the important property that, if added to the Hamiltonian ($H_h\rightarrow H-hO$), they do not change its local character. Moreover, this kind of perturbation typically leads to a sizable change of the ground-state energy per site E_h even in the linear regime $E_h=E_0-h\langle O\rangle/L+o(h)$, providing a very reliable estimate of the ground-state expectation value $\langle O\rangle$, as the energy $E(h)$ can be accurately determined for few values of the field h.

So far, in the literature,[12,13,10] the ground-state expectation value of the squared order parameter O^2 is estimated on an approximate ground state $\tilde{\psi}_0$, by taking, simply, its bare expectation value $\langle\tilde{\psi}_0|O^2|\tilde{\psi}_0\rangle$. For long-range operators such as O^2, this may lead to very poor approximations, unless the method is almost exact.

In order to detect superconducting long-range order with a more controlled approximation, we perform simulations in the grand canonical ensemble and add to H a short-range operator which creates or destroys a *d*-wave singlet Cooper pair:

$$H(h)=H-h(\Delta^+ +\Delta)-\mu\hat{N}, \quad (2)$$

where $\Delta^+=\Sigma_{\langle i,j\rangle}M_{ij}(c^+_{i\uparrow}c^+_{j\downarrow}+c^+_{j\uparrow}c^+_{i\downarrow})$ and $M_{ij}=1$ or -1 if the bond $\langle i,j\rangle$ is in the x or y direction, respectively, while μ is the chemical potential and $\hat{N}$ the particle operator. FN and GFMCSR allow to compute quite accurately the ground-state energy $E(h)$ also in presence of the field h. To this purpose a fundamental role is played by the guiding wave function which allows to perform importance sampling. We generalize the N particle, *d*-wave symmetry, BCS guiding wave function[14] ($|\text{BCS}\rangle$) to the grand canonical ensemble by introducing a proper weight f_N for each N particle sector:

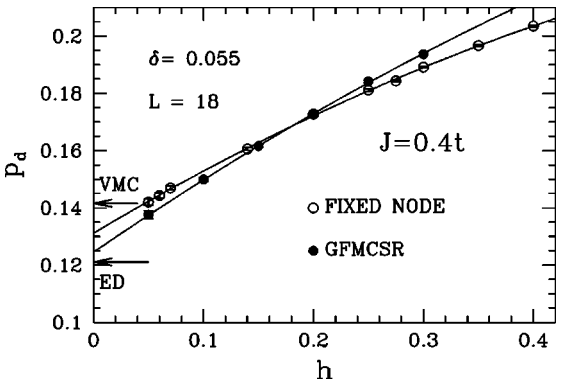

FIG. 1. p_d for $N=16$, $L=18$.

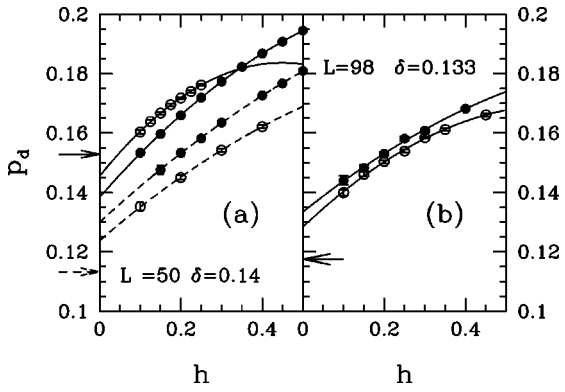

FIG. 2. VMC (arrows), FN (empty dots), and GFMCSR (full dots) calculation of p_d at $J=0.4t$ (see text for details).

$$|\psi_G\rangle = \sum_N f_N P_N \mathcal{P}_G |\mathrm{BCS}\rangle, \tag{3}$$

where $\mathcal{P}_G$ projects out doubly occupied sites and P_N selects the N-particle component of the wave function.

