Hole-hole superconducting pairing in the t-J model induced by spin-wave exchange

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We study numerically the hole pairing induced by spin-wave exchange. The contact hole-hole interaction is taken into account as well. It is assumed that antiferromagnetic order is preserved at all scales relevant to pairing. The strongest pairing is obtained for the d-wave symmetry of the gap. Dependence of the value of the gap on hole concentration and temperature is presented. For the critical temperature we obtain $T_c \sim 100$ K at the hole concentration $\delta \sim 0.2$–0.3.

I. INTRODUCTION

Magnetic fluctuations are believed to be a very likely mechanism of pairing in cuprate superconductors. There have been many studies[1–9] of predominantly phenomenological nature supporting this idea. In the present work we study spin-wave-mediated hole pairing using results obtained from *first principles* for the undoped t-J model.

We base our study on the results of previous papers.[10,11] It was shown in Ref. 10 that because of spin-wave exchange there is an effective long-range attraction between two holes with opposite spins,

$$U_{\rm eff}(r) = \frac{\lambda}{r^2}, \qquad \lambda < 0. \tag{1}$$

In this potential there is an infinite series of two-hole bound states. However, they have very large sizes and very small binding energies and thus are not directly responsible for high-T_c superconductivity. Very strong pairing in the many-hole problem due to the same potential (1) was demonstrated in Ref. 11, where an infinite set of solutions for the superconducting gap was found. The strongest pairing was either in the d-wave or g-wave sector. The pairing induced by spin-wave exchange is a long-range phenomenon. However, the attractive potential (1) is too singular and the wave function is known to collapse to the origin. On the one hand, this "collapse" effect substantially enhances pairing. On the other hand, it leads to a dependence of superconducting gap on short-range dynamics which cannot be studied analytically. For this reason analytical calculations[11] can only estimate the numerical value of the gap and cannot distinguish between d- and g-wave pairing (which have the same long-range behavior but a different short-range one). In the present work, we calculate the gap numerically, taking into account both spin-wave exchange and contact hole-hole interaction. The d-wave pairing is shown to be the strongest.

Recently, d-wave pairing was studied in Ref. 12. Although many results are similar, we believe the spin-wave exchange interaction which we use is more realistic than the atomic limit interaction employed in Ref. 12.

Our paper has the following structure. In Sec. II we present an effective Hamiltonian of the t-J model. In Sec. III we calculate the BCS-type pairing of holes at zero temperature. Section IV presents the results of the calculation of the critical temperature. Finally, our conclusions are given in Sec. V.

II. EFFECTIVE HAMILTONIAN FOR DRESSED HOLES

The underlying microscopic physics is described by the t-J model defined by the Hamiltonian

$$H = H_t + H_J = -t \sum_{\langle nm\rangle\sigma} (d^\dagger_{n\sigma} d_{m\sigma} + \text{H.c.}) + J \sum_{\langle nm\rangle} \mathbf{S}_n \cdot \mathbf{S}_m, \tag{2}$$

where $d^\dagger_{n\sigma}$ is the creation operator of a hole with spin σ ($\sigma = \uparrow, \downarrow$) at site n on a two-dimensional square lattice. The $d^\dagger_{n\sigma}$ operators act in Hilbert space with no double-electron occupancy. The spin operator is $\mathbf{S}_n = \frac{1}{2} d^\dagger_{n\alpha} \sigma_{\alpha\beta} d_{n\beta}$. $\langle nm\rangle$ are the nearest-neighbor sites on the lattice. Below we set $J = 1$ and give all energy values in units of J.

At half-filling (one hole per site) the t-J model is equivalent to the Heisenberg antiferromagnet model which has long-range Néel order in the ground state. Under doping the long-range antiferromagnetic order is destroyed. However, local antiferromagnetic order is preserved. We assume that the magnetic correlation length $\xi_{\rm magn}$ is not smaller than the typical wavelength of holes, $\xi_{\rm magn} \geq 1/p_F \sim 1/\sqrt{\delta}$ ($\delta \ll 1$ is the concentration of holes). Thus we have antiferromagnetic order at all scales relevant to the problem. This assumption does not contradict experimental data.[13]

We treat the J term of the Hamiltonian (2) using the linear spin-wave approximation (see Ref. 14 for a review). Define the Fourier transformations

$$a^\dagger_{\mathbf q} = \sqrt{\frac{2}{N}}\sum_{n\in\uparrow} S^-_n e^{i\mathbf q\cdot\mathbf r_n}, \quad b^\dagger_{\mathbf q} = \sqrt{\frac{2}{N}}\sum_{n\in\downarrow} S^+_n e^{i\mathbf q\cdot\mathbf r_n}, \quad (3)$$

where the notation $n\in\uparrow$ ($n\in\downarrow$) means that site n is on the spin-up (-down) sublattice. Introducing the Bogolubov canonical transformation

$$\alpha^\dagger_{\mathbf q} = U_{\mathbf q} a^\dagger_{\mathbf q} - V_{\mathbf q} b_{-\mathbf q}, \qquad \beta^\dagger_{\mathbf q} = U_{\mathbf q} b^\dagger_{\mathbf q} - V_{\mathbf q} a_{-\mathbf q}, \quad (4)$$

