Superconductivity and superconducting order parameter phase fluctuations in a weakly doped antiferromagnet

V. M. Loktev*
Bogolyubov Institute for Theoretical Physics, Metrologicheskaya street 14-b, Kiev-143 03680, Ukraine

V. M. Turkowski†
Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, Missouri 65211, USA
(Received 30 October 2006; revised manuscript received 22 January 2007; published 25 June 2007)

The superconducting properties of a recently proposed phenomenological model for a weakly doped antiferromagnet are analyzed, taking into account fluctuations of the phase of the order parameter. In this model, we assume that the doped charge carriers cannot move out of the antiferromagnetic sublattice in which they were introduced. This case corresponds to free-carrier spectra with the maximum at $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$, as it was observed in angle-resolved photoemission spectroscopy experiments for some of the cuprates in the insulating state [A. Damascelli *et al.*, Rev. Mod. Phys. **75**, 473 (2003)]. The doping dependence of the superconducting gap and the temperature–carrier density phase diagram of the model are studied in the case of the $d_{x^2-y^2}$ pairing symmetry of the order parameter and different values of the model parameters. A possible relevance of the results to experiments on high-temperature superconductors is discussed.

DOI: 10.1103/PhysRevB.75.224513 PACS number(s): 74.20.−z, 74.20.Fg, 74.20.Rp, 74.72.−h

I. INTRODUCTION

The theoretical description of high-temperature superconductors (HTSCs) remains one of the most important unsolved problems of modern condensed-matter theory. However, despite the lack of complete understanding of this phenomenon, some facts about the cuprate materials are almost generally accepted by the scientific community. First of all, it is believed that superconductivity in these materials is mainly generated in CuO_2 layers, since even samples with the layer spacing of ~ 10 Å demonstrate a very high critical temperature. Second, in the undoped regime, these materials are antiferromagnetic insulators, which transform into superconductors when the doping is larger than some critical value. Experiments indicate the presence of strong antiferromagnetic correlations in the superconducting regime.[2,3] Third, the symmetry of the superconducting order parameter is of a *d*-wave type in many of the compounds.[4,5] It is believed by many researches that these facts contain sufficient information to understand the phenomenon of HTSC. It is almost generally accepted that this phenomenon can be described in the framework of a simple two-dimensional model of strongly correlated electrons (for a recent over-review, see Ref. 6). The antiferromagnetic correlations produce a Bardeen-Cooper-Schrieffer (BCS)-type spin-wave pairing between electrons. One of the most often studied models of HTSCs is the *t-J* model[7,8] (see, for example, Refs. 9–14). It was shown that the solution of this model within different approximations demonstrates the *d*-wave superconductivity in the underdoped regime. This and many other models, however, are rather oversimplified, and they do not take into account some properties of the cuprates. In particular, it is known from angle-resolved photoemission spectroscopy experiments that the free-carrier spectra of some cuprates such as $Sr_2CuO_2Cl_2$ in the insulating phase have the maxima not at the Brillouin zone edge at momenta $\mathbf{k}=(\pm\pi,\pm\pi)$ but at points $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$.[1] This fact suggests that the free-carrier spectra can be approximated as $\varepsilon(\mathbf{k})\sim -4t_2\cos k_x\cos k_y-2t_3(\cos 2k_x+\cos 2k_y)$, i.e., the doped carriers only move within one sublattice where they were born. This situation is similar to the case of collinear antiferromagnetic dielectrics with the Néel ground state, where electronic and spin excitations cannot move out of one sublattice to another. It is important that the excitations must live on nonequivalent sublattices, i.e., on the copper sublattices, which form an antiferromagnet. It is often assumed for several reasons (see below) that doped holes in cuprates occupy sites in the oxygen subsystem of the CuO_2 planes.[15] However, it is known that the next-nearest-neighbor (NNN) hopping parameter for this sublattice is much smaller than the nearest-neighbor (NN) hopping parameter, which excludes the possibility to explain the spectra experiments[1] in this case. One can try to overcome this difficulty by introducing the Zhang-Rice singlet, which consists of a doped oxygen hole coupled to one of the closest copper ions. The hole chooses the ion in such a way that the energy of the singlet is minimal. Such states can only move within their magnetic sublattices. However, these states are unstable due to several reasons. First of all, the "up" and "down" spins of the copper ions enter as a linear combination in the Zhang-Rice singlet in an equivalent way, so a hole with the opposite spin projection will try to form the same singlet with the neighboring localized ion spin from another sublattice. Also, the oxygen ions occupy states that are symmetrical with respect to the neighbor copper ions. Therefore, the total exchange field, which acts on a hole on the oxygen site, is compensated, and the hole becomes frustrated with respect to the choice of the axis of the spin quantization. The proper axis of quantization can be established, but in this case, the hole hybridized with copper states will move in the CuO_2 plane not feeling the magnetic ordering. This also does not allow one to explain the spectra experiments.

These difficulties can be avoided by assuming that the doped holes sit on the copper sites.[16] In fact, in the undoped

state, the CuO_2 planes consist of Cu^{2+} and O^{2-} ions. The doping leads to a change of the valence of some ions, which results in the appearance of movable charges in the system. The assumption that the holes occupy copper ions means that the $Cu^{2+} \rightarrow Cu^{3+}$ transitions take place. These transitions are different from usually considered $O^{2-} \rightarrow O^{-}$ transitions in the case of the holes, which occupy the oxygen sites. The reason for the last assumption follows from the fact that it is believed by many researches that the $Cu^{3+}O^{2-}$ configuration has a higher energy compared to $Cu^{2+}O^{-}$. However, the $Cu^{3+}O^{2-}$ configuration can be preferable if one takes into account the Coulomb attraction V_C inside the configurations. In fact, since $V_C^{Cu^{3+}O^{2-}} \simeq 3V_C^{Cu^{2+}O^{-}} \simeq 6V_C^{Cu^{+}O^{-}}$ and every copper ion is surrounded by four oxygen ions, at the same time as every oxygen ion is surrounded by only two copper ions, one can find that the corresponding Coulomb attraction energy difference for two configurations is of order $20V_C^{Cu^{+}O^{-}}$. This difference in the Coulomb interaction energies can provide the stability of the $Cu^{3+}O^{2-}$ configuration campared to other configurations, i.e., a possibility for the doped holes to move within the copper sublattice. This picture corresponds qualitatively to the *t*-*J*-model case. However, it was usually assumed that the free-carrier dispersion relation in this model corresponds to the NN hopping, which does not allow one to obtain the experimental spectra with the maximum at $\mathbf{k}=(\pm\pi/2, \pm\pi/2)$.

