Indications of $d_{x^2-y^2}$ Superconductivity in the Two Dimensional t-J Model

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Superconducting correlations in the two dimensional t-J model at zero temperature are evaluated using numerical techniques. At the fermionic density $\langle n\rangle \sim \frac{1}{2}$, 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, and flux quantization as indicators of superconductivity. A tentative 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 $YBa_2Cu_3O_7$ 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 discussed [2–5]. It would be important to find a Hamiltonian model of strongly interacting electrons having $d_{x^2-y^2}$ superconductivity in the 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, especially since the strongly interacting character of several realistic models makes most analytical approximations questionable.

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 superconducting correlations are strong in the $d_{x^2-y^2}$ channel, and thus this model may become a physical realization of the d-wave pairing scenarios recently proposed in the literature [2,3]. The superconducting phase observed here appears near the well-known region of phase separation of the t-J model [6,7]. The possible presence of superconducting correlations near phase separation has been discussed in other contexts and theories using several approximations [8–10]. Here, we present the first numerical indications that this phenomenon indeed occurs in the ground state of a realistic model.

The t-J model is defined by the Hamiltonian

$$H = J\sum_{\langle \mathbf{ij}\rangle}(\mathbf{S_i}\cdot\mathbf{S_j} - \tfrac{1}{4}n_\mathbf{i}n_\mathbf{j}) - t\sum_{\langle \mathbf{ij}\rangle,s}(\bar{c}^\dagger_{\mathbf{i},s}\bar{c}_{\mathbf{j},s} + \text{H.c.})\,, \quad (1)$$

where $\bar{c}^\dagger_{\mathbf{i},s}$ denote *hole* operators, $n_\mathbf{i} = n_{\mathbf{i},\uparrow} + n_{\mathbf{i},\downarrow}$, 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 4×4 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 $\Delta_\mathbf{i} = c_{\mathbf{i},\uparrow}(c_{\mathbf{i}+\hat{\mathbf{x}},\downarrow} + c_{\mathbf{i}-\hat{\mathbf{x}},\downarrow} \pm c_{\mathbf{i}+\hat{\mathbf{y}},\downarrow} \pm c_{\mathbf{i}-\hat{\mathbf{y}},\downarrow})$, where + and − corresponds to extended s and $d_{x^2-y^2}$ waves, respectively, and $\hat{\mathbf{x}},\hat{\mathbf{y}}$ are unit vectors along the axis. The pairing-pairing correlation function $C(\mathbf{m}) = (1/N)\sum_\mathbf{i}\langle\Delta^\dagger_\mathbf{i}\Delta_{\mathbf{i}+\mathbf{m}}\rangle$ and its susceptibility $\chi^\alpha_{\rm sup} = \sum_\mathbf{m} C(\mathbf{m})$ 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.

$\chi^d_{\rm sup}$ is shown in Fig. 1(a) as a function of J/t, for several densities. The $d_{x^2-y^2}$ wave susceptibility dominates, presenting at $\langle n\rangle = \frac{1}{2}$ a sharp peak at $J/t \sim 3$. By analyzing several spin and hole correlations, and following other criteria [11], it was verified that the fast decay of $\chi^d_{\rm sup}$ after the peak is induced by the transition to the phase separated region. Changing the fermionic density, it was found that $\chi^d_{\rm sup}$ has its maximum value at $\langle n\rangle = \frac{1}{2}$, as shown in Fig. 1(a). $\chi^s_{\rm sup}$ has been also evaluated at $\langle n\rangle = \frac{1}{2}$. This susceptibility peaks at approximately the same position as $\chi^d_{\rm sup}$ does, but with a smaller intensity [12]. The pairing-pairing correlations as a function of distance are shown explicitly in Fig. 1(b) in the region where the susceptibilities have a sharp maximum, i.e., $J/t = 3.0$ and $\langle n\rangle = \frac{1}{2}$. In agreement with the behavior of $\chi^d_{\rm sup}$, Fig. 1(a), the dominant correlation function at the maximum distance on the 4×4 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 larger distances. For completeness, in Fig. 1(b) the correlation corresponding to d_{xy} symmetry is also presented [13]. These correlations seem more heavily suppressed than for the $d_{x^2-y^2}$ and extended s channels. In Fig. 1(c), the d-wave pairing correlations are shown at $\langle n\rangle = \frac{1}{2}$, as a function of J/t. Their maximum value is obtained at the same coupling where $\chi^d_{\rm sup}$ peaks, as expected. The symmetry of the ground state (obtained