we write the Heisenberg Hamiltonian H_J as

$$H_J = E_0 + \sum_{\mathbf q} \omega_{\mathbf q}(\alpha^\dagger_{\mathbf q}\alpha_{\mathbf q} + \beta^\dagger_{\mathbf q}\beta_{\mathbf q}), \quad (5)$$

where E_0 is the antiferromagnetic background energy. The summation over $\mathbf q$ is restricted to the Brillouin zone of one sublattice $[\gamma_{\mathbf q} = \frac{1}{2}(\cos q_x + \cos q_y) \geq 0]$. The spin-wave dispersion and the transformation coefficients are given by

$$\omega_{\mathbf q} = 2\sqrt{1-\gamma^2_{\mathbf q}}, \qquad \omega_{\mathbf q} \approx \sqrt{2}|\mathbf q| \quad \text{at } |\mathbf q| \ll 1,$$
$$U_{\mathbf q} = \sqrt{\frac{1}{\omega_{\mathbf q}} + \frac{1}{2}}, \qquad V_{\mathbf q} = -\mathrm{sgn}(\gamma_{\mathbf q})\sqrt{\frac{1}{\omega_{\mathbf q}} - \frac{1}{2}}. \quad (6)$$

The spin waves created by $\alpha^\dagger_{\mathbf q}$ and $\beta^\dagger_{\mathbf q}$ have definite values of spin projection. Due to Eqs. (3) and (4), $\alpha^\dagger_{\mathbf q}|0\rangle$ has $S_z = -1$ and $\beta^\dagger_{\mathbf q}|0\rangle$ has $S_z = +1$. Here $|0\rangle$ is the wave function of the quantum Néel state.

Single-particle properties in the t-J model are by now well established (see Ref. 15). A single hole is a magnetic polaron of a small radius, i.e., a "bare" hole that is "dressed" by virtual spin excitations. A single hole has a ground state with a momentum of $\mathbf k = (\pm\pi/2, \pm\pi/2)$. The energy is almost degenerate along the line $\cos k_x + \cos k_y = 0$ which is the edge of the magnetic Brillouin zone (see, e.g., Refs. 16–23). The hole dispersion may be well approximated by the analytical expression[21]

$$\epsilon_{\mathbf k} = \sqrt{\Delta_0^2/4 + 4t^2(1+y)}$$
$$-\sqrt{\Delta_0^2/4 + 4t^2(1+y) - 4t^2(x+y)\gamma^2_{\mathbf k}}$$
$$+\frac{1}{4}\beta_2(\cos k_x - \cos k_y)^2,$$
$$\Delta_0 \approx 1.33, \quad x \approx 0.56, \quad y \approx 0.14, \quad (7)$$

where the parameters Δ_0, x, y are some combinations of the ground state spin correlators.[21] Near the band bottom $\mathbf k_0 = (\pm\pi/2, \pm\pi/2)$ the dispersion (7) can be presented in the usual quadratic form

$$\epsilon_{\mathbf p} \approx \frac{1}{2}\beta_1 p_1^2 + \frac{1}{2}\beta_2 p_2^2, \qquad \beta_2 \ll \beta_1, \quad (8)$$

where p_1 (p_2) is the projection of $\mathbf k - \mathbf k_0$ on the direction orthogonal (parallel) to the face of the magnetic Brillouin zone (Fig. 1). From Eq. (7) for $t \gg \Delta_0/4$ we have

$$\beta_1 = \frac{x+y}{\sqrt{1+y}}t \approx 0.65t. \quad (9)$$

According to Refs. 18 and 23, $\beta_2 \approx 0.1t$ at $t \geq \Delta_0/4$. The wave function of a single hole may be written in the form $\psi_{\mathbf k\sigma} = h^\dagger_{\mathbf k\sigma}|0\rangle$. At large t the composite hole operator $h^\dagger_{\mathbf k\sigma}$ has complex structure. For example at $t/J = 3$ very roughly, the weight of a bare hole in $\psi_{\mathbf k\sigma}$ is about 25%; the weight of configurations "bare hole + 1 magnon" is ~50%, and of configurations "bare hole + 2 or more magnons" ~25%. These estimations are based on the approach with a minimal string ansatz[21] and further renormalization due to additional magnons.[24] However, other approaches like finite cluster diagonalization[17] or numerical solution of Dyson's equation[16,18,19,22] give very close results. We have to stress that the dressed hole is a normal fermion.

The interaction of a composite hole with spin waves is of the form (see, e.g., Refs. 18, 19, 24, 25)

$$H_{h,sw} = \sum_{\mathbf k,\mathbf q} g_{\mathbf k,\mathbf q}(h^\dagger_{\mathbf k+\mathbf q\downarrow}h_{\mathbf k\uparrow}\alpha_{\mathbf q} + h^\dagger_{\mathbf k+\mathbf q\uparrow}h_{\mathbf k\downarrow}\beta_{\mathbf q} + \text{H.c.}),$$
$$g_{\mathbf k,\mathbf q} = 2f\sqrt{\frac{2}{N}}(\gamma_{\mathbf k}U_{\mathbf q} + \gamma_{\mathbf k+\mathbf q}V_{\mathbf q}). \quad (10)$$

For arbitrary t the coupling constant f was calculated in Refs. 24, 25. The plot of f as a function of t is presented in Fig. 2. For large t the coupling constant is t-independent $f \approx 2$.