Our purpose is to compute the anomalous average of the order parameter $p_d = |\langle N+2|\Delta^+|N\rangle|/L$, where $|N\rangle$ and $|N+2\rangle$ are the N and $N+2$ particle ground state, respectively. p_d can be nonzero even on a finite size and zero external field. Moreover, if superconducting long-range order occurs, p_d remains finite for $L\to\infty$.

In order to compute p_d on finite-size systems we have implemented the following simple strategy. We choose the chemical potential μ in a way that the ground-state energies per site E_N and E_{N+2} for the N and $N+2$ particles are degenerate. In order to reduce the ground-state energy statistical error we optimize the variational parameters f_N by restricting ourselves to the subspaces of N and $N+2$ particles relevant for the matrix element p_d, f_N being zero otherwise. In the guiding function f_N and f_{N+2} are then determined by requiring that the average particle number $\langle \psi_G|\hat{N}|\psi_G\rangle$ is equal to $N+1$. The first-order correction to the energy due to the perturbation (2) in this restricted Fock space is given by the eigenvalues of the secular matrix:

$$\begin{vmatrix} E_N & \pm h p_d \\ \pm h p_d & E_{N+2} \end{vmatrix}. \tag{4}$$

It easily follows that $E(h)=E_N - h p_d$, meaning that the anomalous average of the order parameter can be computed as an energy difference $[E_N - E(h)]/h$ for $h\to 0$. *A long-range property of the model can be probed by studying the ground-state energy change under the effect of a local perturbation.* We expect this scheme to be a much more controlled and accurate way to characterize the long-distance behavior of a model.

As can be seen from the comparison with the exact results in Fig. 1(a), at $J=0.4t$, the VMC highly overestimates the order parameter. The FN reduces this value. The GFMCSR, implemented by reconfiguring the unperturbed energy of the two subspaces at N and $N+2$ particles in an independent way, is almost exact.

In order to attempt a finite-size scaling for the order parameter we compute p_d for much larger sizes (Fig. 2). As can be seen in the $L=50$ lattice case both the FN and the GFMCSR reduce the variational value. We have tested the accuracy of the calculation and the dependency of the results from the chosen guiding wave function, by reducing the optimal energy variational parameter $\Delta_{DW}=0.65$ [dots connected by full lines in Fig. 2(a)] to the value of $\Delta_{DW}=0.3$ (dashed lines). This implies a sizable reduction of p_d within VMC. The FN evaluation of p_d correctly enhances this value, getting closer to the more reliable estimate obtained with the optimal energy variational parameter. The GFMCSR method, the most accurate technique used here, is, remarkably, rather insensitive to the choice of the guiding function, being the difference for the two GFMCSR results a conservative estimate of the possible error in the determination of p_d. GFMCSR seems to improve by the same amount the FN estimate of p_d, both for the 18 sites (Fig. 1) and 50 sites [Fig. 2(a)], and this improvement is expected to remain even for larger sizes, being GFMCSR, as well as FN, a size consistent approximation. The 98-site calculation shows that the VMC value of p_d is enhanced both by the FN and GFMCSR calculation and remarkably the computed value is very close to the one obtained for the 50 site lattice.

Our results at this doping and J/t value display, *all* consistently, stronger and stronger *d*-wave correlations, as the accuracy of our numerical techniques are improved and lattice size increased. We believe that this represents a robust evidence of *d*-wave superconductivity in the 2D *t-J* model. However the limited number of lattice sizes considered does not allow us to perform an accurate finite-size scaling. As shown in Fig. 3, size effects are present also at the variational level and the true order parameter may be much below the value ~ 0.12 reported in the picture.

Since the *t-J* model originates from the doping of an antiferromagnetic Mott insulator it is interesting to understand if the antiferromagnetic character of the undoped ground state is resistant upon doping. Following a similar procedure to the one used for the superconducting long-range order, we added to the Hamiltonian a short-range perturbation coupled to the staggered magnetization: $m_h = 1/L \Sigma_R s^z_R (-)^R$, namely $H \to H - h \Sigma_R s^z_R (-)^R$, and compute m_h in presence of the field h either by differentiating the energy per site $m_h = -dE(h)/dh$ or by using the forward walking technique, whenever possible (FN).[15] For this quantity the FN and GFMCSR are consistent for small field, meaning that the FN is already enough accurate for the magnetic phase diagram.