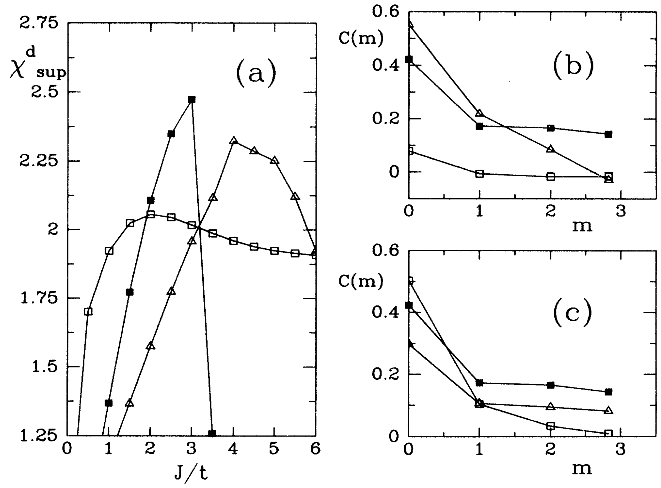

FIG. 1. (a) $d_{x^2-y^2}$ superconducting susceptibility, χ^d_{sup}, as a function of J/t, at densities $\langle n\rangle=0.25$ (△), $\langle n\rangle=\frac{1}{2}$ (■), and $\langle n\rangle=0.75$ (□). (b) Pairing-pairing correlation function $C(\mathbf{m})$ as a function of distance, at density $\langle n\rangle=\frac{1}{2}$ and $J/t=3.0$. ■ denotes $d_{x^2-y^2}$ pairing correlations, △ indicates extended s correlations, while □ corresponds to d_{xy} correlations. (c) Pairing-pairing correlation function $C(\mathbf{m})$ in the $d_{x^2-y^2}$ channel, as a function of distance, at density $\langle n\rangle=\frac{1}{2}$. △, ■, and □ are results for $J/t=1.0$, 3.0, and 4.0, respectively.

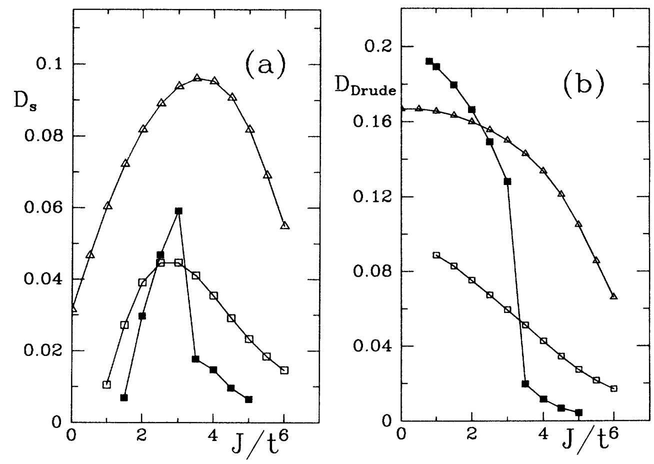

FIG. 2. (a) Superfluid density, D_s, vs J/t, at several fermionic densities. ■ corresponds to $\langle n\rangle=\frac{1}{2}$, △ denotes results for $\langle n\rangle=0.25$, while □ indicates $\langle n\rangle=0.75$. (b) Drude peak, D_{Drude}, as a function of J/t for several densities. The notation is as in (a).

with the Lanczos method) under a rotation of the lattice in $\pi/2$ has been also studied. In the region where superconducting correlations exists, the ground state is odd under this operation, but invariant under reflections with respect to both axis. Then, the ground state at $\langle n\rangle=\frac{1}{2}$ belongs to the B_{1g} ($d_{x^2-y^2}$) representation of the C_{4v} group.

