Superconductivity in the cuprates

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Abstract

We evaluate numerically several superconducting correlation functions in a generalized $t - J$ model derived for hole-doped CuO$_2$ planes. The model includes a three-site term $t''$ similar to that obtained in the large $U$ limit of the Hubbard model but of opposite sign for realistic O-O hopping. For realistic parameters we obtain strong evidence of superconductivity of predominantly $d_{x^2-y^2}$ character. The ground state has a large overlap with a very simple resonating-valence-bond wave function with off-diagonal long-range order. This function reproduces the main features of the magnetic and superconducting correlation functions.

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In spite of a considerable effort, no indisputable evidence of superconductivity has been found in strongly correlated models for the cuprates for realistic parameters. The numerical methods are so far the most reliable to treat strong correlations, and clear indications of \(d_{x^2-y^2}\) superconductivity have been found in the \(t-J\) model for a \(4 \times 4\) cluster, but only for values of \(J\) which are an order of magnitude larger than the realistic values and for too large doping \(x = 0.5\). Variational Monte Carlo results in the large \(U\) limit of the Hubbard model suggest that it might be necessary to solve larger clusters to obtain superconductivity for realistic parameters, and favor mixed \(s-d\) superconductivity \([2]\). On the other hand, Monte Carlo results in the three-band Hubbard model \([3,4]\) with O-O hopping \(t_{pp} = 0\) favor \(s\)-wave superconductivity, although the dependence of the superconducting correlation functions with distance has not been investigated \([5]\). In this Letter we present numerical evidence of superconductivity and at the same time a resonating-valence-bond (RVB) state \([6]\) in a realistic model.

After the original derivation of the \(t-J\) model \([7]\), it became clear that this model should be supplemented by other terms to accurately represent the physics of the three-band Hubbard model \([8-12]\), and experimental data \([12-14]\). Including the most important terms, the Hamiltonian can be written in the form \([11]\):

\[
H = t \sum_{\delta \sigma} c_{i+\delta \sigma}^\dagger c_{i \sigma} + t' \sum_{\gamma \sigma} c_{i+\gamma \sigma}^\dagger c_{i \sigma} \\
+ t'' \sum_{\delta \neq \delta'} c_{i+\delta' \sigma}^\dagger c_{i \delta \sigma} \left( \frac{1}{2} - 2 \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \right) \\
+ \frac{J}{2} \sum_{i \delta \sigma} (\mathbf{S}_i \cdot \mathbf{S}_{i+\delta} - \frac{1}{4} n_i n_j) .
\]

\(H\) acts on a square lattice on which double occupancy is forbidden \((c_{i\sigma}^\dagger n_i = 0)\). The vectors \(\delta(\gamma)\) connect a site with each of its four nearest neighbors (next-nearest neighbors). While the sign of \(t\) can be absorbed in a change of phase of half the creation operators, the signs of \(t'\) and \(t''\) are relevant and depend on the form chosen for the restricted Hilbert space and the precise meaning of \(c_{i\sigma}^\dagger\). Here this operator creates a \(particle\) at the vacant site \(i\) \([15]\).

A recent systematic analytical study of the mapping of the three-band Hubbard model
to $H$ shows that for O-O hopping $t_{pp} \gtrsim 0.3\text{eV}$, the mapping using localized non-orthogonal Zhang-Rice singlets is more accurate than the one which uses orthogonal O Wannier functions [12]. Using the former mapping, $t_{pp}$ gives rise to a positive contribution to $t''$ due to the non-orthogonality of the states. As shown in Fig. 1, numerical fitting of the parameters of $H$ agrees very well with the analytical calculations and both show that $t'$ and $t''$ change sign for increasing $t_{pp}$. Constrained density-functional calculations predict $t_{pp} = 0.65\text{eV}$ [9] and this results in positive values of $t'$ and $t''$. A positive $t'$ [15] agrees with calculations of other authors [9,14], with the form of the Fermi surface [14], and with calculations of different normal state properties [13]. Also, the fact that $t' > 0$ for hole-doped systems while $t' < 0$ in electron doped systems [9,12,14] allows to understand the different relative stability of the Neel order upon doping in both types of systems [12,14]. Thus, the parameters taken here: $J = 0.4, t' \sim 0.2$, and $t'' \sim 0.1$ in units of $t = 1$, are close to those which best describe the hole-doped cuprates.

The effect expected from the correlated hopping $t''$ becomes clear writing the corresponding term in the form of a hopping of nearest-neighbor singlets:

$$H_{t''} = 2t'' \sum_{i\delta \neq i'\delta'} b_{i\delta}^\dagger b_{i'\delta'}; \quad b_{i\delta}^\dagger = \frac{1}{\sqrt{2}}(c_{i+\delta\uparrow}^\dagger c_{i\downarrow}^\dagger - c_{i+\delta\downarrow}^\dagger c_{i\uparrow}^\dagger).$$

(2)

Thus, $H_{t''}$ is expected to favor a Bose condensate of singlets with $d_{x^2-y^2}$ ($s$) symmetry for $t'' > 0$ ($t'' < 0$), similar to the RVB state constructed by Anderson [3]. This agrees with mean-field calculations [16], and the above mentioned results for the Hubbard model [2] (for which $t'' = -J/4$) and the three-band Hubbard model with $t_{pp} = 0$ [3] (implying also $t'' < 0$ in the effective model $H$). Instead $J$ at most tends to stabilize static singlets, while $t$ and part of the terms proportional to $t'$, break the singlets. Since $d$-wave pairing is expected to arise from antiferromagnetic spin fluctuations at small doping [1,17], one expects that a positive $t''$ would interfere constructively with any superconducting mechanism already present in $H - H_{t''}$.