A simple phenomenological Hamiltonian that corresponds to charge carriers that move within fixed sublattices was proposed in order to describe superconductivity in some cuprates at low carrier densities in Ref. 16. In this paper, the effective attraction between the doped electrons on different sublattices was assumed to be equal to the antiferromagnetic coupling *J* between nearest site spins. In fact, the carrier doping in the antiferromagnet leads to breakdown of the antiferromagnetic coupling *J* between nearest site spins. This results in increase of the energy of the system. This energy increase is minimal when two empty sites are nearest neighbors, because the minimal number of the antiferromagnetic spin-spin (exchange) interaction bonds is broken in this case. This phenomenological attraction was introduced for the first time by Trugman in Ref. 18 (see also recent papers[19–21]). As it was shown in Ref. 22, the order parameter, which corresponds to the pairs produced by such an interaction, has a *d*-wave symmetry.

Below, the doping dependence of the *d*-wave superconducting gap in the model at different values of coupling and $T=0$ is studied. In addition, we analyze the temperature-doping phase diagram of the model by taking into account fluctuations of the phase of the order parameter according to the Emery-Kiveson scenario.[23] We identify the temperature region between the mean-field critical temperature T_c^{MF}, at which the modulus of the superconducting order parameter is created, and the Berezinskii-Kosterlitz-Thouless (BKT) critical temperature T_{BKT}, below which the order parameter phases are algebraically correlated, as the lower part of the pseudogap phase with a critical temperature T_0, which is a few times larger than T_c (see, for example, Refs. 6, 24, and 25). It is shown that the width of this temperature region between $T_c^{MF} \equiv T_0$ and $T_{BKT} \equiv T_c$ strongly depends on the carrier concentration. We make a qualitative comparison of the results with experimental results on some HTSCs.

II. MODEL

The Hamiltonian of noninteracting doped *d*-hole carriers in HTSCs can be approximated by

$$H_d = \varepsilon_d \sum_{\mathbf{n}} \sum_{\sigma_\mathbf{n}} d^\dagger_{\mathbf{n}\sigma_\mathbf{n}} d_{\mathbf{n}\sigma_\mathbf{n}} - \frac{1}{2} \sum_{\mathbf{n},\mathbf{m}} \sum_{\sigma_n,\sigma_m} t_{\mathbf{nm}} \langle \sigma_\mathbf{n} | \sigma_\mathbf{m} \rangle d^\dagger_{\mathbf{n}\sigma_n} d_{\mathbf{m}\sigma_m}, \tag{1}$$

where $d^\dagger_{\mathbf{n}\sigma_n}(d_{\mathbf{n}\sigma_n})$ is the creation (annihilation) operator of the electron on site $\mathbf{n}$ with spin $\sigma_\mathbf{n}$, ε_d is the electron on-site energy, $t_{\mathbf{nm}}$ is the hopping parameter, and $\langle \sigma_\mathbf{n} | \sigma_\mathbf{m} \rangle$ is the spin-spin correlation function calculated in the ion system of coordinates (see Ref. 16). This Hamiltonian can be transformed to the following form in terms of the Hubbard operators in the laboratory system of spin coordinates:

$$H_d = H_{coh} + H^{(1)}_{int} + H^{(2)}_{int}, \tag{2}$$

where

$$H_{coh} = (\varepsilon_d - \mu) \sum_{\mathbf{n}} X^{2,2}_{\mathbf{n}} - \frac{1}{2} \sum_{\mathbf{n},\mathbf{m}} t_{\mathbf{nm}} \cos \frac{\mathbf{Q}_{AFM}(\mathbf{n}-\mathbf{m})}{2} X^{2,1/2}_{\mathbf{n}} X^{1/2,2}_{\mathbf{m}} \tag{3}$$

is a part of the Hamiltonian which describes motion of free holes in an antiferromagnetically ordered medium, $\mathbf{Q}_{AFM}\mathbf{a} = (\pm\pi, \pm\pi)$, $\mathbf{a}$ is the lattice constant of a square lattice, and

$$H^{(1)}_{int} = -\frac{1}{2} \sum_{\mathbf{n},\mathbf{m}} t_{\mathbf{nm}} \sin \frac{\mathbf{Q}_{AFM}(\mathbf{n}-\mathbf{m})}{2} (X^{2,1/2}_{\mathbf{n}} X^{1/2,2}_{\mathbf{m}} S^-_{\mathbf{m}} - X^{2,1/2}_{\mathbf{n}} X^{1/2,2}_{\mathbf{m}} S^+_{\mathbf{n}}) \tag{4}$$

and

$$H^{(2)}_{int} = -\frac{1}{2} \sum_{\mathbf{n},\mathbf{m}} t_{\mathbf{nm}} \cos \frac{\mathbf{Q}_{AFM}(\mathbf{n}-\mathbf{m})}{2} X^{2,1/2}_{\mathbf{n}} X^{1/2,2}_{\mathbf{m}} S^+_{\mathbf{n}} S^-_{\mathbf{m}} \tag{5}$$

describe noncoherent inter-ion hole transitions with one and two spin excitations, correspondingly. $S^+_\mathbf{n}$ and $S^-_\mathbf{m}$ are spin creation and annihilation operators. It is important that expressions (2)–(5) are written in terms of the Hubbard operators, which directly take into account the antiferromagnetic ordering in the system. The ion spin projections in both magnetic sublattices are equal to 1/2 in the ground state of the crystal (we use local systems of coordinates for each sublattice). The spin conservation is also taken into account, which results in the fact that the electrons can move only on the magnetic sublattice on which they were born (for details, see Ref. 16).