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 [14] in the analysis of the superfluid density, D_s, using linear response theory allows 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 [15]. Following Scalapino, White, and Zhang [14], it can be shown that D_s is given by

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

where e is the electric charge, the current operator in the x direction with momentum $\mathbf{q}$ is $j_x(\mathbf{q})=\sum_{l,\sigma}e^{i\mathbf{q}\cdot\mathbf{l}}(\bar{c}^\dagger_{l,\sigma}\times\bar{c}^\dagger_{l+\hat{x},\sigma}-\bar{c}^\dagger_{l+\hat{x},\sigma}\bar{c}_{l,\sigma})$, $\langle -T\rangle$ is the kinetic energy operator of Eq. (1), $|n\rangle$ are eigenstates of Eq. (1) with energy E_n (where $n=0$ corresponds to the ground state), and the rest of the notation is standard. The momentum $\mathbf{q}=(q_x,q_y)$ of the current operator is selected such that $q_x=0$ and $q_y\rightarrow 0$. The constraint of having a small but nonzero q_y is necessary to avoid a trivial cancellation of D_s due to rotational and gauge invariance [14]. On the 4×4 cluster, the minimum value of q_y is $\pi/2$, and that is the momentum used here. 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 [15]. In Fig. 2(a), D_s is shown as a function of J/t for several densities. In good agreement with χ^d_{sup}, the superfluid density D_s presents a sharp maximum in the neighborhood of phase separation at $\langle n\rangle=\frac{1}{2}$ 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, $\langle n\rangle=0.25$, perhaps due to the higher mobility of pairs in that regime. D_s is small in the phase separated region, as expected.

The resistivity of the model has also been analyzed. From previous studies of the optical conductivity in strongly interacting models [15], it can be shown that the Drude peak is given by a simple modification of Eq. (2), i.e., it is enough to replace $D_s\rightarrow D_{\mathrm{Drude}}$, and consider zero momentum, $\mathbf{q}=(0,0)$, in the current [14,15]. In Fig. 2(b), 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_{Drude} in the bulk limit implies zero resistivity, $\rho=0$, since $\sigma(\omega\rightarrow 0)=\rho^{-1}=D_{\mathrm{Drude}}\delta(\omega)$. Figure 2(b) 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 ρ 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 [14]. To further complete the present analysis, the response of the system to an external magnetic *flux* ϕ

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 [16]. In Fig. 3(a), the ground state energy $\Delta E(\phi)=E(\phi)-E(\phi=0)$, in the zero momentum subspace, is shown as a function of ϕ, at density $\langle n\rangle=\frac{1}{2}$. In the region of pairing, $J/t=3.0$, the energy presents two minima, one located at $\phi=0$ (mod2π), 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 [17].

What is the nature of the superconducting state at $\langle n\rangle\sim\frac{1}{2}$? 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 eventually leads to phase separation when the coupling is increased [6]. In this respect, the antiferromagnetic coupling can be considered as an attractive interaction in the Hamiltonian at low densities, and thus the presence of superconductivity in the model should not be too surprising. At small density and large J/t, but before phase separation occurs, pairs of electrons 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 have some features of bipolaronic pairing. The pairs should be