We have used the Lanczos method to obtain the ground state of $H$ for a $4 \times 4$ cluster with periodic boundary conditions in each subspace defined by the $z$ projection of the total spin.
and the irreducible representation of the space group. In Fig. 2 we show the susceptibility
\[
\chi_{\text{sup}}^d = \frac{\langle \sum_{i<j,\delta,\delta'} f(\delta) f(\delta') | g \rangle}{\langle b_{i\delta}^\dagger b_{j\delta'} | g \rangle} / L
\]
where \( | g \rangle \) is the ground state, \( L \) the size of the system, \( f(\delta) = 1 \) if \( \delta \parallel \hat{\mathbf{x}} \) and \( f(\delta) = -1 \) if \( \delta \parallel \hat{\mathbf{y}} \) as a function of \( t'' \).

The abrupt increase in \( \chi_{\text{sup}}^d \) is apparent. After this increase, \( \chi_{\text{sup}}^d \) reaches values similar or larger than the maximum one obtained previously in the \( t - J \) model (\( \chi_{\text{sup}}^d \sim 2.5 \) for \( J = 3, x = 0.5, t' = t'' = 0 \)) [1]. Also, the qualitative behavior of the superconducting correlation functions (shown below) changes and they saturate rapidly with distance for \( x = 0.25 \) but not for \( x \geq 0.5 \). As will be described in detail elsewhere, except for very particular values of the parameters, \( \chi_{\text{sup}}^d \) has its maximum value at a doping level \( x \sim 0.25 \) in agreement with experiment. For \( x = 0.75, \chi_{\text{sup}}^d \sim 10^{-2} \) for \( t' = 0.2 \). For all parameters considered here the system is far from the region of phase separation [1], which is reduced by \( t'' \).

Our results suggest that as \( t'' \) is increased, there is a continuous, although abrupt transition from a disordered spin liquid to a RVB state with off-diagonal long range order (ODLRO). To support this conclusion we consider the following simple generalization to \( x \neq 0 \) and ODLRO of Sutherland’s RVB wave function [18]:

\[
|RVB0\rangle = P_N \prod_{j \in A} (1 + \sum_\delta g(\delta) b_{i\delta}^\dagger) |0\rangle,
\]

where \( P_N \) is the projector over a definite even number of particles \( N, j \in A \) indicates that the product over sites is restricted to one sublattice \( g(\delta) = 1 \) for each “horizontal” singlet (\( \delta \parallel \hat{\mathbf{x}} \)) and \( g(\delta) = i \) for each “vertical” singlet (\( \delta \parallel \hat{\mathbf{y}} \)). Eq. (3) is clearly not an optimum wave function, since unlike Anderson’s one [1] it contains no wave-vector dependence. In spite of this we find that from its real part and the first few powers of \( H \) applied to it, an excellent variational function for \( t'' > 0.12 \) can be constructed. The real (imaginary) part of \( |RVB0\rangle \) has an even (odd) number of vertical singlets. For \( N = L, Im |RVB0\rangle = 0 \). It is easy to check that if the number of singlets \( N/2 \) is a multiple of four, \( Re |RVB0\rangle \) transforms like the representation \( \Gamma_1 \) (invariant) of the space group, while \( Im |RVB0\rangle \) transforms like \( \Gamma_3 (x^2 - y^2) \). Instead for \( N/2 \) even but not multiple of four, the real (imaginary) part of
$\text{RVB}\,0 >$ transforms like $\Gamma_3$ ($\Gamma_1$) under the symmetry operations of the space group. In the $4 \times 4$ cluster we find that for $N = 12\, (x = 0.25)$ and $N = 8\, (x = 0.5)$ for $t'' \geq 0.1$, the ground state $g >$ belongs to the same irreducible representation as $\text{Re} \, | \text{RVB}0 >$. The simplest function which contains configurations with even and odd number of vertical bonds with the correct symmetry, and takes advantage of $H_{t''}$ has the form:

$$| \text{RVB}1 > = F\left(1 - \frac{\alpha}{t''}\right)\text{Re} \, | \text{RVB}0 > ,$$

where $F$ is a normalization factor. We have determined $\alpha$ maximizing the square of the overlap $S^2 = |< g | \text{RVB}1 >|^2$. This quantity as a function of $t''$ is shown in Fig. 3. Taking into account the simplicity of Eq. (4), that there is only one free parameter, and that the size of the Hilbert space is huge, the magnitude of $S^2$ after the transition is noticeable.

