INDICATIONS OF $d_{x^2-y^2}$ SUPERCONDUCTIVITY IN THE TWO DIMENSIONAL $t$-$J$ MODEL

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ABSTRACT: Superconducting correlations in the two dimensional $t$ – $J$ model at zero temperature are evaluated using numerical techniques. At the fermionic density $\langle n \rangle \sim 1/2$, strong signals of $d_{x^2-y^2}$ superconductivity were observed in the ground state. These conclusions are based on a study of static pairing correlations, the Meissner effect, flux quantization, and other indicators of superconductivity. It is argued that these results can be explained using a spin dimer “liquid” state. A phase diagram of the two dimensional $t$ – $J$ model is presented.

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The study of high-$T_c$ superconductors continues attracting considerable attention. Recent calculations suggest that non s-wave symmetry pairing interactions with nodes, may explain some of the unusual properties of the cuprate compounds, in particular the behavior of relaxation rates in the YBa$_2$Cu$_3$O$_7$ material, as well as the systematic presence of spectral weight inside the superconducting gap.$^1$ More specifically, the possibility of $d_{x^2−y^2}$ superconductivity in the cuprate materials has been recently discussed.$^2,3$ Most of these calculations have been performed without specifying the details of the interaction, but analyzing a BCS-like gap equation for different pairing symmetries. Thus, it would be important to find a realistic model of strongly interacting electrons having a $d_{x^2−y^2}$ symmetric superconducting state as ground state. From the properties of this state, dynamical responses of a d-wave condensate could be studied, and concrete predictions would be made to contrast theory with experiments. In this scenario, numerical studies are important to decide whether a given electronic model presents a superconducting phase, specially since the strongly interacting character of several realistic models makes most analytical approximations questionable. The one band Hubbard model is a typical example of these problems, i.e. while for some time it was assumed that the ground state at finite hole doping superconducts, Quantum Monte Carlo simulations have not supported these claims. Then, the issue of whether purely electronic models of high-$T_c$ materials present a superconducting ground state is still open.

The purpose of this paper is to present numerical results suggesting that the widely studied two dimensional $t−J$ model has a superconducting phase in a previously unexplored region of parameter space. The symmetry of the condensate is $d_{x^2−y^2}$, and thus this model may become a physical realization of the d-wave pairing scenarios recently proposed in the literature.$^3,2$ The superconducting phase observed here appears near the well-known region of phase separation of the $t−J$ model.$^4,5$ The possible presence of superconducting correlations near phase separation has been recently discussed in other contexts and
theories, but here the first numerical indications are provided that this phenomenon may occur in the ground state of a realistic model of strongly correlated electrons. The $t - J$ model is defined by the Hamiltonian,

$$H = J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) - t \sum_{\langle ij \rangle,s} (\bar{c}_{i,s}^\dagger \bar{c}_{j,s} + h.c.),$$

(1)

where $\bar{c}_{i,s}^\dagger$ denote hole operators; $n_i = n_{i,\uparrow} + n_{i,\downarrow}$; and square clusters of $N$ sites with periodic boundary conditions are considered. The rest of the notation is standard. Here, efforts have been concentrated on the exact diagonalization of $4 \times 4$ lattices, although preliminary results for clusters of 20 and 24 sites are available. It has been repeatedly shown in the literature that these cluster sizes are large enough to capture the essential qualitative physics of several models of strongly correlated electrons. Besides, no other available (and unbiased) numerical technique can handle the involved calculations that have been carried out for the $t - J$ model without making assumptions about the properties of the ground state. To search for indications of superconductivity, let us define the singlet pairing operator $\Delta_i = c_{i,\uparrow}(c_{i+\hat{x},\downarrow} + c_{i-\hat{x},\downarrow} \pm c_{i+\hat{y},\downarrow} \pm c_{i-\hat{y},\downarrow})$, where + and − corresponds to extended-s and $d_{x^2-y^2}$ waves, respectively, and $\hat{x}, \hat{y}$ are unit vectors along the axis. The pairing-pairing correlation function $C(m) = \frac{1}{N} \sum_1 \langle \Delta_i^\dagger \Delta_{i+m} \rangle$, and its susceptibility $\chi^\alpha_{sup} = \sum_m C(m)$ have been calculated (where $\alpha = d$ corresponds to $d_{x^2-y^2}$ wave, and $\alpha = s$ to extended-s wave). $\langle \rangle$ denote expectation values in the ground state, which is obtained using the Lanczos method.

