Superconductivity in a narrow-band system with intersite electron pairing in two dimensions: A mean-field study

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We study a simple model for superconductivity based on the extended Hubbard model with on-site repulsive and intersite attractive interactions for arbitrary electron density using the mean-field approach. We perform detailed numerical studies of anisotropic superconductivity of s, p, and d type for the two-dimensional square lattice with nearest- and next-nearest-neighbor hopping. For a nearly half-filled band the d-wave pairing is most stable. p-wave and then extended s-wave pairings become stable upon decreasing the band filling. While T_c for d- and p-wave pairings smoothly decrease with band filling, s-wave pairing shows strong nonmonotonic behavior of T_c versus electron density. Inclusion of next-nearest-neighbor hopping changes essentially the behavior of T_c and the mutual stability of anisotropic pairings. The competition between superconductivity and the spin-density-wave state is studied. The question of the transition from Cooper pairs to intersite pairs and their Bose condensation is discussed. We also consider the limit of strong correlations and its connection with recent theoretical proposals for the superconductivity in high-T_c oxides. Our findings are discussed in connection with the experimental studies of superconductivity and magnetism in La_2CuO_4-based compounds.

I. INTRODUCTION

The recent discovery of superconducting materials with unexpectedly high transition temperatures[1] has led theorists to seriously reconsider the physical properties of the Hubbard model and its extensions, mainly for the following reason. The new high-T_c superconductors belong to the transition-metal oxides family for which it has been known for some time that a tight-binding approach with strong electron-electron correlations is a more appropriate picture than that of nearly-free-electron metals. The success of the Hubbard model so far concerns primarily the explanation of the magnetic properties of the oxides. The strong polarizability of the oxygens leading to small polaron and bipolaron formation in some of the transition-metal oxides, such as Ti_4O_7 and $Na_xV_2O_5$, could be accounted for by adding to the Hubbard model an electron-lattice coupling. Such electron-lattice coupling results in short-range attractive interaction between the tight-binding electrons. This lattice-induced attractive interaction competes with the repulsive Coulomb interaction and can lead to an overall short-ranged attractive interaction[2-9] which can be modeled by the extended Hubbard Hamiltonian

$$H=\sum_{ij\sigma}(t_{ij}-\mu\delta_{ij})c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}+\frac{1}{2}\sum_{ij\sigma\sigma'}W_{ij}n_{i\sigma}n_{j\sigma'} \tag{1.1}$$

with an attractive ($W<0$) intersite interaction. t_{ij} denotes the transfer integral, μ the chemical potential, and U the renormalized Hubbard on-site Coulomb interaction. The number operator $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. The model (1.1) can be considered as rather general, resulting from a system of narrow-band electrons strongly coupled to a boson field which they polarize, and which in turn acts onto the electrons thereby forming entirely new entities. These new entities are described by a correlated motion of the electrons and their surrounding polarization field and by an induced short-range attraction which can compete with the Coulomb repulsion. The bosonic modes can be phonons, excitons, acoustic plasmons, etc. The induced attractive potential can partially overcome the Coulomb repulsion. This then gives rise to the formation of on-site pairs of electrons if the coupling is strong enough to overcome the Hubbard U.[3,7] For less strong coupling (intermediate-coupling regime) one has essentially intersite pairing due to the short-range effective interaction and on-site as well as long-range Coulomb repulsion.[4,6] Finally, the attractive intersite interaction can also arise from purely electronic mechanisms (chemical bonding) such as possible peroxide formation in the new high-T_c superconducting oxides. This simple extended Hubbard model [Eq. (1.1)] permits one to treat magnetic and superconducting correlations on the basis of a concise model with a minimum of parameters. We believe that such a model might be relevant for the new high-T_c materials where magnetic correlations and superconductivity can be closely linked if not intimately related. The physical origin of electron pairing in the present model is different from the resonating-valence-bond[10] (RVB) picture. Nevertheless, the conclusions about the thermodynamic properties of the present model derived in this paper in the strong correlation limit $U\gg t$ are similar to the ones conjectured for RVB.