As it was mentioned in the Introduction, a simple effective attraction between the doped holes on different sublattices can be introduced.[18] The carrier doping in the antiferromagnet leads to an increasing of the energy of the system, since it breaks the antiferromagnetic coupling *J* between the

nearest site spins. The energy increase is minimal when two doped particles occupy the nearest-neighbor sites, since the minimal number of the antiferromagnetic spin-spin bonds is broken in this case. Therefore, the doping leads to an effective attraction between carriers on different sublattices:

$$H_{attr} = -J \sum_{\mathbf{n},\rho=\mathbf{a},\mathbf{b}} X_{\mathbf{n}}^{2,2} X_{\mathbf{n}+\rho}^{2,2}. \tag{6}$$

The total Hamiltonian of the system is $H=H_d+H_{attr}$. For simplicity, we neglect Eqs. (4) and (5), which do not contribute significantly to the increase of the superconducting critical temperature. The first term corresponds to a BCS-like interaction, which is small at low carrier densities, or Fermi momenta of doped holes k_F. It is proportional to the energy of the spin waves $\Omega_{AFM}(k_F)$, which is much smaller than the exchange energy J. Equation (5), which corresponds to the two-magnon attraction, also does not contribute significantly to the increase of the critical temperature in the d-wave pairing channel.[16,17,26]

Therefore, a simplified version of the Hamiltonian of a doped antiferromagnet can be written as

$$H = (\varepsilon_d - \mu)\sum_{\mathbf{n}} X_{\mathbf{n}}^{2,2} - \frac{1}{2}\sum_{\mathbf{n},\mathbf{m}} t_{\mathbf{nm}} \cos\frac{\mathbf{Q}_{AFM}(\mathbf{n}-\mathbf{m})}{2} X_{\mathbf{n}}^{2,1/2} X_{\mathbf{m}}^{1/2,2} - J \sum_{\mathbf{n},\rho=\mathbf{a},\mathbf{b}} X_{\mathbf{n}}^{2,2} X_{\mathbf{n}+\rho}^{2,2}. \tag{7}$$

In the case of an antiferromagnet on a square lattice, the free particle energy spectrum, which corresponds to the first two terms in Eq. (7), is

$$\varepsilon(\mathbf{k}) = \varepsilon_d - 4t_2 \cos k_x \cos k_y - 2t_3(\cos 2k_x + \cos 2k_y) - \mu, \tag{8}$$

where μ is the chemical potential, and t_2 and t_3 are the NNN and next NNN hopping parameters, correspondingly. We use the units in which the lattice constant is equal to one: $a=1$. In order to have $\varepsilon(\mathbf{k})=0$ at $\mathbf{k}=0$, one can choose $\varepsilon_d=4t_2+4t_3$. The chemical potential is connected with the free (or doped) particle number in the system by the following relation:

$$\delta = \sum_{\mathbf{n}} \langle X_{\mathbf{n}}^{2,2} \rangle, \tag{9}$$

where the sum goes over two sublattices. The Hamiltonian [Eq. (7)] has a simpler structure, compared to the t-J-model Hamiltonian, yet it can describe some of the main physical properties of underdoped cuprates.

III. ZERO-TEMPERATURE PROPERTIES

To study the superconducting properties of the system described by the Hamiltonian [Eq. (7)], it is convenient to introduce generalized Nambu-Hubbard hole operators:

$$\Psi_{\mathbf{n}}(t) = \begin{pmatrix} X_{\mathbf{n}}^{2,1/2}(t) \\ X_{\mathbf{n}}^{1/2,2}(t) \end{pmatrix}, \quad \Psi_{\mathbf{n}}^{\dagger}(t) = (X_{\mathbf{n}}^{1/2,2}(t), X_{\mathbf{n}}^{2,1/2}(t)), \tag{10}$$

where $\mathbf{n}$ are lattice sites and t is time. In this case, the time-ordered Green function $\hat{G}_{\mathbf{nm}}(t,t') = -i\langle T(\Psi_{\mathbf{n}}(t)\Psi_{\mathbf{m}}^{\dagger}(t')\rangle$ is

$$\hat{G}_{\mathbf{nm}}(t,t') = -i \begin{pmatrix} \langle TX_{\mathbf{n}}^{2,1/2}(t)X_{\mathbf{m}}^{1/2,2}(t')\rangle & \langle TX_{\mathbf{n}}^{2,1/2}(t)X_{\mathbf{m}}^{2,1/2}(t')\rangle \\ \langle TX_{\mathbf{n}}^{1/2,2}(t)X_{\mathbf{m}}^{1/2,2}(t')\rangle & \langle TX_{\mathbf{n}}^{1/2,2}(t)X_{\mathbf{m}}^{2,1/2}(t')\rangle \end{pmatrix}. \tag{11}$$

The Green function [Eq. (11)] satisfies the following equation of motion:

$$i\frac{\partial}{\partial t}\hat{G}_{\mathbf{nm}}(t,t') = \delta(t-t')\delta_{\mathbf{nm}}\hat{I} + \langle T[\Psi_{\mathbf{n}}(t),H]\Psi_{\mathbf{m}}^{\dagger}(t')\rangle, \tag{12}$$

where, as it was mentioned above, H is defined by Eq. (7), and

$$\hat{I} = \begin{pmatrix} \langle X_{\mathbf{n}}^{1/2,1/2}(t) + X_{\mathbf{n}}^{2,2}(t)\rangle & 0 \\ 0 & \langle X_{\mathbf{n}}^{1/2,1/2} + X_{\mathbf{n}}^{2,2}\rangle \end{pmatrix}. \tag{13}$$

This equality can be derived by using the commutation relations for the Hubbard operators.

In the generalized mean-field theory approximation, the last term in Eq. (12) can be linearized in the following way (see, for example Ref. 27):

$$\langle T[\Psi_{\mathbf{n}},H]\Psi_{\mathbf{m}}^{\dagger}\rangle(\omega) \simeq \sum_{\mathbf{l}} \hat{E}_{\mathbf{nl}}\hat{G}_{\mathbf{lm}}(\omega), \tag{14}$$

where

$$\hat{E}_{\mathbf{nm}} = \langle\{[\Psi_{\mathbf{n}},H],\Psi_{\mathbf{m}}^{\dagger}\}\rangle \tag{15}$$

is the energy matrix. The nonlinear (dynamical) corrections to the self-energy in Eq. (14) can be taken into account.[12] We assume that the generalized mean-field approximation [Eq. (14)] is good enough in the case of low carrier densities, when the free quasiparticle excitations can be described by the fields represented by the Hubbard operators [Eq. (10)].