Let us stress that even for $t > J$ the interaction (10) between quasiholes and spin waves has the form as for $t \ll J$ (i.e., as for bare hole operators) with an added

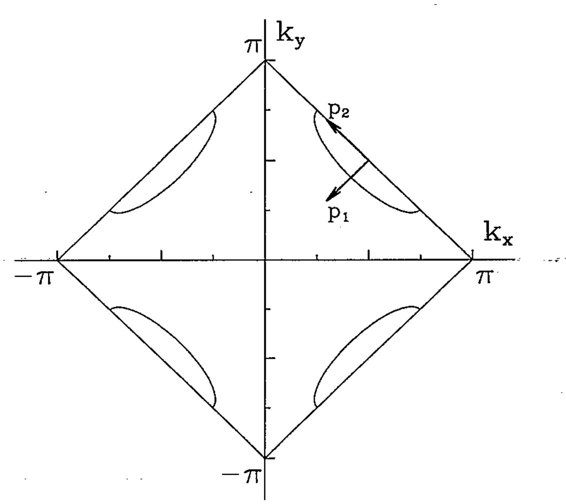

FIG. 1. The Brillouin zone of a hole in the t-J model.

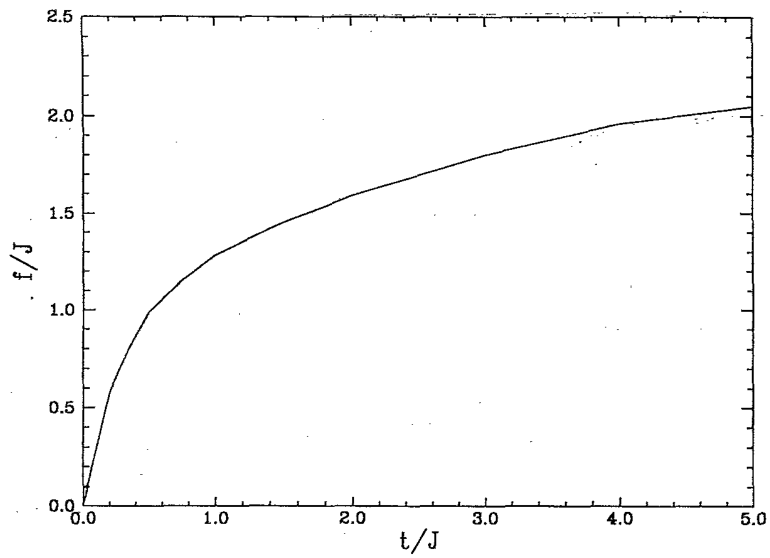

FIG. 2. The plot of the hole–spin-wave coupling constant f.

renormalization factor (of the order of J/t for $t \gg J$). This is a remarkable property of the t-J model which is due to the absence of a single-loop correction to the vertex. This property was first found perhaps in Ref. 16. In Refs. 18, 19, 25 it was demonstrated explicitly that vertex corrections with different kinematic structure are of the order of few percent at $t/J \approx 3$. There is also a weak q dependence of the coupling constant f. The plot in Fig. 2 corresponds to the long-wavelength limit $q = 0$ because, as we will see later, the small q's are most important for pairing. At $q \sim \pi$, the factor f is (10-17)% bigger than at $q = 0$ [see the discussion between Eqs. (13) and (14) of Ref. 10]. The influence of this correction on the pairing is negligible.

Note that the hole scattering between different pockets makes a large contribution to the pairing. However, in the two-sublattice formalism which we use, there are no spin waves with $\mathbf{q} = \mathbf{g} = (\pm\pi, \pm\pi)$ and such scattering takes place via umklapp processes with $q \sim p_F \ll 1$. One could use another description: Expand the Brillouin zone for spin waves and include $\mathbf{q} \approx \mathbf{g}$ into consideration explicitly. Then, due to antiferromagnetic order the points $\mathbf{q} = 0$ and $\mathbf{q} = \mathbf{g}$ are equivalent, and the coupling constants in the effective Hamiltonian (10) are exactly equal, $f_{\mathbf{q}=0} = f_{\mathbf{q}=\mathbf{g}}$. Certainly the kinematic structure of the vertex (10) reflects this symmetry: $g_{\mathbf{k},\mathbf{q}} = g_{\mathbf{k},\mathbf{q}+\mathbf{g}}$.

Interaction between two holes can be caused by exchange of one spin wave. Alongside that there is a contact hole-hole interaction. One can say that it is due to exchange of several hard spin-wave excitations. The Hamiltonian of the contact hole-hole interaction was derived in Refs. 26, 10 using a variational approach:

$$H_{h,h} = \frac{8}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \left[A\gamma_{\mathbf{k}_1-\mathbf{k}_3} + \frac{1}{2}C(\gamma_{\mathbf{k}_1+\mathbf{k}_3} + \gamma_{\mathbf{k}_2+\mathbf{k}_4})\right] h^\dagger_{\mathbf{k}_3\uparrow} h^\dagger_{\mathbf{k}_4\downarrow} h_{\mathbf{k}_2\downarrow} h_{\mathbf{k}_1\uparrow} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}, \tag{11}$$

$$A = 16t\nu\mu^3(1 - 7\mu^2) - \frac{1}{4} - 2\mu^2 - 18.5\mu^4 + 84\mu^6 + 10\alpha t\nu^3\mu^3, \quad C = \frac{2}{3}\alpha t\nu\mu^3,$$