The major objective of this paper is to study the superconductivity of a system with intersite pairing. This is different from both the Cooper pairing in the Bardeen-Cooper-Schrieffer (BCS) theory and its extreme opposite, the superconductivity of local pairs which has been derived on the basis of a Hubbard model with $U<0$.[4,7-9] Our study will be concerned with a two-dimensional (2D) square lattice employing the usual type of random phase approximation (RPA) for superconductivity assuming nearest-neighbor attractive interaction. Superconductivity in two dimensions due to intersite attraction represents a problem of fundamental importance, in particular with regard to the formation of intersite pairs and eventually their Bose condensation. Many of the recent theoretical propositions[10-13] for the new high-T_c materials intrinsically contain such an idea of a Bose condensation. The model proposed here is certainly also relevant for heavy-fermion systems[14,15] and perhaps ^{3}He (Ref. 16) and spin-polarized fermions on a lattice.[17] The paper is organized in the following way. In Sec. II we present the mean-field formalism within the framework of a broken-symmetry Hartree-Fock approach, appropriate for the weak- (intermediate-) coupling regime, i.e., $8t>U$. Our approach is similar to previous works on heavy-fermion systems which, however, were limited to three-dimensional systems and essentially to the half-filled-band case.[14,15] In Sec. III we give a detailed discussion of the various anisotropic s-, p-, and d-wave pairings and the spin-density-wave state. This will be done for the square lattice with nearest-neighbor hopping and arbitrary band filling. The effects of next-nearest-neighbor hopping on the anisotropic superconductivity will be studied in Sec. IV. In Sec. V we briefly discuss the limit of strong electron correlations $U/t\gg 1$. In Sec. VI, we comment on the relation of the present model to both BCS and local pair superconductivity, and discuss the possible relevance of this model to high-T_c superconducting oxides.

II. MEAN-FIELD THEORY

Within the framework of the broken-symmetry Hartree-Fock approach the mean-field Hamiltonian including the spin-density-wave (SDW) ordering, the singlet superconductivity, and the triplet superconductivity is given by

$$\begin{aligned}\tilde{H}=&\sum_{\mathbf{k}\sigma}A_{\mathbf{k}}^{\sigma}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}-Um_{\mathbf{Q}}\sum_{\mathbf{k}\sigma}\sigma c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}+\mathbf{Q},\sigma}\\&-\sum_{\mathbf{k}}(\Delta_{\mathbf{k}}c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}+\text{H.c.})\\&-\tfrac{1}{2}\sum_{\mathbf{k}\sigma}[\Delta_t^{\sigma}(\mathbf{k})c_{\mathbf{k}\sigma}^{\dagger}c_{-\mathbf{k}\sigma}^{\dagger}+\text{H.c.}]+C\ ,\end{aligned}\tag{2.1}$$

where

$$A_{\mathbf{k}}^{\sigma}=\varepsilon_{\mathbf{k}}-\frac{1}{N}\sum_{\mathbf{q}}W_{\mathbf{k}-\mathbf{q}}\langle c_{\mathbf{q}\sigma}^{\dagger}c_{\mathbf{q}\sigma}\rangle-\bar{\mu}\ ,\tag{2.2a}$$

$$\bar{\mu}=\mu-n(U/2+W_0)\ ,\tag{2.2b}$$

where n is the number of electrons per lattice site.