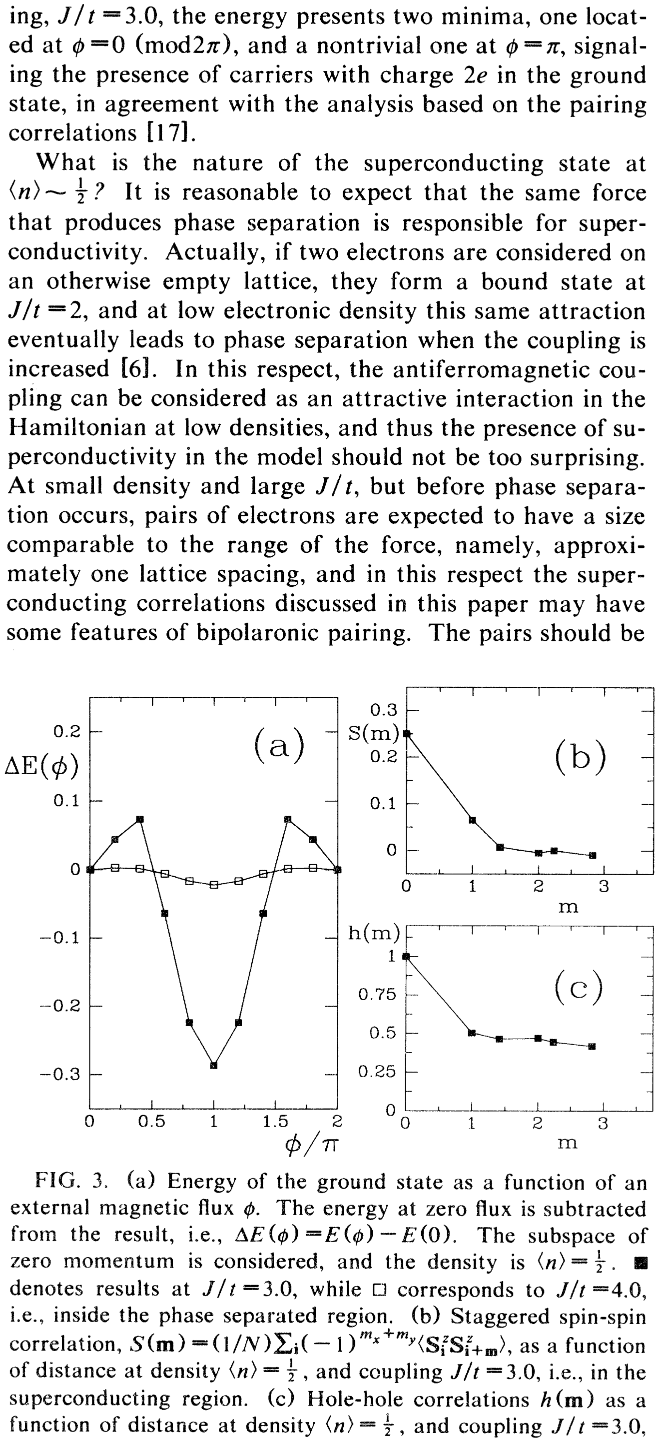

FIG. 3. (a) Energy of the ground state as a function of an external magnetic flux ϕ. The energy at zero flux is subtracted from the result, i.e., $\Delta E(\phi)=E(\phi)-E(0)$. The subspace of zero momentum is considered, and the density is $\langle n\rangle=\frac{1}{2}$. ■ denotes results at $J/t=3.0$, while □ corresponds to $J/t=4.0$, i.e., inside the phase separated region. (b) Staggered spin-spin correlation, $S(\mathbf{m})=(1/N)\sum_{\mathbf{i}}(-1)^{m_x+m_y}\langle S^z_{\mathbf{i}}S^z_{\mathbf{i}+\mathbf{m}}\rangle$, as a function of distance at density $\langle n\rangle=\frac{1}{2}$, and coupling $J/t=3.0$, i.e., in the superconducting region. (c) Hole-hole correlations $h(\mathbf{m})$ as a function of distance at density $\langle n\rangle=\frac{1}{2}$, and coupling $J/t=3.0$, i.e., in the superconducting region.