where

$$\nu = \frac{1}{2}\left[\frac{3/2 + 2S_t}{S_t}\right]^{1/2}, \mu = \frac{t}{[S_t(3/2 + 2S_t)]^{1/2}},$$

$$S_t = [9/16 + 4t^2]^{1/2}. \tag{12}$$

The coefficients A and C in Eq. (11) were derived in first order in α, where α is the coefficient in front of the transverse part to the Heisenberg interaction: $\mathbf{S}_n\mathbf{S}_m \to S^z_n S^z_m + \frac{\alpha}{2}(S^+_n S^-_m + S^-_n S^+_m)$. Since the physical value is $\alpha = 1$, contributions of higher orders are important. In order to estimate them, we will set $\alpha = 0.6$. This choice is made so that results for the binding energy of short-range two-hole bound states obtained by finite lattice diagonalizations[27–31] would agree with results obtained[26,10] by using the effective interaction (11). Actually at $\alpha = 0.6$ the contact interaction $H_{h,h}$ is very small and practically does not influence the pairing.

To summarize, we conclude that the dynamics of holes on the antiferromagnetic background is described by the effective Hamiltonian

$$H_{\text{eff}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} h^\dagger_{\mathbf{k}\sigma} h_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}}(\alpha^\dagger_{\mathbf{q}}\alpha_{\mathbf{q}} + \beta^\dagger_{\mathbf{q}}\beta_{\mathbf{q}}) + H_{h,\text{sw}} + H_{h,h}, \tag{13}$$

which is expressed in terms of the composite hole $h_{\mathbf{k}\sigma}$ and spin-wave $\alpha_{\mathbf{q}}, \beta_{\mathbf{q}}$ operators. It includes free holes and spin waves and their interactions $H_{h,\mathrm{sw}}$ and $H_{h,h}$ [given by Eqs. (10) and (11)].

III. SUPERCONDUCTING STATE

For the small concentrations $\delta \ll 1$ under consideration, holes are localized in momentum space in the vicinity of the minima of the band, $\mathbf{k}_0 = (\pm\pi/2, \pm\pi/2)$, and the Fermi surface consists of ellipses (see Fig. 1). The Fermi energy and Fermi momentum of noninteracting holes are

$$\epsilon_F = \frac{1}{2}\pi(\beta_1\beta_2)^{1/2}\delta, \qquad p_F \sim (\pi\delta)^{1/2}. \tag{14}$$

The Fermi momentum p_F is measured from the center of the corresponding ellipse. Let us stress that the numerical value of ϵ_F is very small. For realistic superconductors $t/J \approx 3$ (see, e.g., Refs. 32–34). Therefore at $\delta = 0.1$ and $J = 0.15$ eV one gets $\epsilon_F \approx 15$ meV ≈ 175 K. In pairing, the exchange of spin waves with typical momentum $q \sim p_F \ll 1$ is the most important. The energy of such spin waves is much higher than the typical energy of a pair,

$$\omega_q \sim p_F \sim (\pi\delta)^{1/2} \gg \epsilon_F \sim (\beta_1\beta_2)^{1/2}\delta. \tag{15}$$

The situation is quite similar to that for the two-hole bound state problem[10] and much different from the situation with the usual phonon-induced pairing where Debye's frequency is much lower than the Fermi energy.

The interaction between two holes with opposite spins and opposite momenta is[10]

$$V_{\mathbf{k},\mathbf{k}'} = -2\frac{g_{\mathbf{k},\mathbf{q}}g_{\mathbf{k}',-\mathbf{q}}}{-\omega_{\mathbf{q}} - E_{\mathbf{k}} - E_{\mathbf{k}'}} + \frac{8}{N}(A\gamma_{\mathbf{k}-\mathbf{k}'} + C\gamma_{\mathbf{k}+\mathbf{k}'}). \tag{16}$$

The first term here is due to the spin-wave exchange diagrams shown in Fig. 3. The minus sign before this term takes into account the fact that spin-wave exchange makes the spin flip for both holes. For the same reason, the momentum transfer is the sum (not the difference) of the hole momenta, $\mathbf{q} = \mathbf{k} + \mathbf{k}'$. The energy denominator in Eq. (16) takes into account the energy of the spin wave $\omega_{\mathbf{q}}$, and the energies $E_{\mathbf{k}}$ and $E_{\mathbf{k}'}$ of the two holes in an intermediate unpaired state. In fact, the account of $E_{\mathbf{k}}$ and $E_{\mathbf{k}'}$ is the account of retardation. We discuss this question below. The second term in Eq. (16) is the contact interaction (11).

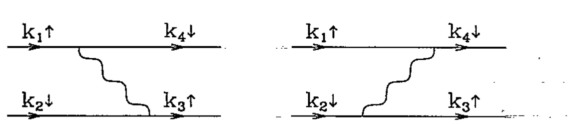

FIG. 3. Interaction between two holes via a single spin-wave exchange.

We use the usual BCS wave function for the ground state of the many-hole system,

$$|\Psi\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}h^{\dagger}_{\mathbf{k}\uparrow}h^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle. \tag{17}$$

Thus we suppose that all quasiparticles are in the condensate. For strong interactions the validity of this assumption is under question because there is no parameter to justify it. We believe that numerically the wave function (17) is good. Anyway one may consider the wave function (17) as a trial one in the variational method. In this case the large gain in energy which we get is a justification of the wave function.