The expression for the energy matrix [Eq. (15)] can be found by solving the Heisenberg equations of motion for the X operators. In terms of the energy matrix [Eq. (15)], the Green function can be written as

$$\hat{G}_{\mathbf{nm}}(\omega) = \frac{\hat{I}}{\omega\delta_{\mathbf{nm}} - \hat{E}_{\mathbf{nm}}}. \tag{16}$$

To find the explicit expression for the Green function [Eq. (16)], let us write down the equations of motion for the Hubbard operators:

$$i\hbar\frac{\partial}{\partial t}X_{\mathbf{n}}^{1/2,2}(t) = (\varepsilon_d - \mu)X_{\mathbf{n}}^{1/2,2} - \frac{1}{2}\sum_{\mathbf{l}} t_{\mathbf{nl}} \cos\frac{Q_{AFM}(\mathbf{n}-\mathbf{l})}{2}(X_{\mathbf{n}}^{1/2,1/2} + X_{\mathbf{n}}^{2,2})X_{\mathbf{l}}^{1/2,2} - 2J\sum_{\rho} X_{\mathbf{n}+\rho}^{2,2}X_{\mathbf{n}}^{1/2,2}, \tag{17}$$

$$i\hbar\frac{\partial}{\partial t}X_{\mathbf{n}}^{2,1/2}(t) = -(\varepsilon_d-\mu)X_{\mathbf{n}}^{2,1/2} + \frac{1}{2}\sum_{\mathbf{l}} t_{\mathbf{ln}}\cos\frac{Q_{AFM}(\mathbf{l}-\mathbf{n})}{2}X_{\mathbf{l}}^{2,1/2}(X_{\mathbf{n}}^{1/2,1/2} + X_{\mathbf{n}}^{2,2}) + 2J\sum_{\rho} X_{\mathbf{n}}^{2,1/2}X_{\mathbf{n}+\rho}^{2,2}. \quad (18)$$

Substitution of the expressions on the right-hand side in Eqs. (17) and (18) instead of the commutators $(i\partial X/\partial t = [X,H])$ into Eq. (15) and evaluation of the anticommutators give the following expression for the energy matrix:

$$\hat{E}_{\mathbf{nm}} = \begin{pmatrix} \tilde{E}_{\mathbf{nm}} & -\tilde{\Delta}_{\mathbf{nm}} \\ \tilde{\Delta}_{\mathbf{nm}} & -\tilde{E}_{\mathbf{nm}} \end{pmatrix}, \quad (19)$$

where

$$\tilde{E}_{\mathbf{nm}} = -\delta_{\mathbf{nm}}(\varepsilon_d-\mu)\langle X_{\mathbf{n}}^{1/2,1/2} + X_{\mathbf{n}}^{2,2}\rangle + \frac{1}{2}\delta_{\mathbf{nm}}\sum_{\mathbf{l}} t_{\mathbf{ln}}\cos\frac{\mathbf{Q}_{AFM}(\mathbf{l}-\mathbf{n})}{2}\langle X_{\mathbf{l}}^{2,1/2}X_{\mathbf{n}}^{1/2,2}\rangle + 2\delta_{\mathbf{nm}}\sum_{\mathbf{l}} J_{\mathbf{nl}}\langle X_{\mathbf{n}}^{1/2,1/2}X_{\mathbf{l}}^{2,2}\rangle + \frac{1}{2}t_{\mathbf{mn}}\cos\frac{\mathbf{Q}_{AFM}(\mathbf{m}-\mathbf{n})}{2}\langle X_{\mathbf{m}}^{1/2,1/2}(X_{\mathbf{n}}^{1/2,1/2} + X_{\mathbf{n}}^{2,2})\rangle, \quad (20)$$

$$\tilde{\Delta}_{\mathbf{nm}} = -\frac{1}{2}\delta_{\mathbf{nm}}\sum_{\mathbf{l}} t_{\mathbf{ln}}\cos\frac{\mathbf{Q}_{AFM}(\mathbf{l}-\mathbf{n})}{2}\langle X_{\mathbf{l}}^{2,1/2}X_{\mathbf{n}}^{2,1/2}\rangle - 2J_{\mathbf{nm}}\langle X_{\mathbf{n}}^{2,1/2}X_{\mathbf{m}}^{2,1/2}\rangle \quad (21)$$

are the renormalized energy and the superconducting gap matrices. In Eqs. (20) and (21), we have introduced the following NN attraction matrix operator: $J_{\mathbf{nm}}=J\delta_{\mathbf{n},\mathbf{m}+\boldsymbol{\rho}}$. Despite their complicated formal structure, it is possible to show that the terms in Eqs. (20) and (21) have a very simple physical interpretation. In particular, the second and third terms in Eq. (20), which are proportional to δ, lead to a renormalization of the chemical potential $\mu\rightarrow\mu'=\mu+\delta\mu$. The average $\langle X_{\mathbf{m}}^{1/2,1/2}(X_{\mathbf{n}}^{1/2,1/2}+X_{\mathbf{n}}^{2,2})\rangle$ multiplied by the hopping operator $t_{\mathbf{mn}}$ in the last term of Eq. (20) leads to a renormalization of the quasiparticle bandwidth in the limit of low doping. However, one can set $\langle X_{\mathbf{m}}^{1/2,1/2}(X_{\mathbf{n}}^{1/2,1/2}+X_{\mathbf{n}}^{2,2})\rangle\simeq 1$ in this limit, since in the limit of low carrier concentrations, $X_{\mathbf{n}}^{1/2,1/2}+X_{\mathbf{n}}^{2,2}\simeq 1$, and the renormalization of the quasiparticle band is not strong. Therefore, the energy function $\tilde{E}_{\mathbf{nm}}$ defined in Eq. (20) can be approximated by the free-energy spectra expression [Eq. (8)] multiplied by −1 in the momentum space. It is also assumed that the chemical potential in Eq. (8) is renormalized.