The gap function for the singlet pairing is

$$\Delta_k=\frac{1}{N}\sum_{\mathbf{q}}V_{\mathbf{kq}}^{s}\langle c_{-\mathbf{q}\downarrow}c_{\mathbf{q}\uparrow}\rangle\ ,\tag{2.3a}$$

where

$$V_{\mathbf{kq}}^{s}=-U-W_{\mathbf{k}-\mathbf{q}}\ .\tag{2.3b}$$

The gap function for the triplet pairing is

$$\Delta_t^{\sigma}(\mathbf{k})=\frac{1}{N}\sum_{\mathbf{q}}V_{\mathbf{kq}}^{t}\langle c_{-\mathbf{q}\sigma}c_{\mathbf{q}\sigma}\rangle\tag{2.4}$$

and

$$V_{\mathbf{kq}}^{t}=\tfrac{1}{2}(W_{\mathbf{k}+\mathbf{q}}-W_{\mathbf{k}-\mathbf{q}})\ .\tag{2.5}$$

The SDW order parameter is given by

$$m_{\mathbf{Q}}=\frac{1}{2N}\sum_{\mathbf{k}\sigma}\sigma\langle c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}+\mathbf{Q}\sigma}\rangle\ ,\tag{2.6}$$

where $\mathbf{Q}$ is half the reciprocal-lattice vector, $W_{\mathbf{k}}$ is the Fourier transform of W_{ij}, and $W_{\mathbf{k}}=W\gamma_{\mathbf{k}}$, where $\gamma_{\mathbf{k}}=\sum_{\delta}e^{-i\mathbf{k}\cdot\delta}$ with δ representing the vectors linking nearest neighbors. C is a constant arising from the Gorkov-type factorization and is given by

$$\begin{aligned}C=&-NU(\tfrac{1}{4}n^2-m_{\mathbf{Q}}^2)-\frac{U}{N}\sum_{\mathbf{kq}}\langle c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}\rangle\langle c_{\mathbf{q}\downarrow}c_{-\mathbf{q}\uparrow}\rangle\\&+\frac{1}{2N}\sum_{\mathbf{kq}\sigma\sigma'}W_{\mathbf{k}-\mathbf{q}}\langle c_{\mathbf{k}\sigma}^{\dagger}c_{-\mathbf{k}\sigma'}^{\dagger}\rangle\langle c_{-\mathbf{q}\sigma}c_{\mathbf{q}\sigma'}\rangle\\&-\tfrac{1}{2}W_0n^2N+\frac{1}{2N}\sum_{\mathbf{kq}\sigma}W_{\mathbf{k}-\mathbf{q}}\langle c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}\rangle\langle c_{\mathbf{q}\sigma}^{\dagger}c_{\mathbf{q}\sigma}\rangle\end{aligned}\tag{2.7}$$

and N is the total number of lattice sites. In the following section we give the solutions for the pure phases only.

A. Singlet-superconducting phase

The gap equation has the following form:

$$\Delta_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{q}}V_{\mathbf{kq}}^{s}\Delta_{\mathbf{q}}F_{\mathbf{q}}\ ,\tag{2.8}$$

where

$$F_{\mathbf{q}}=(2E_{\mathbf{q}})^{-1}\tanh(\beta E_{\mathbf{q}}/2)\ ,\tag{2.9}$$

$$E_{\mathbf{q}}=\sqrt{\bar{\varepsilon}_{\mathbf{q}}^2+|\Delta_{\mathbf{q}}|^2}\ ,\tag{2.10}$$

$$\bar{\varepsilon}_{\mathbf{q}}=\varepsilon_{\mathbf{q}}+p|W|\gamma_{\mathbf{q}}/\gamma_0-\bar{\mu}\ ,$$

$$\varepsilon_{\mathbf{q}}=-t\gamma_{\mathbf{q}}\ ,\tag{2.11}$$

$$V_{\mathbf{kq}}^{s}=-U+|W|\gamma_{\mathbf{k}-\mathbf{q}}\ .$$

$E_{\mathbf{q}}$ denotes the quasiparticle energy and $\beta=1/k_BT$. The Fock parameter

$$p=\frac{1}{N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}\langle c_{\mathbf{q}\sigma}^{\dagger}c_{\mathbf{q}\sigma}\rangle\ ,\tag{2.12}$$

and the chemical potential μ satisfy

$$p=-\frac{1}{N}\sum_{\mathbf{q}}\bar{\varepsilon}_{\mathbf{q}}\gamma_{\mathbf{q}}F_{\mathbf{q}}\ ,\tag{2.13}$$

$$n-1=-\frac{2}{N}\sum_{\mathbf{q}}\bar{\varepsilon}_{\mathbf{q}}F_{\mathbf{q}}\ .\tag{2.14}$$