mostly 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 $-\frac{1}{4}$ of the on-site correlation, and it should vanish at larger distances. The results shown in Fig. 3(b) obtained at $\langle n\rangle=\frac{1}{2}$ and $J/t=3.0$ are in good agreement with this picture. However, note that such a sharp decay of the spin correlations implies a finite spin gap, which seems contrary to the notion of a d-wave condensate. There are two possible explanations for this "paradox." One possibility is that a difficult to observe small power-law tail exists in Fig. 3(b), due to the existence of spin singlets in the ground state at distances larger than one lattice spacing. This behavior has been observed in one dimension [12]. Another is some variation on the scenario given by Schrieffer, Wen, and Zhang in their discussion of d-wave superconductivity [4]. They proposed that the nodes in the superconducting order parameter in momentum space may correspond to regions where other interactions have opened a large gap (in their case due to a spin density wave) creating a nodeless d-wave condensate. More work is necessary to clarify these results. Another issue to address is the possible formation of a "crystal" structure. Is there any special order in the position of the electrons? For that purpose hole-hole correlations, $h(m)=\langle n_h(0)\times n_h(m)\rangle$ (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. 3(c), $h(m)$ is shown at $\langle n\rangle=\frac{1}{2}$ 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 $\langle n\rangle=\frac{1}{2}$, in the electronic distribution).

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 $\langle n\rangle=\frac{1}{2}$, and near phase separation [6,7]. The Meissner effect, as well as flux quantization calculations support this scenario. The dominant symmetry of the pairing correlations is $d_{x^2-y^2}$. These results have several implications: (i) They are the first numerical evidence that the t-J model superconducts in two dimensions [18]; (ii) since the symmetry of the superconducting condensate is $d_{x^2-y^2}$, 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 [6,7] the currently available information for the phase diagram of the two dimensional t-J model at zero temperature is sketched in Fig. 4. The notation is explained in the caption. The "binding" region denotes a regime

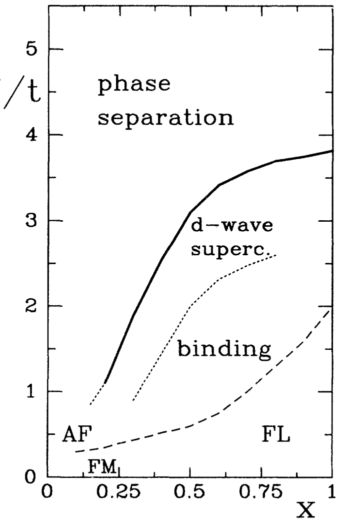

FIG. 4. Schematic phase diagram of the t-J model in two dimensions at zero temperature, as a function of coupling J/t, and hole density $x=1-\langle n\rangle$. The curves separating the region at small J/t, presumably a Fermi liquid, FL, from the "binding" region, as well as the separation between binding and $d_{x^2-y^2}$ wave superconductivity, are rough estimations based on the study of binding energies, and the strength of $\chi^d_{\rm sup}$. The transition leading to phase separation is more accurate, and in qualitative agreement with high-temperature expansions [7]. Near half filling, the calculations are more difficult, and it is only known that antiferromagnetic, AF, and ferromagnetic, FM, correlations are important.

where pairs are formed, but they are not condensed in a superconducting state. We consider it very important to continue the study of this model in the novel region of superconductivity using other techniques, and also to increase the size of the clusters to analyze the influence of finite-size effects. The details of this phase diagram close to half filling are more difficult to address numerically than at $\langle n\rangle=\frac{1}{2}$. However, the possibility that the model superconducts also at low hole doping is not excluded. Whether there is an analytical continuation between $\langle n\rangle=\frac{1}{2}$ 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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[11] See Assaad and Würtz, Ref. [10], where correlation functions at a fixed density are used, instead of energies at several densities as in the compressibility.

[12] Details will be presented in an extended version of this paper (to be published).

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