The gap $\Delta_{\mathbf{k}}$ corresponding to the wave function (17) satisfies the conventional BCS equation

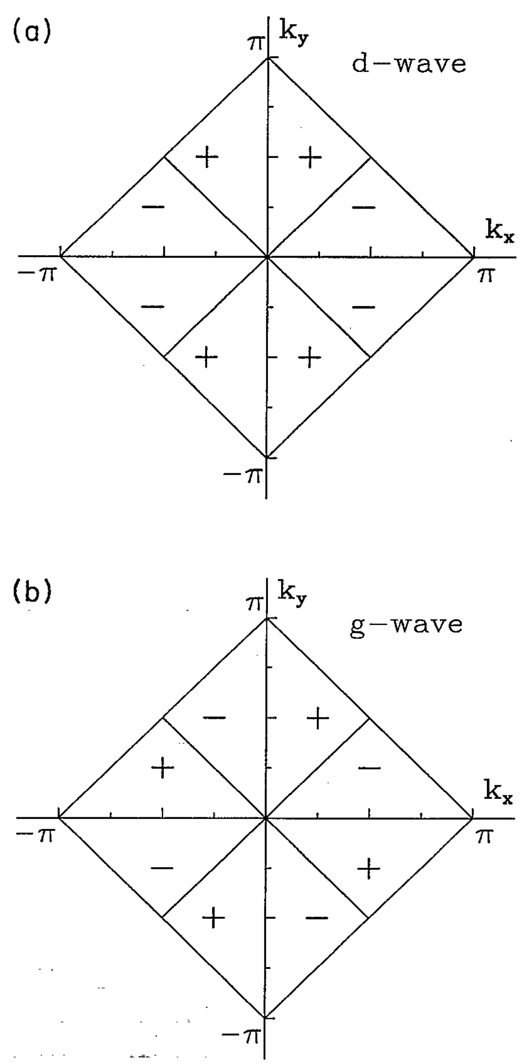

FIG. 4. The gap symmetry. (a) B_1 type (d wave), (b) A_2 type (g wave).

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{\sqrt{\xi_{\mathbf{k}'}^2+\Delta_{\mathbf{k}'}^2}}, \tag{18}$$

where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, μ being the chemical potential fixed by the hole density

$$\delta = 2\sum_{\mathbf{k}} v_{\mathbf{k}}^2. \tag{19}$$

It is well known that the excitation energy of fermions in BCS theory is $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$. Just this energy enters Eq. (16) for the effective hole-hole interaction. Equation (18) is obtained by variation of the average value of the Hamiltonian with respect to the parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$,

$$\frac{\delta}{\delta u_{\mathbf{k}}}\langle\Psi|H-\mathcal{E}|\Psi\rangle = \frac{\delta}{\delta v_{\mathbf{k}}}\langle\Psi|H-\mathcal{E}|\Psi\rangle = 0. \tag{20}$$

Here $\mathcal{E}$ is the energy of the ground state. The effective interaction (16) itself depends on the parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ via the dependence of $E_{\mathbf{k}}$ on the gap $\Delta_{\mathbf{k}}$. Nevertheless, in the variational equations (20) we have to set

$$\frac{\delta}{\delta u_{\mathbf{p}}}V_{\mathbf{k}\mathbf{k}'} = \frac{\delta}{\delta v_{\mathbf{p}}}V_{\mathbf{k}\mathbf{k}'} = 0, \tag{21}$$

and therefore we get the usual BCS equation (18). Explanation of the condition (21) is as follows. The spin-wave exchange part of the interaction (16) is due to the second order of perturbation theory. Therefore, the actual denominator in the spin-wave contribution is $\mathcal{E}-\mathcal{E}_{\text{excited}}$, and it does not depend explicitly on $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. The self-consistency condition $\mathcal{E}-\mathcal{E}_{\text{excited}} = -\omega_{\mathbf{q}} - E_{\mathbf{k}} - E_{\mathbf{k}'}$ appears after solving Eqs. (20) and (21). From the practical point of view this question is not important because due to the condition (15) the dependence of $V_{\mathbf{k},\mathbf{k}'}$ on the gap is very weak.

An iterative numerical solution of Eq. (18) is straightforward. We present results for $t = 3$ corresponding to realistic superconducting systems.[32–34] Since the inverse mass β_2 [see Eqs. (7),(8)] is known with rather poor accuracy, we use several values of the mass ratio $a = \beta_1/\beta_2$. We take β_1 from Eq. (9) and then set $\beta_2 = \beta_1/a$. The constant of the hole-magnon interaction (10) is $f = 1.80$ at $t = 3$.

The symmetry group of the square lattice is C_{4v}. The solutions of Eq. (18) belong to certain representations of this group. In agreement with Ref. 11 the strongest pairing is in the B_1 representation [d wave, Fig. 4(a)] and in the A_2 representation [g wave, Fig. 4(b)]. Consider first the d-wave pairing. The map of the gap for the hole concentration $\delta = 0.1$ and the mass ratio $a = \beta_1/\beta_2 = 7$ is presented in Fig. 5. In Fig. 6 for the same parameters we give the map of $v_{\mathbf{k}}^2$ which is the mean occupation number of a single-hole quantum state. We observe that despite a big value of gap the hole density distribution changes quite sharply at crossing the Fermi surface. For other mass ratios and hole concentrations Fig. 5 is also approximately valid because it gives the gap in units of $\Delta_{\max}$ and we found that with changing δ and a, the whole gap function is multiplied by some factor but the $\mathbf{k}$ dependence is not much changed,