$\chi^d_{sup}$ is shown in Fig.1a as a function of $J/t$, for several densities. In this study, it was observed that the $d_{x^2-y^2}$ wave susceptibility dominates, presenting at $\langle n \rangle = 1/2$ a sharp peak at $J/t \sim 3$. By analyzing several spin and hole correlations, and following other criteria it was verified that the fast decay of $\chi^d_{sup}$ after the peak is induced by the transition to the phase separated region. Changing the fermionic density, it was observed that $\chi^d_{sup}$ has its maximum value at $\langle n \rangle = 1/2$, as shown in Fig.1a. $\chi^s_{sup}$ has been also
evaluated at $\langle n \rangle = 1/2$. This susceptibility peaks at approximately the same position as $\chi_{sup}^d$ does, but with a smaller intensity.\textsuperscript{10} The pairing-pairing correlations as a function of distance are shown explicitly in Fig.1b in the region where the susceptibilities have a sharp maximum, i.e $J/t = 3.0$ and $\langle n \rangle = 1/2$. As expected from the behavior of $\chi_{sup}^d$, Fig.1a, the dominant correlation functions at the maximum distance on the $4 \times 4$ cluster corresponds to $d_{x^2-y^2}$ symmetry. On the other hand, the correlations for extended-s operators are strong at short distances, but decay rapidly at large distances. For completeness, in Fig.1b the correlation corresponding to $d_{xy}$ symmetry is also presented.\textsuperscript{11} These correlations seem more heavily suppressed than for the $d_{x^2-y^2}$ and extended-s channels. In Fig.1c, the d-wave pairing correlations are shown at $\langle n \rangle = 1/2$, as a function of $J/t$. Their maximum value is obtained at the same coupling where $\chi_{sup}^d$ peaks, as expected.

The symmetry of the ground state (obtained with the Lanczos method) under a rotation of the lattice in $\pi/2$ has been studied. In the region where superconducting correlations exists, the ground state is odd under this operation, but it is invariant under reflexions with respect to the x and y-axis. Then, the ground state at $\langle n \rangle = 1/2$ belongs to the $B_{1g}$ representation of the $C_{4v}$ group, usually denoted by $d_{x^2-y^2}$, in agreement with the previous conclusions studying pairing correlations. However, it is worth noticing that the state with the lowest energy in the subspace invariant under rotations and reflexions (i.e. s-wave) is close in energy to the ground state. More specifically, at $\langle n \rangle = 1/2$ and $J/t = 3.0$, the energy of the d-wave ground state is $-26.413t$, the lowest s-wave state has energy $-26.127t$, while, for comparison, the lowest spin one state in the spectrum carries an energy $-25.188t$. Then, a scenario where s + id pairing occurs in the bulk limit is not excluded, although it is clear that the $d_{x^2-y^2}$ correlations seem stronger.

The pairing correlations found in the two dimensional $t - J$ model suggest the existence of a superconducting phase near phase separation. To complete the analysis, it is necessary to show that a Meissner effect occurs in that region. Recent progress\textsuperscript{12} in the analysis
of the superfluid density, $D_s$, using linear response theory allow us to carry out such a study using techniques similar to those required to analyze the Drude peak in the optical conductivity, $\sigma(\omega)$, of strongly interacting electrons. Following Scalapino et al., it can be shown that $D_s$ is given by

$$\frac{D_s}{2\pi e^2} = \frac{\langle -T \rangle}{4N} - \frac{1}{N} \sum_{n \neq 0} \frac{1}{E_n - E_0} |\langle n|j_x(q)|0\rangle|^2,$$