The free energy is given by

$$\frac{F}{N}=\tfrac{1}{4}(U-2|W|\gamma_0)n^2+\bar{\mu}(n-1)-|W|p^2/\gamma_0 +\frac{1}{N}\sum_{\mathbf{k}}\frac{|\Delta_{\mathbf{k}}|^2}{2E_{\mathbf{k}}}\tanh(\beta E_{\mathbf{k}}/2) -\frac{2}{\beta N}\sum_{\mathbf{k}}\ln[2\cosh(\beta E_{\mathbf{k}}/2)] \ . \tag{2.15}$$

The pairing potential $V^{\xi}_{\mathbf{kq}}$ takes on the separable form in $d=2$ for the square lattice and the nearest-neighbor interaction

$$V^{\xi}_{\mathbf{kq}}=-U+\frac{|W|}{4}(\gamma_{\mathbf{k}}\gamma_{\mathbf{q}}+\eta_{\mathbf{k}}\eta_{\mathbf{q}}) +2|W|(\sin k_x\sin q_x+\sin k_y\sin q_y) \ , \tag{2.16}$$

where $\gamma_{\mathbf{k}}=2(\cos k_x+\cos k_y)$ and $\eta_{\mathbf{k}}=2(\cos k_x-\cos k_y)$. Equation (2.8) can be solved by an ansatz

$$\Delta_{\mathbf{k}}=\Delta_0+\Delta_\gamma\gamma_{\mathbf{k}}+\Delta_\eta\eta_{\mathbf{k}} \ , \tag{2.17}$$

where the particular terms refer to on-site extended s-wave and d-wave pairing, respectively. The self-consistent equations are

$$\Delta_0=-U\phi_1 \ , \tag{2.18a}$$

$$\Delta_\gamma=\frac{|W|}{4}\phi_\gamma \tag{2.18b}$$

for the s-wave pairing, and

$$\Delta_\eta=\tfrac{1}{4}|W|\phi_\eta \tag{2.18c}$$

for the d-wave pairing.

In Eqs. (2.18a)–(2.18c),

$$\phi_1=\frac{1}{N}\sum_{\mathbf{q}}\Delta_{\mathbf{q}}F_{\mathbf{q}},\quad \phi_\gamma=\frac{1}{N}\sum_{\mathbf{q}}\Delta_{\mathbf{q}}\gamma_{\mathbf{q}}F_{\mathbf{q}},\quad \phi_\eta=\frac{1}{N}\sum_{\mathbf{q}}\Delta_{\mathbf{q}}\eta_{\mathbf{q}}F_{\mathbf{q}} \ .$$

The transition temperature for the onset of pure s-wave pairing is given by

$$\begin{pmatrix} 1+U\phi_1(T_c) & U\phi_2(T_c) \\ -\frac{|W|}{4}\phi_2(T_c) & 1-\frac{|W|}{4}\phi_\gamma(T_c)\end{pmatrix}\begin{pmatrix}\Delta_0\\ \Delta_\gamma\end{pmatrix}=0 \ , \tag{2.19a}$$

where

$$\phi_1(T_c)=\frac{1}{N}\sum_{\mathbf{q}}F_{\mathbf{q}}(T_c) \ , \tag{2.19b}$$

$$\phi_2(T_c)=\frac{1}{N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}F_{\mathbf{q}}(T_c) \ , \tag{2.19c}$$

$$\phi_\gamma(T_c)=\frac{1}{N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}^2F_{\mathbf{q}}(T_c) \ , \tag{2.19d}$$

and

$$F_{\mathbf{q}}(T_c)=(2\bar{\varepsilon}_{\mathbf{q}})^{-1}\tanh(\beta_c\bar{\varepsilon}_{\mathbf{q}}/2) \ . \tag{2.20}$$