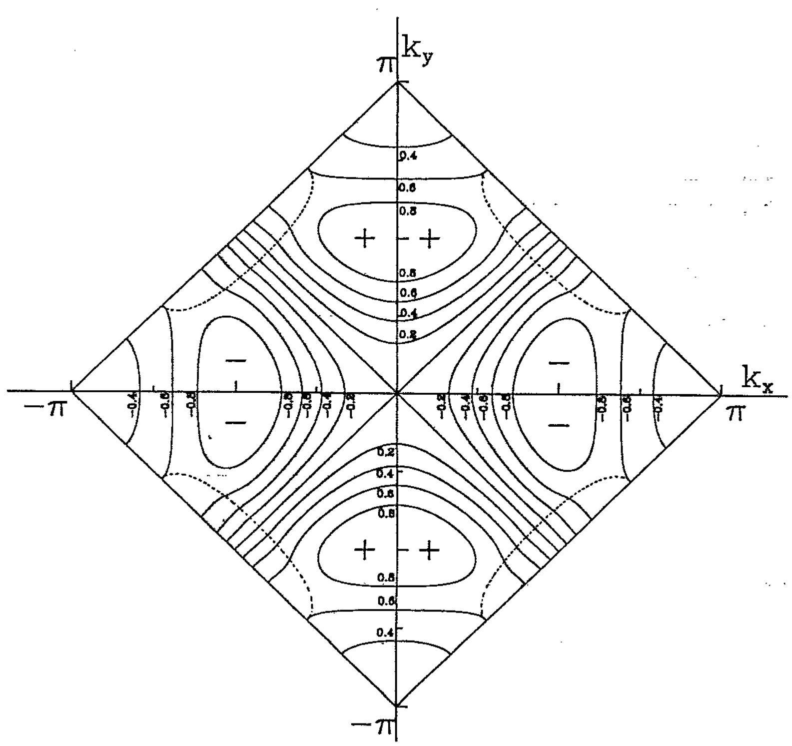

FIG. 5. The contour plot of the d-wave gap for $t/J = 3$, the mass ratio $a = \beta_1/\beta_2 = 7$, and hole concentration $\delta = 0.1$. The levels are presented in units of the maximum gap value $\Delta_{\max}$ (at these parameters, $\Delta_{\max} = 0.0661$). Dashed curves represent the Fermi surface for the case when one considers the holes like an ideal gas.

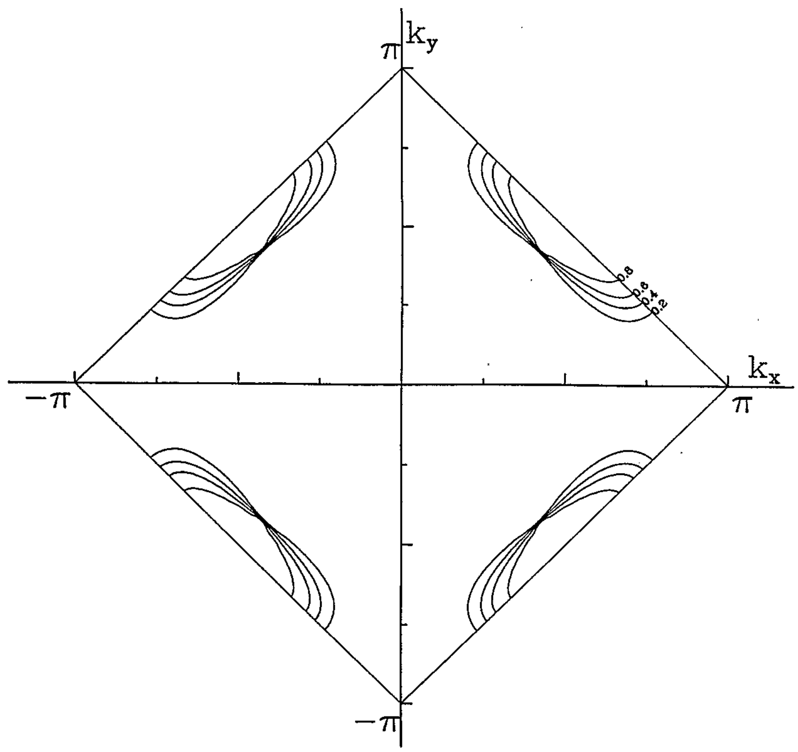

FIG. 6. The contour plot of a single-hole quantum state mean occupation number $v_{\mathbf{k}}^2$. Parameters are the same as in Fig. 5.

$$\Delta_{\mathbf{k}}(\delta, a) \approx \frac{\Delta_{\max}(\delta, a)}{\Delta_{\max}(\delta', a')} \Delta_{\mathbf{k}}(\delta', a'). \tag{22}$$

Due to interaction between holes, the ideal gas relation (14) between the chemical potential μ and the hole concentration is not valid. The correct relation follows from Eq. (19). Plots of μ as a function of δ are given in Fig. 7.