The expression for the gap function [Eq. (21)] can be also simplified. In fact, as it was shown in Ref. 22, attraction (6) favors a superconducting pairing with the d-wave symmetry of the order parameter. Therefore, we assume that the strongest pairing in the system takes place in the d-wave channel and neglect the first term in Eq. (21), which does not contribute to the pairing in this channel. In this case, the gap function in the momentum representation can be approximated in the following way:

$$\Delta(\mathbf{k}) = -2\sum_{\mathbf{q}} J(\mathbf{k}-\mathbf{q})\langle X_{-\mathbf{q}}^{2,1/2}X_{\mathbf{q}}^{2,1/2}\rangle, \quad (22)$$

where we introduced a NN attraction kernel, $J(\mathbf{k})=2J[\cos(k_x-q_x)+\cos(k_y-q_y)]$. Thus, the Green function [Eq. (16)] has the following form in the momentum space:

$$G(\omega,\mathbf{k}) = \frac{1}{\omega+\varepsilon(\mathbf{k})\tau_z + i\Delta(\mathbf{k})\tau_y}, \quad (23)$$

where $\hat{\tau}_y$ and $\hat{\tau}_z$ are the Pauli matrices and we assumed that in the limit of low carrier densities, the normalization matrix is approximately equal to the unit matrix $\hat{I}\simeq\hat{1}$.

To find the unknown gap function $\Delta(\mathbf{k})$ and the renormalized chemical potential μ', one can write down and solve the system of equations for these functions using the fluctuation-dissipation theorem:

$$\langle AB\rangle = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\frac{\Im G_{AB}(\omega)}{e^{(\omega-\mu)/T}+1}. \quad (24)$$

The zero-temperature equations, which connect $\Delta(\mathbf{k})$ and μ with the parameters t_2, t_3, J, and δ, follow from Eqs. (9) and (22):

$$\Delta(\mathbf{k}) = 2\sum_{\mathbf{q}} J(\mathbf{k}-\mathbf{q})\frac{\Delta(\mathbf{q})}{\sqrt{\varepsilon^2(\mathbf{q})+\Delta^2(\mathbf{q})}}, \quad (25)$$

$$\delta = \sum_{\mathbf{k}}\left[1+\frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k})+\Delta^2(\mathbf{k})}}\right]. \quad (26)$$

Since we consider the case when the pairing in the system takes place in the d-wave channel, we set $\Delta(\mathbf{k})=\Delta_d\gamma_d(\mathbf{k})$, where $\gamma_d(\mathbf{k})=(\cos k_x-\cos k_y)$, in Eqs. (25) and (26). In this case, in order to satisfy Eqs. (25) and (26), one must extract the d-wave piece from the interaction kernel and approximate it by the function $J(\mathbf{k}-\mathbf{q})\rightarrow 2J\gamma_d(\mathbf{k})\gamma_d(\mathbf{q})$. In this approximation, Eq. (25) for the superconducting order parameter acquires a rather simple form,

$$1 = 4J\sum_{\mathbf{q}}\gamma_d^2(\mathbf{q})\frac{1}{\sqrt{\varepsilon^2(\mathbf{q})+\Delta_d^2\gamma_d^2(\mathbf{q})}}. \quad (27)$$

The solution of the set of Eqs. (26) and (27) at different values of interaction and hopping t_2 is presented in Fig. 1. As it follows from this figure, the gap is not very sensitive to the values of the NNN hopping parameter, but it strongly depends on the interaction potential. Superconductivity is suppressed when the carrier density is smaller than some critical value. This value also increases when the effective attractive interaction J decreases. This situation is, in principle, similar to the case with attracting electrons, when there is no antiferromagnetic background for the carrier motion (see, for example, Refs. 31 and 32).

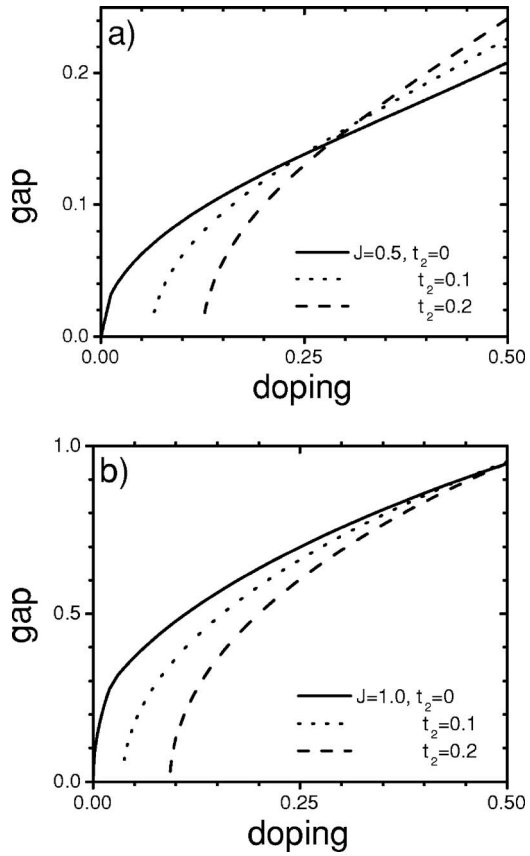

FIG. 1. The gap parameter Δ_d as a function of the carrier density at $t_3=1$ and different values of t_2 and J. Here and in Figs. 2(b), 5(b), and 6(b), we do not present results in the case when the gap or the critical temperature is very small for some values of the model parameters, since it was difficult to get an accurate numerical solution in these cases.

IV. TEMPERATURE–CARRIER DENSITY PHASE DIAGRAM

In this section, we study the finite-temperature properties of the model. It is known that there are two critical temperatures in the two-dimensional superconducting systems: the mean-field critical temperature T_c^{MF}, below which the uncorrelated pairs start to form, and the Berezinskii-Kosterlitz-Thouless critical temperature $T_{BKT}<T_c^{MF}$, below which the phases of the pair wave functions become algebraically ordered (for over-review, see, for example, Ref. 28). Since such an order is the only possible order in our system, as it was stated above, we have to set $T_{BKT}=T_c$. As it was mentioned in the Introduction, we use this scenario in order to describe the low-temperature part of the pseudogap phase in some of the HTSCs. It was established experimentally that some of the cuprates demonstrate a strong Nernst effect below a temperature T_0, which is a few orders higher than T_c, and which can be naturally identified with T_c^{MF}. In fact, experimental data suggest that the physical properties of the system in the region of temperature $T_c<T<T_0$ are defined by the phase fluctuations of the order parameter (see Refs. [6,24,25] and references therein). It is necessary to stress that the temperature T_0 is much lower than the upper pseudogap temperature T^*, which is caused by nonsuperconducting effects.[6] Moreover, as it follows from experiments, these two temperatures have different doping dependencies. Namely, T^* grows and T_0 decreases with doping decreasing. As it will be shown below, our results for the doping dependence of T_c^{MF} are in a qualitative agreement with experimental results for the temperature T_0. It is out of the scope of the present paper to describe the temperature region $T_0<T<T_c^*$ of the phase diagram of cuprate superconductors. In this region, the physical properties of the system are defined by nonsuperconducting effects. In particular, some of the researchers believe that the system behavior in this region is dominated by the spin singlet formation.[6] Below, we study the phase diagram of the present model at temperatures $T<T_c^{MF}$.