T_c for the d-wave pairing is

$$\frac{4}{|W|}=\frac{1}{N}\sum_{\mathbf{q}}\eta_{\mathbf{q}}^2F_{\mathbf{q}}(T_c) \ . \tag{2.21}$$

Notice that the strict separation of the transition temperatures implies that T_c for d-wave pairing is independent of U. An ansatz of the form of Eq. (2.17) amounts to neglecting the relative phases of d- and s-wave order parameters, and hence is not the most general one.[18] Such a phase coupling could be of importance for studying the mixed s-d wave state below T_c.

B. Equal-spin (triplet) pairing

We consider here the case of $|\Delta_t^{\uparrow}|=|\Delta_t^{\downarrow}|$ and require $\Delta_t^{\uparrow}(\mathbf{k})=\Delta_t(\mathbf{k})$, $\Delta_t^{\downarrow}(\mathbf{k})=\Delta_t^*(\mathbf{k})$.[19] Indeed $\Delta_t(\mathbf{k})=-\Delta_t(-\mathbf{k})$. The self-consistent equation for $\Delta_t(\mathbf{k})$ is

$$\Delta_t(\mathbf{k})=\frac{1}{N}\sum_{\mathbf{q}}V^{t}_{\mathbf{kq}}\Delta_t(\mathbf{q})F_{\mathbf{q}} \ , \tag{2.22}$$

where $F_{\mathbf{q}}$ is given by (2.9) and

$$E_{\mathbf{q}}=\sqrt{\bar{\varepsilon}_{\mathbf{q}}^2+|\Delta_t(\mathbf{q})|^2},\quad V^{t}_{\mathbf{kq}}=\tfrac{1}{2}(W_{\mathbf{k}+\mathbf{q}}-W_{\mathbf{k}-\mathbf{q}}) \ . \tag{2.23}$$

The equations for p and μ are the same as for the singlet pairing; moreover, the free energy takes on the form of Eq. (2.15) if $\Delta_{\mathbf{k}}$ is replaced by $\Delta_t(\mathbf{k})$. For the $d=2$ square lattice one obtains after substituting $\Delta_t(\mathbf{k})=\Delta_x^p\sin k_x+\Delta_y^p\sin k_y$:

$$\Delta_\alpha^p=\frac{2|W|}{N}\sum_{\mathbf{q}}\sin^2(q_\alpha)\Delta_{\mathbf{q}}^pF_{\mathbf{q}},\quad \alpha=x,y \tag{2.24}$$

with $\Delta\mathbf{q}^p$ having p-like character. T_c for the onset of p-wave pairing is determined by

$$\frac{1}{2|W|}=\frac{1}{N}\sum_{\mathbf{q}}\sin^2(q_x)F_{\mathbf{q}}(T_c) \ , \tag{2.25}$$

where $F_{\mathbf{q}}(T_c)$ is given by Eq. (2.20).

C. SDW state

The order parameter m_Q is given by

$$m_{\mathbf{Q}}=\frac{Um_{\mathbf{Q}}}{4N}\sum_{\mathbf{q}}\frac{1}{x_{\mathbf{q}}}[\tanh(\beta E_{\mathbf{q}}^+/2)-\tanh(\beta E_{\mathbf{q}}^-/2)] \ . \tag{2.26}$$