where $e$ is the electric charge; the current operator in the $x$-direction with momentum $q$ is given by $j_x(q) = \sum I, \sigma e^{iq^1_1} \bar{c}_{I=1+\tilde{x}, \sigma} - \bar{c}_{I, \sigma}^\dagger \hat{x}, \sigma \sigma$; $\langle -T \rangle$ is the kinetic energy operator of Eq.(1); $|n\rangle$ are eigenstates of the $t-J$ Hamiltonian with energy $E_n$ (where $n = 0$ corresponds to the ground state), and the rest of the notation is standard. The momentum $q = (q_x, q_y)$ of the current operator is selected such that $q_x = 0$ and $q_y \to 0$. The constraint of having an infinitesimal but nonzero $q_y$ is necessary to avoid a trivial cancellation of $D_s$ due to rotational and gauge invariance. On the $4 \times 4$ cluster, the minimum value of $q_y$ is $\pi/2$, and that is the momentum used in the present analysis. $D_s$ given by Eq.(2) can be evaluated numerically using the continued fraction expansion technique previously used to extract dynamical information from finite clusters. In Fig.2a, $D_s$ is shown as a function of $J/t$ for several densities. In good agreement with $\chi_{sup}^d$, the superfluid density $D_s$ presents a sharp maximum in the neighborhood of phase separation at $\langle n \rangle = 1/2$ giving support to the previous conclusions regarding the existence of superconductivity in this model. It is interesting to note that the signal is stronger for lower densities, e.g. $\langle n \rangle = 0.25$, perhaps due to the higher mobility of pairs in that regime. In the phase separated region, $D_s$ is small, as expected.

The resistivity of the model has also been analyzed. From previous studies of the optical conductivity in strongly interacting models, it can be shown that the Drude peak is given by a simple modification of Eq.(2), i.e. it is enough to replace $D_s \to D_{Drude}$, and consider zero momentum, $q = (0, 0)$, in the current. In Fig.2b, $D_{Drude}$ is shown as
a function of \( J/t \), for several densities. In the region of phase separation, the conductivity is small as expected, while for smaller values of \( J/t \), the Drude peak is considerably larger. A finite value of \( D_{\text{Drude}} \) in the bulk limit implies a zero resistivity, \( \rho = 0 \), since \( \sigma(\omega \to 0) = a e^{-1} = D_{\text{Drude}} \delta(\omega) \). Fig.2b suggests that this result will hold not only in the superconducting region, but it will survive a further reduction of the coupling into the small \( J/t \) regime, i.e. even in a phase without pairing. This example shows that \( \rho \) is not enough to distinguish between a “perfect metal” and a “superconductor”, and thus the previously discussed study of the superfluid density is crucial to show unambiguously the presence of superconducting correlations in the model.\(^{12}\) To further complete the present analysis, the response of the system to an external magnetic flux \( \phi \) was studied. For this purpose, a phase factor \( e^{i\phi/N} \) is introduced in the kinetic energy hopping terms of Eq.(1), but only in the x-direction. This is equivalent to allowing a nonzero flux across one of the “holes” of the torus.\(^{15}\) In Fig.3a, the ground state energy \( \Delta E(\phi) = E(\phi) - E(\phi = 0) \), in the zero momentum subspace, is shown as a function of \( \phi \), at density \( \langle n \rangle = 1/2 \). In the region of pairing, \( J/t = 3.0 \), the energy presents two minima, one located at \( \phi = 0 \) (mod \( 2\pi \)), and a nontrivial one at \( \phi = \pi \), signaling the presence of carriers with charge \( 2e \) in the ground state, in agreement with the analysis based on the pairing correlations.