A very important characteristic is the maximal value Δ_1 of the gap on the Fermi surface. Its value is directly related to the critical temperature of the superconducting transition,[11]

$$T_c \approx 0.5\Delta_1(T = 0). \tag{23}$$

According to Fig. 5, $\Delta_1 \approx 0.7\Delta_{\max}$. The dependence of Δ_1 on the concentration is given in Fig. 8. Comparing the plots of the gap Δ_1 and the chemical potential μ (Fig. 7), we conclude that $\Delta_1 \sim 0.7\mu$. This is really a very strong coupling limit and virtually all holes are involved in pairing. This is to be contrasted with the usual situation when only a small portion of electrons $\frac{\omega_D}{\epsilon_F}$ take part in pairing and the gap is proportional to the Debye frequency.

The g-wave pairing is weaker and we will not present complete results for this case. Due to the above mentioned similarity of the long-range (small q) behavior of the d and g waves which arises from having the same number of zeros at the Fermi surface, the value of the gap for the g wave for the above parameters is of the same order as for the d wave. It is also interesting that the g wave does not depend on details of the contact part of the interaction (16) while the d-wave gap is substantially suppressed by adding repulsion to the short-range interaction. Thus, under certain conditions the g-wave solution may be relevant to the problem. Table I gives more information about solutions at several parameters including the difference of the free energy $F = \langle\Psi|H - \mu N_h|\Psi\rangle$ (N_h is the number of holes) between the superconducting and normal states,

$$F_S - F_N = 2\sum_{\mathbf{k}} \xi_{\mathbf{k}} v_{\mathbf{k}}^2 + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}. \tag{24}$$

It is convenient to calculate free energy per *hole* and use the difference $f_S - f_N = \frac{1}{N\delta}(F_S - F_N)$.

TABLE I. Influence of short-range interaction. Changes in the short-range interaction are introduced by increasing the parameter α [see discussion after Eq. (11)] which makes the contact interaction more repulsive. All data are for $T = 0$, $a = 7$, $\mu = 0.058$ (this is the chemical potential at which in the absence of interaction the hole concentration would be $\delta_0 = 0.05$).

Symmetry	α	$f_S - f_N$	δ	$\Delta_{\max}$	Δ_1
d-wave	$\alpha = 0.6$	-4.42×10^{-3}	0.0606	0.0523	0.0377
d-wave	$\alpha = 0.8$	-2.01×10^{-3}	0.0552	0.0317	0.0222
g-wave	$\alpha = 0.6$	-1.79×10^{-3}	0.0547	0.0259	0.0210
g-wave	$\alpha = 0.8$	-1.79×10^{-3}	0.0547	0.0259	0.0210

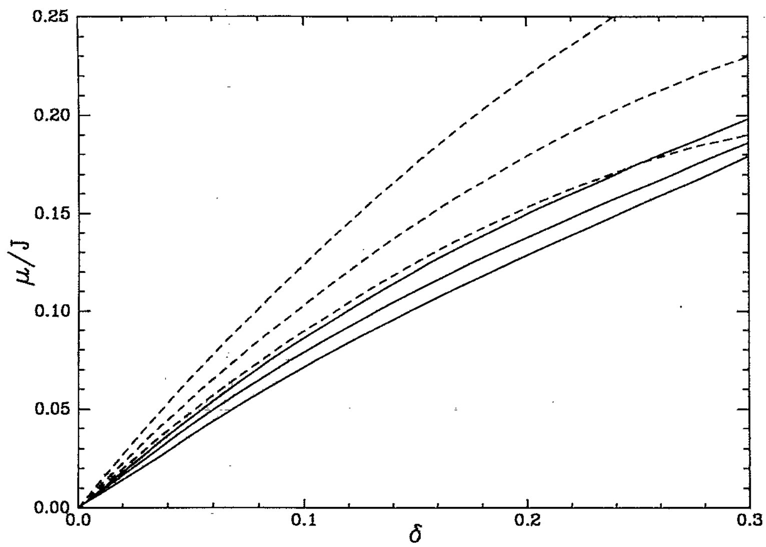

FIG. 7. The chemical potential μ as a function of hole concentration δ. Dashed curves correspond to an ideal gas of holes. Deviation of dashed curves from linear dependence (14) is due to the deviation of the dispersion relation (7) from the quadratic expansion (8). The dependence with pairing taken into account is presented by solid lines. All the curves correspond to $t/J = 3$. The mass ratio is (from top to bottom) $a = \beta_1/\beta_2 = 5, 7, 9$.

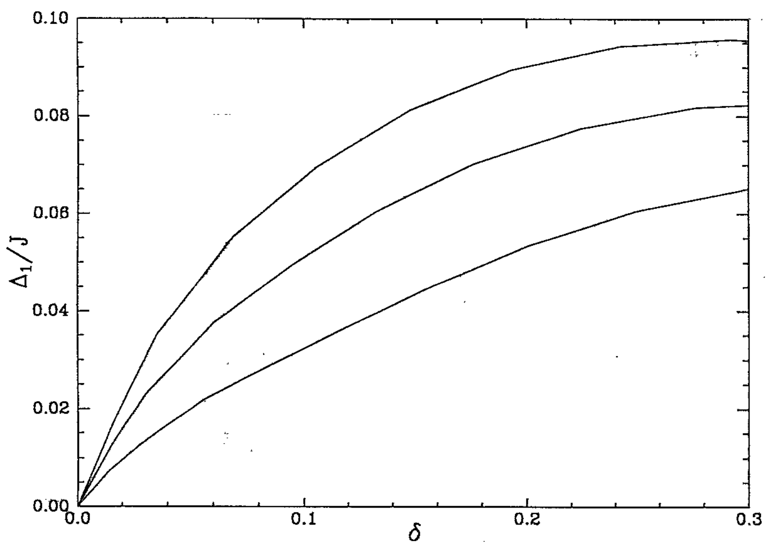

FIG. 8. The maximal value of the gap on the Fermi surface, Δ_1, vs hole concentration for $t/J = 3$; the mass ratio is (from top to bottom) $a = \beta_1/\beta_2 = 5, 7, 9$.