The chemical potential satisfies

$$n-1=-\frac{1}{2N}\sum_{\mathbf{q}}[\tanh(\beta E_{\mathbf{q}}^+/2)+\tanh(\beta E_{\mathbf{q}}^-/2)] \ , \tag{2.27}$$

where the quasiparticles energies are given by

$$E_{\mathbf{q}}^{\pm}=\tfrac{1}{2}(\bar{\varepsilon}_{\mathbf{q}}+\bar{\varepsilon}_{\mathbf{q}+\mathbf{Q}})\pm x_{\mathbf{q}} \ , \tag{2.28a}$$

$$x_{\mathbf{q}}=\sqrt{\tfrac{1}{4}(\bar{\varepsilon}_{\mathbf{q}}-\bar{\varepsilon}_{\mathbf{q}+\mathbf{Q}})^2+U^2m_{\mathbf{Q}}^2} \ , \tag{2.28b}$$

and $\bar{\varepsilon}_{\mathbf{q}}=\varepsilon_{\mathbf{q}}+p|W|\gamma_{\mathbf{q}}|/\gamma_0-\bar{\mu}$. The Fock parameter satisfies the equation

$$p=-\frac{1}{2N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}[\tanh(\beta E_{\mathbf{q}}^+/2)+\tanh(\beta E_{\mathbf{q}}^-/2)] +\frac{1}{4N}\sum_{\mathbf{q}}\frac{\gamma_{\mathbf{q}}(\bar{\varepsilon}_{\mathbf{q}}-\bar{\varepsilon}_{\mathbf{q}+\mathbf{Q}})}{x_{\mathbf{q}}}[\tanh(\beta E_{\mathbf{q}}^-/2) -\tanh(\beta E_{\mathbf{q}}^+/2)] \ . \tag{2.29}$$

The free energy is given by

$$\frac{F}{N}=\tfrac{1}{4}(U-2|W|\gamma_0)n^2+\bar{\mu}(n-1)-|W|p^2/\gamma_0+Um_Q^2 -\frac{1}{\beta N}\sum_{\mathbf{q}}\{\ln[2\cosh(\beta E_{\mathbf{q}}^{+}/2)] +\ln[2\cosh(\beta E_{\mathbf{q}}^{-}/2)]\} . \quad (2.30)$$

In the above equations summation over $\mathbf{q}$ is not restricted to the inner half of the Brillouin zone. The equation for the transition temperature T_N is obtained upon assumption of the continuous transition, i.e., $m_Q \to 0$. For the $d=2$ lattice such a transition has only formal meaning within the mean-field theory, at least for finite-range hopping, since the fluctuations destroy the SDW ordering for any $T\neq 0$, and no transition is allowed even in the Kosterlitz-Thouless sense. Interplanar couplings, however, can easily stabilize the SDW state. Another view is that the range of nonzero solutions for SDW's indicates the role of the spin fluctuations. T_N is determined by

$$\frac{1}{U}=\frac{1}{N}\sum_{q}\left(\frac{1}{\bar{\varepsilon}_{\mathbf{q}}-\bar{\varepsilon}_{\mathbf{q}+\mathbf{Q}}}\right)\tanh\left(\frac{\beta_N\bar{\varepsilon}_{\mathbf{q}}}{2}\right) \quad (2.31)$$

together with μ and p which are given by Eqs. (2.13) and (2.14) with $F_q(T_N)=(2\bar{\varepsilon}_{\mathbf{q}})^{-1}\tanh(\beta_N\bar{\varepsilon}_{\mathbf{q}}/2)$.

Finally, for the nonordered state we have the following set of equations:

$$\frac{F}{N}=\tfrac{1}{4}(U-2|W|\gamma_0)n^2+\bar{\mu}(n-1)-|W|p^2/\gamma_0 -\frac{2}{\beta N}\sum_{\mathbf{q}}\ln[2\cosh(\beta\bar{\varepsilon}_{\mathbf{q}}/2)] ,$$
$$n-1=-\frac{2}{N}\sum_{\mathbf{q}}\bar{\varepsilon}_{\mathbf{q}}F_{\mathbf{q}}(T) , \quad (2.32)$$
$$p=-\frac{1}{N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}\bar{\varepsilon}_{\mathbf{q}}F_{\mathbf{q}}(T) ,$$

where $F_{\mathbf{q}}(T)=(2\bar{\varepsilon}_{\mathbf{q}})^{-1}\tanh(\beta\bar{\varepsilon}_{\mathbf{q}}/2)$. In the subsequent sections we shall analyze these different types of orderings for the case of nearest- and next-nearest-neighbor hopping.