What is the nature of the superconducting state at \( \langle n \rangle \sim 1/2 \)? It is reasonable to expect that the same force that produces phase separation, is responsible for superconductivity. Actually, if two electrons are considered on an otherwise empty lattice, they form a bound state at \( J/t = 2 \), and at low electronic density this same attraction leads to phase separation when the coupling is increased.\(^{4}\) In this respect, the antiferromagnetic coupling should be considered as an attractive interaction in the Hamiltonian at low densities, and thus the presence of superconductivity in the model is easily understood. At large \( J/t \), pairs of electrons (at least for small \( \langle n \rangle \)) are expected to have a size comparable to the range of the force, namely approximately one lattice spacing, and in this respect the superconducting
correlations discussed in this paper may be of the bipolaronic type. The pairs should be coupled in short spin singlets forming dimers. To check these ideas let us analyze the spin-spin correlations. In this scenario, each electron is coupled with only one other particle in a spin singlet, but due to rotational invariance, that particle can be located at any of the four possible nearest neighbors. Then, the correlation at distance of one lattice spacing, should be 1/4 of the on-site correlation, and it should vanish at larger distances. The results shown in Fig.3b obtained at \( \langle n \rangle = 1/2 \) and \( J/t = 3.0 \), are in excellent agreement with this picture. Another issue to address is the possible formation of a “crystal” structure. Is there any special order in the position of these dimers? For that purpose hole-hole correlations, \( h(m) = \langle n_{h}(0)n_{h}(m) \rangle \) (where \( n_{h} \) is the hole number operator) were studied, i.e. once a hole is located at a given site 0, then correlations with other holes are evaluated. Asymptotically, \( h(m) \) should decay to \( \langle n \rangle \) at large distance. In Fig.3c, \( h(m) \) is shown at \( \langle n \rangle = 1/2 \) and \( J/t = 3.0 \). The hole-hole correlations rapidly decay to its asymptotic value, showing that there is no special pattern in the hole distribution (or, equivalently at \( \langle n \rangle = 1/2 \), in the electronic distribution). The spin-gap in the neighborhood of phase separation has also been studied. Although to obtain conclusive results a careful finite size scaling analysis is necessary, the data suggest the presence of a finite spin-gap,\(^{16}\) compatible with the idea of small size dimers as responsible for the superconducting correlations.\(^{17}\) To summarize these ideas, in Fig.4a a snapshot of the “dimer liquid” state that here is claimed to be compatible with the numerical results is presented.\(^{18}\) Note that this state explains the observed maximum that \( \chi_{sup}^{d} \) presents at \( \langle n \rangle = 1/2 \), since at that density the model has the maximum number possible of mobile dimers. At smaller densities, there are fewer dimers contributing to the signal; while closer to \( \langle n \rangle = 1 \), the pairs of electrons have less mobility for lack of space. A similar state, although defined in a rigid crystal pattern, was previously discussed in the context of the \( t-J-V \) model.\(^{7,6}\)

Summarizing, in this paper numerical evidence suggesting that the \( t-J \) model in two
dimensions has a superconducting phase at zero temperature has been discussed. The pairing correlations are the strongest at density \( \langle n \rangle = 1/2 \), and near phase separation.\(^{4,5}\) The symmetry of the pairing state corresponds to \( d_{x^2-y^2} \). The Meissner effect, as well as flux quantization calculations support this scenario. The size of the pairs seem small at \( \langle n \rangle = 1/2 \) as suggested by the spin-spin correlations, and they are in a disordered state. Thus, a liquid of dimers may represent the physics of this condensate. These results have several implications: i) they are the first numerical evidence that the \( t - J \) model superconducts in two dimensions. Previous numerical studies\(^{13}\) concentrated their efforts near \( \langle n \rangle \sim 1 \), but in that regime the signal for superconductivity would be too weak to be detectable; ii) In addition, it was found that the symmetry of the superconducting condensate is \( d_{x^2-y^2} \), and thus this model may become a realization of recent proposals to explain the phenomenology of high-\( T_c \) materials making use of non s-wave pairing interactions with nodes.\(^{2,3}\) Based on the present calculation and others\(^{4,5}\) the currently available information for the phase diagram of the two dimensional \( t - J \) model at zero temperature is sketched in Fig.4b. The notation is explained in the caption. The “binding” region denotes a regime where pairs are formed, but they are not condensed in a superconducting state. The details of this phase diagram close to half-filling are more difficult to address numerically than at \( \langle n \rangle = 1/2 \). However, the possibility that the model superconducts also at low hole doping is not excluded. Whether there is an analytical continuation between \( \langle n \rangle = 1/2 \) and large \( J/t \), and densities closer to half-filling and smaller couplings is a crucial issue for the success of the \( t - J \) model as a phenomenological model of high-\( T_c \) superconductors. This important subject will be addressed in future publications.

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9. See F. Assaad and D. Würtz, see Ref.8, where correlation functions at a fixed density are used, instead of energies at several densities as in the compressibility.
10. Details will be presented in an extended version of this paper, in preparation.

11. A possible $d_{x^2-y^2} + i d_{xy}$ pairing mechanism in the $t-J$ model has been recently suggested by R. Laughlin (private communication). For $d_{xy}$ symmetry, the pairing operator is odd under both axis-reflexions and $\pi/2$ rotations, and the carriers are located at a distance of $\sqrt{2}$ lattice spacings from each other.

