From antiferromagnetism to d-wave superconductivity in the 2D t–J model

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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-Tc 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 density with clear absence of antiferromagnetism at $\delta > \sim 0.1$.

71.10.Fd,71.10.Hf,75.10.Lp

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. However, after many years of theoretical studies and experimental efforts the most obvious question is still unclear: whether the occurrence of high Tc 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 2D t-J model [3]:

$$H = J \sum_{<i,j>} (S_i \cdot S_j - \frac{1}{4} n_i n_j) - t \sum_{<i,j>} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.),$$

where $c_{i\sigma}^\dagger$ creates an electron of spin $\sigma$ on the site $i$, $n_i$ and $S_i$ being the electron number and spin operators respectively. Double occupations are forbidden and $<i,j>$ 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) [3] 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 [3], which is strictly variational on the ground state energy, the constrained path quantum Monte Carlo [3] and the Green function Monte Carlo with stochastic reconfiguration GFMC/SGFMC [7], which has been developed to improve the accuracy of the FN. Both the FN and GFMC/SGFMC techniques will be extensively used in this work. Similar approximations on the ground state wavefunction can be obtained by applying one (or more) Lanczos steps (LS) to the variational wavefunction [8], 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 to draw reasonable conclusions on the interesting long range properties of the model, see e.g. [6]. 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 like, 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 ($H_h \rightarrow H - hO$) 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 $E_h = E_0 - h <O>/L + o(h)$, providing a very reliable estimate of the ground state expectation value $<O>$, as the energy $E(h)$ can be accurately determined for few values of the field $h$.

So far, in the literature the ground state expectation value of the squared order parameter $O^2$ is estimated on an approximate ground state $\psi_0$, by taking, simply, its bare expectation value $<\psi_0|O^2|\psi_0>$. 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 grandcanonical ensemble and add to $H$ a short range operator which creates or destroys a $d$-wave singlet Cooper pair:

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

where $\Delta^+ = \sum_{<i,j>} M_{ij} (c_{i\uparrow}^\dagger c_{j\downarrow} + c_{i\downarrow}^\dagger c_{j\uparrow})$ and $M_{ij} = 1$ or $-1$ if the bond $<i,j>$ is in the $x$ or $y$ direction re-
spectively, while $\mu$ 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 wavefunction which allows to perform importance sampling. We generalize the $N$ particle, d-wave symmetry, BCS guiding wavefunction [4] ($BCS$) to the grand canonical ensemble by introducing a proper weight $f_N$ for each $N$ particle sector:

$$|\psi_G\rangle = \sum_N f_N P_N \mathcal{P}_G |BCS\rangle$$

(3)

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

![FIG. 1. $p_d$ for $N = 16$, $L = 18$](image)

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 non zero 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 $\mu$ 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 $\langle \psi_G |N \psi_G \rangle$ is equal to $N + 1$. The first order correction to the energy due to the perturbation $\Delta$ in this restricted Fock space is given by the eigenvalues of the secular matrix:

$$\begin{pmatrix} E_N & \pm hp_d \\ \pm hp_d & E_{N+2} \end{pmatrix}$$

(4)

It easily follows that $E(h) = E_N - hp_d$, 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.

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

As can be seen from the comparison with the exact results in Fig. 2(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 wavefunction, by reducing the optimal energy variational parameter $\Delta_{DV} = 0.65$ (dots connected by full lines in Fig. 2(a) to the value of $\Delta_{DV} = 0.3$ (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 maybe below the value $\sim 0.12$ 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: $m_h = 1/L \sum_{R} s^z_{R}(-)^{R}$, namely $H \rightarrow H - h \sum_{R} s^z_{R}(-)^{R}$, 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). 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 field $h \rightarrow h \cdot L$ lies on a universal curve which weakly depends on the system size. This size dependence is almost negligible if compared to the one affecting the squared order parameter (Fig. 3 b) [13]. This feature strengthen 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. 3 (b), in qualitative agreement with experimental findings ($\delta_{\text{exp}} \sim 3 - 5\%$). For a quantitative agreement, other terms must be probably added to the Hamiltonian, as suggested in [15]. 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.

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

![FIG. 4. Staggered magnetization $m_h$ for $\bar{x} = \hbar JL = 0.392$ (a). $m_h$ for $\delta = 0$ (b). The horizontal dotted line represents the squared order parameter value. Remaining lines are guides to the eye.](image)
effective. We have verified this picture (on smaller sizes) by adding to the \( t-J \) model a repulsive nearest-neighbor interaction \( V \sum_{<ij>} n_i n_j \) 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.\cite{13} In order to test this possibility we have compared our results with the DMRG ones on a \( 12 \times 6 \) 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 especially the ones described by short range operators, where our approximations seem to be quite reliable. Within this 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\cite{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, appeared in the early days of HTc superconductivity, namely that the strong correlation \textit{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 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 like 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.\ref{fig:instability}b). This strong suppression of \( d-wave \) pairing, can be easily shown at the variational level (see Fig.\ref{fig:instability}) 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, F. Becca for useful discussion and A. Parola for careful reading of the manuscript. This work was supported by INFN (PRA HTCS), and partly by MURST COFIN97 and COFIN99.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{instability.png}
\caption{Instability (PS) of the uniform phase evaluated by GFMC\( \sigma \)R using the Maxwell construction for the 98 site lattice. Errors are estimates of finite size effects and correspond to twice the difference between the 98 and 50 site critical doping \( \delta = 0.14 \) were \( p_d \) has been computed, AF label the antiferromagnetic region.}
\end{figure}