A. Mean-field critical temperature

To find the doping dependence of the critical temperature T_c^{MF} in the d-wave pairing channel, one needs to solve the finite-temperature version of the set of Eqs. (25) and (26). These equations follow from Eqs. (9), (22), and (24):

$$1 = 4J\sum_{\mathbf{q}} \gamma_d^2(\mathbf{q}) \tanh\left[\frac{\sqrt{\varepsilon^2(\mathbf{q})+\Delta_d^2\gamma_d^2(\mathbf{q})}}{2T}\right]\frac{1}{\sqrt{\varepsilon^2(\mathbf{q})+\Delta_d^2\gamma_d^2(\mathbf{q})}}, \tag{28}$$

$$\delta = \sum_{\mathbf{k}}\left\{1+\tanh\left[\frac{\sqrt{\varepsilon^2(\mathbf{q})+\Delta_d^2\gamma_d^2(\mathbf{q})}}{2T}\right]\frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k})+\Delta_d^2\gamma_d^2(\mathbf{k})}}\right\}. \tag{29}$$

The system of equations for T_c^{MF} and μ' can be obtained from Eqs. (28) and (29) by setting the amplitude of the order parameter equal to zero: $\Delta_d=0$. The solution of the system of these equations shows that the doping dependence of the mean-field critical temperature (Figs. 2–6) has qualitatively the same form as the zero-temperature gap (Fig. 1).

It is important that superconductivity is suppressed at low carrier densities in the d-wave pairing channel at some values of the hopping parameters. To understand this qualitatively, one can notice that at low doping, the function $\gamma_d^2(\mathbf{q})$ in the equation for the mean-field critical temperature [Eq. (28)] can be approximated as $\gamma_{\mathbf{q}} \simeq q^2\cos(2\varphi_{\mathbf{q}})/2 \sim m^*\epsilon_F\cos(2\varphi_{\mathbf{q}_F})/2$, where ϵ_F is the Fermi energy and m^* is an effective quasiparticle mass, which is directly connected with t_2 and t_3 (see Sec. IV B). In this case, Eq. (28) has the form of a standard BSC equation for the critical temperature in the s-wave pairing channel with a renormalized coupling $J\rightarrow Jm^{*2}\epsilon_F^2/4$. Therefore, the mean-field critical temperature is an exponentially small function of the square of the carrier density $\delta^2\sim\epsilon_F^2$ in this case.

In Figs. 2–6, we present the doping dependence of the mean-field critical temperature at different values of t_2, t_3, and J. As it follows from these figures, the critical value of the doping, below which superconductivity is suppressed, grows with decreasing J. Also, it grows with increasing t_2 at fixed t_3 and with increasing t_3 at fixed t_2.

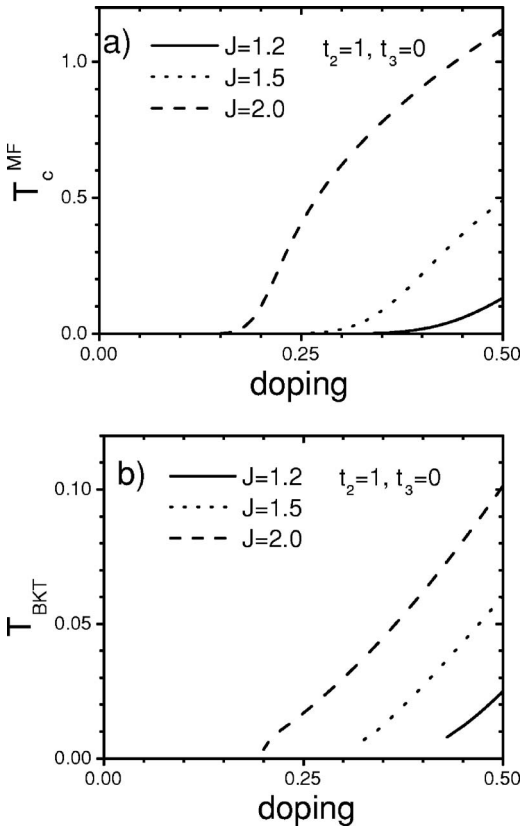

FIG. 2. The mean-field (a) and the BKT (b) critical temperatures as functions of the carrier density at $t_2=1$, $t_3=0$, and different values of J.

B. Critical temperature

In order to study the BKT transition in the system, it is necessary to consider the superconducting order parameter transfer phase fluctuations. The phase of the order parameter $\theta_{\mathbf{nm}}$ can be introduced in analogy with the fermion case, when the fermion operator can be presented as a product of a neutral fermion operator $\chi(\tau,\mathbf{n})$ and its phase $\exp[i\theta(\tau,\mathbf{n})/2]$ (see, for example, Ref. 28). In our case:

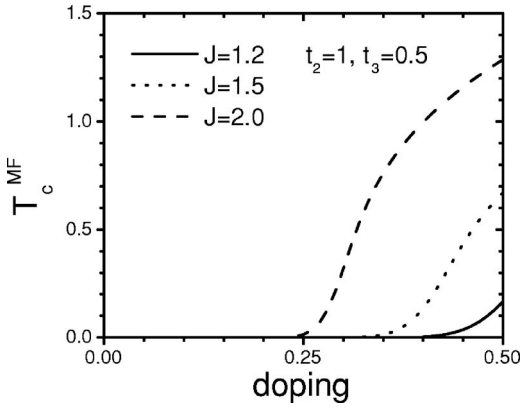

FIG. 3. The doping dependence of the mean-field critical temperature T_c^{MF} at $t_2=1$, $t_3=0.5$, and different values of J.