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14. A good test of the programs used to compute $D_s$ consists of taking $\mathbf{q} = (\pi/2, 0)$ as the current momentum. This is equivalent to using a “trivial” gauge field, i.e. one that does not induce neither electric nor magnetic fields in the problem. In such a case $D_s$ should vanish identically (we thank D. Scalapino for this remark).

15. For more details see D. Poilblanc et al., *Phys. Rev. B* **44**, 466 (1991).

16. Even if the spin-gap vanishes for the $t-J$ model, the addition of a small density-density repulsion is enough to open a gap. See Ref.6, and H. Tsunetsugu and M. Troyer, private communication, for similar conclusions in the 1D $t-J-V$ model.

17. In addition, studying the ground state in the subspace with two less electrons, clear indications of a “Goldstone particle” in the spectrum with the proper symmetry for $d$-wave pairing were observed, due to the presence of superconductivity in the ground state (see A. Moreo, Ref.8).

18. Note the similarity with the RVB states discussed, for example, by L. Pauling, Proc. R. Soc. London *A* **196**, 343 (1949); P. W. Anderson, Science **235**, 1196 (1987); and S. Kivelson, D. Rokhshar, and J. Sethna, Phys. Rev. *B* **35**, 8865 (1987).
Figure Captions

1a $d_{x^2-y^2}$ superconducting susceptibility, $\chi_{\text{sup}}^d$, as a function of $J/t$, at densities $\langle n \rangle = 0.25 (\triangle)$, $\langle n \rangle = 1/2 (\blacksquare)$, and $\langle n \rangle = 0.75 (\square)$.

1b Pairing-pairing correlation function $C(m)$ as a function of distance $m$, at density $\langle n \rangle = 1/2$ and $J/t = 3.0$. $\square$ denotes $d_{x^2-y^2}$ pairing correlations, $\triangle$ indicates extended $s$ correlations, while $\blacksquare$ corresponds to $d_{xy}$ correlations.

1c Pairing-pairing correlation function $C(m)$ in the $d_{x^2-y^2}$ channel, as a function of distance $m$, at density $\langle n \rangle = 1/2$. $\triangle$, $\blacksquare$ and $\square$ are results for $J/t = 1.0$, 3.0 and 4.0, respectively.

2a Superfluid density, $D_s$, versus $J/t$, at several fermionic densities. $\square$ corresponds to $\langle n \rangle = 1/2$, $\triangle$ denotes results for $\langle n \rangle = 0.25$, while $\blacksquare$ indicates $\langle n \rangle = 0.75$.

2b Drude peak, $D_{\text{Drude}}$, as a function of $J/t$ for several densities. The notation is as in Fig.2a.

3a Energy of the ground state as a function of an external magnetic flux $\phi$. The energy at zero flux is subtracted from the result i.e. $\Delta E(\phi) = E(\phi) - E(0)$. The subspace of zero momentum is considered, and the density is $\langle n \rangle = 1/2$. $\square$ denotes results at $J/t = 3.0$, while $\blacksquare$ corresponds to $J/t = 4.0$ i.e. inside the phase separated region.

3b Spin-spin correlation $S(m)$ as a function of distance at density $\langle n \rangle = 1/2$, and coupling $J/t = 3.0$ i.e. in the superconducting region.

3c Hole-hole correlations $h(m)$ as a function of distance at density $\langle n \rangle = 1/2$, and coupling $J/t = 3.0$ i.e. in the superconducting region.

4a Qualitative representation of a “dimer liquid” state, presumed to be the ground state in the superconducting region discussed in this paper.
Schematic semi-quantitative phase diagram of the $t-J$ model in two dimensions at zero temperature, as a function of coupling $J/t$, and hole density $x = 1 - \langle n \rangle$. The curves separating the region at small $J/t$, presumably a Fermi liquid, FL, from the “binding” region, as well as the separation between binding and $d_{x^2-y^2}$ wave superconductivity, are rough estimations based on the study of binding energies, and the strength of $\chi_{\text{sup}}^d$. The transition leading to phase separation is more accurate, and in qualitative agreement with high temperature expansions. Near half-filling, the calculations are more difficult, and it is only known that antiferromagnetic, AF, and ferromagnetic, FM, correlations are important.