For the Heisenberg antiferromagnet, where broken symmetry occurs, the magnetization as a function of the rescaled

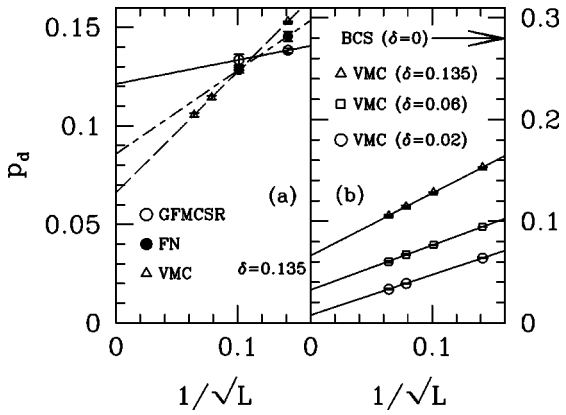

FIG. 3. Size scaling of p_d at $J=0.4t$. The lines connecting FN and GFMCSR in (a) are guides to the eye, least square fit for the variational method in (b).

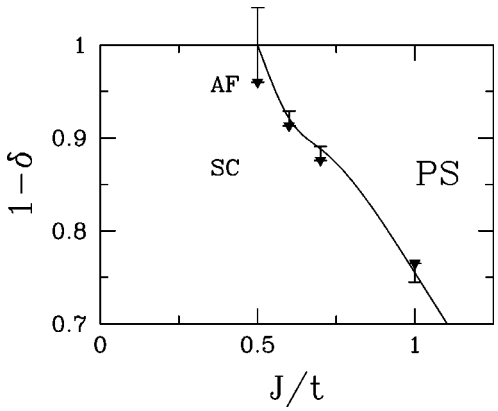

FIG. 5. Instability (PS) of the uniform phase evaluated by GFMCSR using the Maxwell construction for the 98 site lattice. The errors are estimates of finite-size effects and correspond to twice the difference between the 98 and 50 site critical doping (Ref. 22). The SC label represents $\delta=0.14$, where p_d has been computed, and the AF label is the antiferromagnetic region.

field $h\rightarrow hL$ lies on a universal curve[16] which weakly depends on the system size. This size dependence is almost negligible if compared to the one affecting the squared order parameter [Fig. 4(b)].[15,17] This feature strengthens the validity of our results that are *all* based upon ground-state expectation values of short-range operators in presence of a field. At finite doping, computationally heavier, we have chosen to work with a single field for each size and tuned at zero doping in order to reproduce on the available finite systems the infinite size order parameter: $h=\bar{x}/JL$ with $\bar{x}=0.392$. It turns out that the antiferromagnetic correlations are present even at finite doping up to $\delta_c=0.10$ see Fig. 4(b), in qualitative agreement with experimental findings ($\delta_c^{exp}\sim 3-5\,\%$). For a quantitative agreement, other terms must be probably added to the Hamiltonian, as suggested in Ref. 18. In the optimal doping region the staggered magnetization is vanishingly small even in presence of a sizable magnetic field, meaning that long-range order has disappeared favoring a pure *d*-wave superconducting state.

The interplay between antiferromagnetism and superconductivity appears to be a fundamental point in the phase diagram of the *t-J* model. For small doping the matrix element $\langle N+2|\Delta^+|N\rangle$, is strongly suppressed but antiferromagnetism is still present. Close to the Mott insulator ($\delta=0$), as pointed out previously,[19–22] there is a strong tendency to have a phase-separation instability between a hole rich uniform phase and an undoped antiferromagnetic insulator. In the phase diagram shown in Fig. (5), that we have obtained with the same method (GFMCSR using only the energy in the reconfiguration scheme) used for the computation of the *d*-wave order parameter, the PS boundary is quite far from the optimal doping region at $J/t=0.4$. However the compressibility of the electron system is very large ($d\mu/dn\approx 0.54t$) *about 20 times larger than the corresponding spinless fermion compressibility*, in surprising numerical agreement with a spinless fermion model with renormalized flat band.[23] Thus the proximity to an antiferromagnetic insulator strongly enhances charge fluctuations determining—for physical J/t values—a *d*-wave superconducting phase before the PS instability.