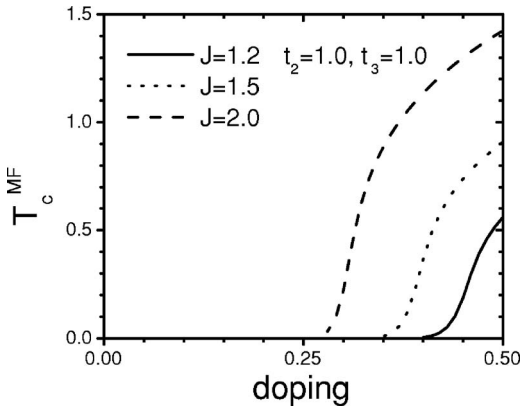

FIG. 4. The mean-field critical temperature T_c^{MF} as a function of the carrier density at $t_2=1$, $t_3=1$, and different values of J.

$$X_{\mathbf{n}}^{2,1/2} = (X_{\mathbf{n}}^{1/2,2})^{\dagger} = \chi(\tau,\mathbf{n})\exp[i\theta(\tau,\mathbf{n})/2].$$

In this case, the superconducting order parameter can be presented as a product of its amplitude and phase:

$$\langle X_{\mathbf{n}}^{2,1/2} X_{\mathbf{m}}^{2,1/2}\rangle = \delta_{\mathbf{n},\mathbf{m}+\rho}\Delta_{\mathbf{nm}}\exp(i\theta_{\mathbf{nm}}). \tag{30}$$

It can be shown that the phase dependence of the thermodynamic potential of the fermion system with the Green function [Eq. (23)] and the gap function [Eq. (30)] in the

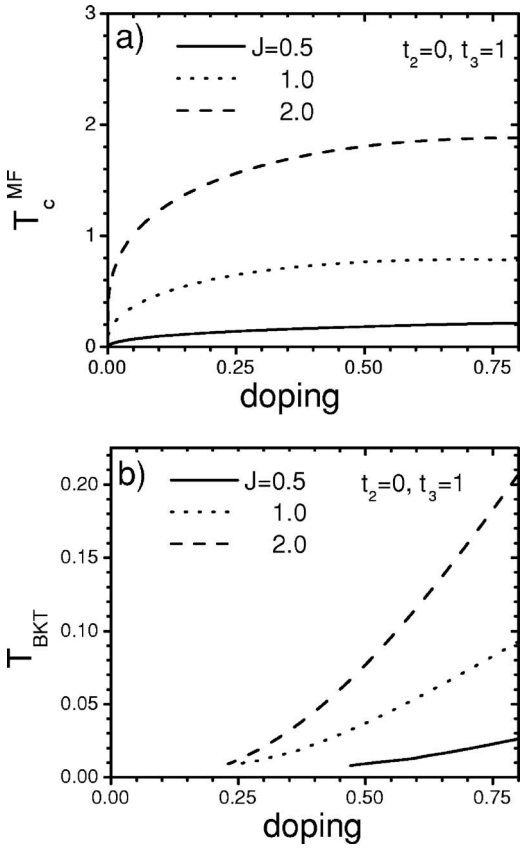

FIG. 5. The mean-field (a) and the BKT (b) critical temperatures as functions of doping at zero hopping parameter t_2 and different values of coupling J.

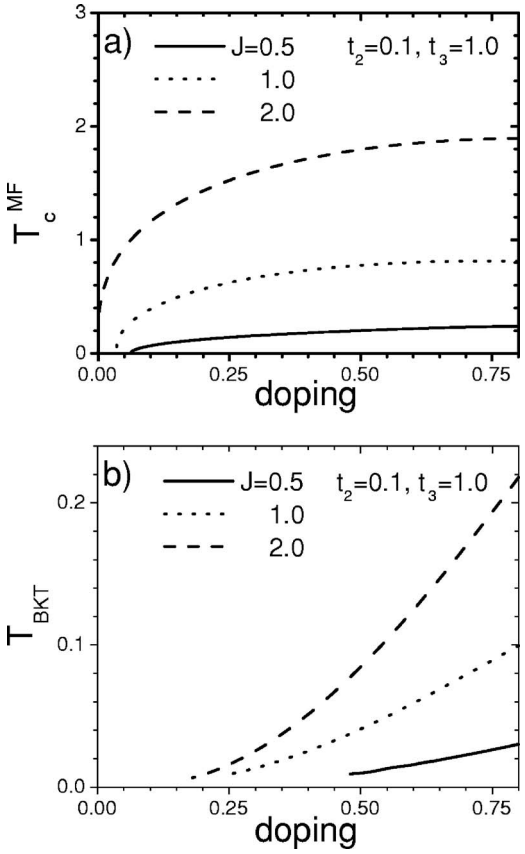

FIG. 6. The mean-field (left) and the BKT (right) critical temperatures as functions of doping in the case of small but nonzero hopping parameter t_2 and different values of coupling J.

limit of small fluctuations of the phase of the order parameter is equal to

$$\Omega(\Delta,\theta)=\frac{\mathcal{J}}{2}\int d^2r(\nabla\theta)^2, \tag{31}$$

where the stiffness in the long-wave limit is

$$\mathcal{J}=\frac{\delta}{4m^*}-\frac{1}{16m^{*2}}\frac{1}{T}\int\frac{d^2k}{(2\pi)^2}\frac{\mathbf{k}^2}{\cosh^2[\sqrt{\varepsilon(\mathbf{k})^2+\Delta_d^2\gamma_d^2(\mathbf{k})}/2T]}. \tag{32}$$

(see, for example, Ref. 29). In our case, the effective mass of the free quasiparticles is $m^*=1/[4(t_2+2t_3)]$.

In analogy with the two-dimensional spin XY model,[30] the equation for the BKT transition critical temperature, below which the phases of order parameter (the spin orientation in the XY-model case) become algebraically ordered, has the following form:

$$T_c=\frac{\pi}{2}\mathcal{J}(\Delta_d,\mu',T_c), \tag{33}$$

where function $\mathcal{J}$ is defined in Eq. (32).