$| \text{RVB}1 >$ can be improved considerably if a variational function is constructed with $H^n | \text{RVB}1 >\, (n = 0$ to $3)$. The generalized RVB state thus obtained correctly takes into account the effects of $t$ and $t'$ and practically coincides with $| g >$. However, we will show that $| \text{RVB}1 >$ reproduces already, at least qualitatively, the main numerical results. $\chi_{\text{sup}}^d$ obtained from $| \text{RVB}1 >$ is compared in Fig. 2. Note that the expectation value of $b_{\delta}^\dagger b_{\delta'}$ in $| \text{RVB}1 >$ for $\delta \perp \delta'$ vanishes for $\alpha = 0$, implying equal amounts of $s-$ and $d$-wave superconductivity. For $t'' > 0.12$ the $d$-wave component of $| \text{RVB}1 >$ dominates but there is always some $s$ component.

In Fig. 4 we show how after the transition with increasing $t''$, a peak in $(\pi, \pi)$ develops in the magnetic structure factor, which is in excellent agreement with the result of $| \text{RVB}1 >$. This peak is probably related with the strong peak in the staggered spin susceptibility $\chi(\pi, \pi)$ assumed in the phenomenological spin-fluctuation theories [17]. For $t'' = 0$, $S(\pi, \pi)$ slightly decreases with increasing $t'$. The absence of a structure in $S(\pi/2, \pi/2)$ for $| \text{RVB}1 >$, is due to the lack of magnetic correlations beyond nearest neighbors in this function, and is restored if $| \text{RVB}1 >$ is improved including the effect of $t$.

In Fig. 5 we show the distance dependence of the $d$-wave superconducting correlation functions $c(m) = \sum_{i\delta\delta'} f(\delta)f(\delta') < g | b_{\delta}^\dagger b_{i+m\delta'} | g >$ and the corresponding expectation
value in $|RVB1>$. One can see that $c(m)$ saturates at large distances, suggesting ODLRO for the infinite system. The significant overlap of $|g>$ with a function which has ODLRO in the thermodynamic limit is another important indication. Instead, the corresponding s-wave correlation functions decay steadily with distance.

In summary, we have found strong evidence of $d$-wave superconductivity in the model Eq. (1) for reasonable $t'' > 0.12$ and experimentally relevant doping $x = 0.25$, and parameters $J = 0.4, t' \sim 0.2$ in units of $t$. The possibility of some amount of $s$-wave superconductivity remains open. The model and parameters are close to the most realistic ones for the cuprates. The superconductivity is rather insensitive to $t'$ and preliminary results suggest that it persists if a repulsion between nearest-neighbor Zhang-Rice singlets smaller than $J$ is included in the model. The ground state of the system for the above mentioned parameters is a generalized superconducting RVB state $\frac{3}{2}$. A similar conclusion has been recently obtained for single-rung $t-J$ ladders $\frac{19}{19}$. As noted by Anderson, the RVB state is favored by electron-phonon interaction, particularly if the system is near an instability against a Cu dimerization mode $\frac{6}{6}$. Theoretical calculations have suggested that this might well be the case $\frac{20,21}{20,21}$. Also a RVB state allows for a qualitative explanation of the phase diagram of the high-Tc systems at mean-field level $\frac{22}{22}$, and is consistent with a strongly enhanced $\chi(\pi, \pi) \frac{17}{17}$ and with the spin gap observed in YBaCuO $\frac{23}{23}$. To our knowledge this is the first time that large superconducting correlations at distances of a few lattice parameters and the physics of the RVB is unambiguously obtained numerically in the ground state of a model for hole-doped CuO$_2$ planes for parameters close to the optimum ones.

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FIGURE CAPTIONS

Fig. 1: Parameters of $H$ determined from the three-band Hubbard model as a function of the O-O hopping $t_{pp}$. The remaining parameters were taken from Ref. 3 and the Cu-O hopping $t_{pd}$ was taken as the unit of energy. Full line: numerical fit of the energy levels of a Cu$_4$O$_8$ cluster. Dashed line: analytical results from a mapping using localized non-orthogonal Zhang-Rice singlets.

Fig. 2: $d$-wave susceptibility as a function of $t''$ for $t = 1, J = 0.4$ and doping $x = 0.25$. Full line: $t' = 0.2$. Dashed line: $t' = 0$. Dotted line: result using $|RVB1>$ (Eq. (4)) with $t' = 0.2$.

Fig. 3: Square of the overlap between the ground state and $|RVB1>$ as a function of $t''$ for $t' = 0.2$. Other parameters as in Fig. 2.

Fig. 4: Magnetic structure factor $\sum_{ij} <g | S_i^z S_j^z e^{iq(\mathbf{R}_i-\mathbf{R}_j)} | g>/L$ as a function of wave vector. Dashed line: $t' = t'' = 0$. Full line: $t' = t'' = 0.2$. Dotted line: result using $|RVB1>$ with $t' = t'' = 0.2$. Other parameters as in Fig. 2.

Fig. 5: $d$-wave superconducting correlation functions as functions of the distance. Parameters are the same as in Fig. 4.