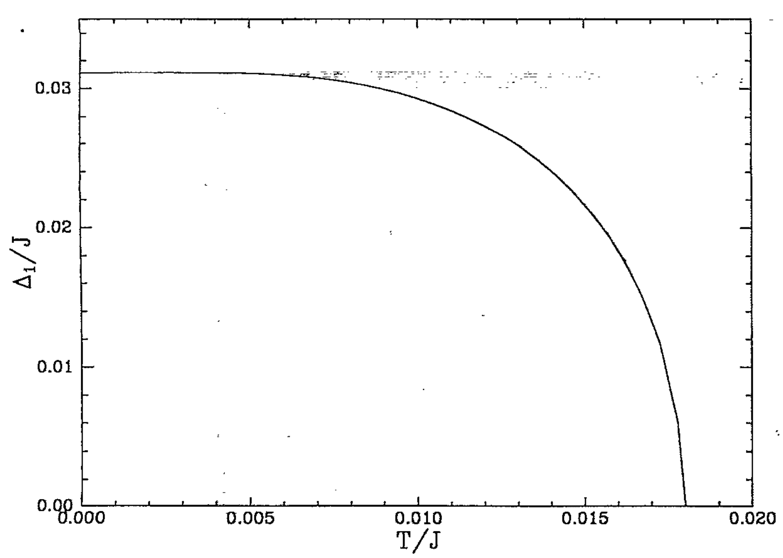

FIG. 9. The maximal value of the gap on the Fermi surface, Δ_1, as a function of temperature. The hole concentration is $\delta = 0.05$, $t/J = 3$, the mass ratio $a = \beta_1/\beta_2 = 7$.

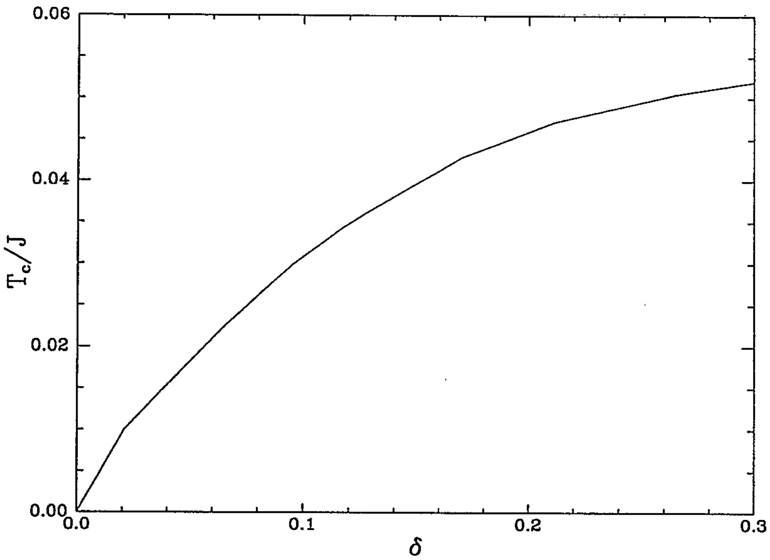

FIG. 10. The critical temperature vs hole concentration. $t/J = 3$, the mass ratio $a = \beta_1/\beta_2 = 7$.

IV. CRITICAL TEMPERATURE

Due to the condition (15) the spin-wave frequency in the hole-hole interaction (16) is large in comparison with the hole excitation energy: $\omega_{\mathbf{q}} \gg E_{\mathbf{k}}$. It means that retardation is small and the interaction is almost instantaneous. It is well known that in this case the equation for the gap at $T \neq 0$ is

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}}\tanh\frac{E_{\mathbf{k}'}}{2T}. \qquad (25)$$

In Fig. 9 we present the calculated dependence of Δ_1 on temperature at hole concentration $\delta = 0.1$. Figure 10 gives the dependence of the critical temperature T_c on hole concentration. The approximate relation (23) derived analytically in Ref. 11 is qualitatively fulfilled. In real units ($J = 0.15$ eV), Fig. 10 gives (taking $a = 7$) $T_c = 51$ K at $\delta = 0.1$ and $T_c = 86$ K at $\delta = 0.3$. Let us stress that in our calculation we do not use any fit. The only input is the values of t and J.

V. CONCLUSIONS

Using the single spin-wave exchange mechanism suggested in Refs. 10, 11 we carried out a numerical *ab initio* calculation of superconducting pairing in the t-J model. Both the magnitude of critical temperature and its dependence on hole concentration are in good agreement with experimental data. The calculated critical temperature is still smaller than the highest critical temperature obtained in experiment. However, this may be explained by not knowing the exact parameters. By a relatively small variation of parameters we can get $T_c = 100$–150 K.

The most important remaining problem is the destruction of long-range antiferromagnetic order. Following experimental results[13] we have assumed that antiferromagnetic order is preserved at distances $r \lesssim 1/p_F$. The behavior at larger distances is an open question in the present paper.

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