The doping dependence of the superconducting critical temperature T_c can be found by solving the system of Eqs. (28), (29), and (33). The solution of this set of equations at different values of the interaction shows that the doping dependence of T_c has qualitatively the same form as the doping dependence of T_c^{MF} (Figs. 2, 5, and 6). It is possible to study some limiting cases of the solution of Eq. (33) analytically. In particular, in the limit of rather large carrier densities, when $\Delta_d \ll T_c$ (T_c is close to T_c^{MF}), one can make an expansion in powers of Δ_d/T_c on the right-hand side of Eq. (33). In this case, this equation transforms to

$$T_c^3=A\Delta_d^2(T_c)\delta^3/m^*, \tag{34}$$

where $A\simeq\pi^3/128$. Since the gap parameter depends on the critical temperature as $\Delta_d(T)=\Delta_d(0)[1-(T/T_c^{MF})^2]^{1/\alpha}$, where $\alpha\geqslant 1$, at temperatures close to the mean-field critical temperature ($\alpha\to 2$ at $T\to T_c^{MF}$),[31] the solution of Eq. (34) is

$$T_c\simeq T_c^{MF}\left\{1-\frac{1}{2}\left[\frac{m^*(T_c^{MF})^3}{A\Delta_d^2(0)}\right]^{\alpha/2}\frac{1}{\delta^{3\alpha/2}}\right\}. \tag{35}$$

In other words, the critical temperature approaches the mean-field critical temperature as the doping increases at large carrier densities. It is interesting that Eq. (34) is also valid in the limit of low carrier concentrations when both critical temperatures are suppressed. Therefore, the second term in Eq. (32) is important at any carrier concentration in the d-wave pairing channel, contrary to the s-pairing case, where this term can be omitted at low values of δ which gives $T_c\sim\delta$.

It is important that the amplitude of T_c is much smaller than T_c^{MF}, and the pseudogap region $T_c<T<T_c^{MF}$ is rather large in this case (Figs. 2–6). This is similar to the phase diagram of cuprates, where there is a large pseudogap region above the critical temperature at low carrier densities. It must be stressed that in the case of higher carrier densities, one must consider a model with a more complicated effective interaction compared to Eq. (6). Also, as it was mentioned above, in this paper, we take into account only superconducting order parameter phase fluctuations in order to describe the pseudogap phase of cuprates. Therefore, we are able to describe only the lower part of the pseudogap phase with a critical temperature T_0, which we identify with T_c^{MF}. Our results are in qualitative agreement with experimental results on some cuprates (see, for example, Fig. 20 in Ref. 24). As it was mentioned in Ref. 16, in order to describe experimental spectra, one needs to choose $t_2\ll t_3$. This condition, together with the requirement to get superconductivity to develop at $\delta\simeq 0.05$, can be satisfied if one chooses $t_2\sim 0.1t_3$. In order to make a qualitative comparison with experiments, we use this condition together with an estimated value of $t_3\sim 0.1$ eV and the effective coupling $J\sim 0.5t_3\sim 0.05$ eV. The last estimation can be obtained by choosing the coupling of order of the antiferromagnetic bond energy. This energy has the order of the antiferromagnetic critical temperature of the undoped cuprates, $\sim$300–400 K. The results for the gap and for the critical temperatures for this choice of the parameters are presented in Figs. 1 and 6, correspondingly. As it follows from these figures, the model gives correct amplitudes for the values of the gap parameter ($\sim 0.1t_3\sim 0.01$ eV), but it seems to give an underestimated value for T_c ($\sim 0.01t_3\sim 0.001$ eV) at dopings higher but close to the optimal one

($\delta \sim 0.16$). Another important set of experimental data, which can be compared with our theoretical results, is the ratio of the $2\Delta_d(T=0)/T_c$, which was estimated for the optimally doped cuprates to be equal approximately to 5.5.[33] Our numerical calculations show that this ratio is 2 orders of magnitude larger in the case of realistic parameters given in Fig. 6 [actually, in our case, the ratio is $4\Delta_d(T=0)/T_c$, since the maximal value of the gap is $2\Delta_d(T=0)$]. However, it must be noted that the model in Eq. (7) was derived for the underdoped regime, i.e., at doping values smaller than ~ 0.16. It would be really important to have a trustable set of experimental data for this ratio in the underdoped case at different values of doping in order to test the model. Interestingly, we have found that the ratio $4\Delta_d(T=0)/T_c^{MF}$ changes from approximately 3.5 to 5 when coupling increases for the parameters given in Fig. 6. This value is of the order of the experimental result, 5.5 (see also Ref. 31). In order to make a quantitative comparison with the experiments at higher values of doping, the model Hamiltonian [Eq. (7)] must be modified. In particular, one needs to take into account the NN hopping parameter t_1, which can be set to equal zero in undoped cuprates but which grows with the doping increasing.[16] The doping dependence of t_1 is a separate complicated problem, which is planned to be studied in the future.

V. CONCLUSIONS

To conclude, we have studied the superconducting properties of an effective model introduced in Ref. 16 in order to describe low carrier density properties of some HTSCs. It was shown that the d-wave pairing superconductivity in this model exists when the carrier density is larger than some critical value. This critical value strongly depends on the interaction energy, and it is growing with the interaction decreasing. The amplitude of the lower (superconducting) pseudogap temperature $T_c^{MF} \equiv T_0$ is almost an order of magnitude larger than the value of the critical temperature T_c. Though this result is in a qualitative agreement with experiments on some cuprates,[24] it seems to be overestimated for other systems. This and some other open issues must be resolved. In particular, it is important to understand the origin of the higher pseudogap temperature T^*, which is defined by nonsuperconducting effects. Currently, we are studying this problem by taking into account spin fluctuations in the model at high temperatures. The results will be presented in future publications. Another important problem is how to generalize the results on the case of larger carrier densities, when the antiferromagnetic sublattice breaks down and it is not enough to set the attraction to be equal to the antiferromagnetic bond energy J. The effective antiferromagnetic attraction decreases in this case. Also, the doping increase is accompanied by increase of the number of scattering centers created by dopants, which also leads to a suppression of superconductivity (see, for example, Ref. 31). Another important problem, which is widely discussed nowadays, is the possibility of a nonhomogeneous superconductivity in cuprates (see, e.g., Ref. 34 and references therein). It is also necessary to estimate pairings in other channels with different symmetries of the order parameter. These and some other questions are planned to be studied in the framework of the model discussed in this paper in the near future.

*Electronic address: vloktev@bitp.kiev.ua
†Electronic address: turkowskiv@missouri.edu

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