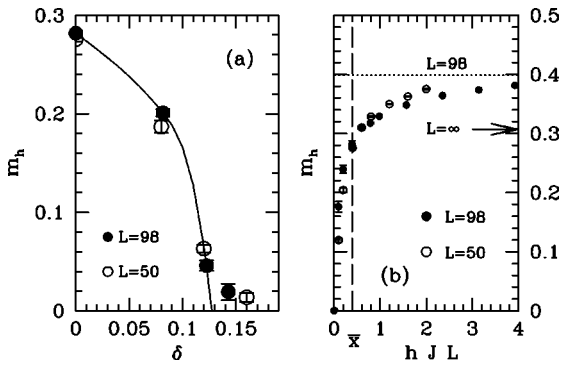

FIG. 4. Staggered magnetization m_h for $\bar{x}=\bar{h}JL=0.392$ (a). m_h for $\delta=0$ (b). The horizontal dotted line represents the squared order parameter value. Remaining lines are guides to the eye.

We believe that a large value of the compressibility is very important to stabilize superconductivity even in presence of long-range Coulomb repulsion, certainly present in the physical system but missing in the *t-J* model. For large compressibility the Thomas-Fermi screening length $\xi=(1/2\pi e^2)d\mu/dn$[24] is very short compared to the Cu-Cu distance, so that the screening is very much effective. We have verified this picture (on smaller sizes) by adding to the *t-J* model a repulsive nearest-neighbor interaction $V\Sigma_{\langle ij\rangle}n_in_j$ and found still strong superconducting correlations, weakly suppressed even for large $V/J\sim 1$.

Another mechanism in competition with superconductivity, is the formation of so called ''stripes'' in the ground state of the *t-J* model, as recently found by White and Scalapino with DMRG.[13] In order to test this possibility we have compared our results with the DMRG ones on a 12×6 system with 8 holes and open boundary conditions at $J/t=0.4$. In this case, DMRG is quite more accurate than our techniques in the energy estimate, but it is not yet clear whether the same is true for correlation functions. Within our accuracy for correlation functions, *we have not found any clear indication of ''stripes.''* in qualitative disagreement with the DMRG results, and confirming our previous work,[22] obtained with periodic boundary conditions. In this case, remarkably, the possibility to use translation invariance, allows

calculations by far more accurate and reliable even compared with the best DMRG results, both for energies and correlation functions.

In this model we thus recover the most simple scenario that appeared in the early days of high T_c superconductivity, namely, that the strong correlation *alone* may drive the system from antiferromagnetism to superconductivity.

The contradictory results present in the literature so far are, in our opinion, mainly due to the general attempt of computing a long-range quantity by using approximations that weakly affect energy estimates but may lead to sizable systematic errors on correlation functions. With our technique we overcome this difficulty by estimating only short-range operators expectation values with energy difference calculations. The short-range operators' expectation values are less sensitive to finite-size effects, and contain the useful information to establish the absence or presence of long-range order.

We finally remark that it is extremely important to use a very accurate method to rule out superconductivity at small doping for a strongly correlated system such as the *t-J* model. Even at the variational level, the superconducting order parameter that is very large before Gutzwiller projection becomes an extremely small quantity after this projection [see Fig. 3(b)]. This strong suppression of *d-wave* pairing, can be easily shown at the variational level (see Fig. 3) and proven at $\delta=0$, and is a crucial property of strongly correlated systems.

We acknowledge S. White for sending us numerical results before publication, M. Fabrizio, L. Capriotti, M. Capone, and F. Becca for useful discussion, and A. Parola for careful reading of the manuscript. This work was supported by INFM (PRA HTCS), and partly by MURST COFIN97 and COFIN99.

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