III. THE NEAREST-NEIGHBOR HOPPING

In the case of the nearest-neighbor hopping $\varepsilon_{\mathbf{k}}=-t\gamma_{\mathbf{k}}$, where $\gamma_{\mathbf{k}}=2(\cos k_x+\cos k_y)$ for $d=2$.[20] The density of states (DOS) $\rho(\varepsilon)$ is then given by

$$\rho(\varepsilon)=\frac{1}{N}\sum_{\mathbf{k}}\delta(\varepsilon-\varepsilon_{\mathbf{k}})=\frac{2}{D\pi^2}K(1-(\varepsilon/D)^2) , \quad (3.1)$$

where $|\varepsilon|\leq D$, and $D=4t$ is the half-bandwidth and K is the complete elliptic integral of the first kind. The DOS exhibits the Van Hove's singularity at $\varepsilon=0$ and $\rho(\varepsilon)$ for $\varepsilon\approx 0$ takes the following form:

$$\rho(\varepsilon)\cong\frac{2}{D\pi^2}\ln\left|\frac{4D}{\varepsilon}\right| . \quad (3.2)$$

Furthermore, we shall present the results for T_c as a function of the band filling for different values of U and W. These results are obtained from the numerical analysis and where it was possible by analytical solutions. In these analyses the Fock parameter has been neglected.

Let us first consider the half-filled band case. For $n=1$, $\bar{\mu}=0$ and T_c for the different pairings can readily be determined from Eqs. (2.19)–(2.21) and (2.25). For $U>0$, the only s-wave pairing is the extended s-wave pairing and T_c is given by

$$\frac{4}{|W|}=\frac{1}{N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}^2F_{\mathbf{q}}(T_c) . \quad (3.3)$$

From Eqs. (3.3) and (2.20) it follows that this pairing can occur for $|W|/D\geq\pi^2/8$ only. For $U<0$, one has the on-site s pairing,

$$\frac{1}{|U|}=\frac{1}{N}\sum_{\mathbf{q}}F_{\mathbf{q}}(T_c) , \quad (3.4)$$

with $F_{\mathbf{q}}(T_c)$ given by (2.20). Upon using the logarithmic approximation for the DOS, Eq. (3.2), one gets

$$\frac{1}{|U|}=\frac{1}{D\pi^2}\left[\ln^2\left(\frac{D}{2k_BT_c}\right) +2\ln\left(\frac{16e^{\gamma}}{\pi}\right)\ln\left(\frac{D}{2k_BT_c}\right)+4.26\right] , \quad (3.5)$$

where $\gamma=0.577$, which can be solved to yield approximate T_c for the on-site pairing

$$k_BT_c/D=0.5\exp[-(\pi^2D/|U|-0.601)^{1/2}+2.205] . \quad (3.6)$$

Equation (3.6) shows an enhancement of T_c due to Van Hove's singularity in two dimensions, i.e., $T_c\sim\exp(-\pi\sqrt{D/U})$, while for $d=3$, $T_c\sim\exp(-D/|U|)$. As far as d-wave and p-wave pairings are concerned, the corresponding equations for T_c for $n=1$ are given by (2.21) and (2.25), and T_c is independent of U. On performing the low-T_c (weak-coupling) and high-T_c (strong-coupling) expansions we obtained that T_c for the p- and d-wave pairings exist from the origin $W/D=0$ onwards and increase with increasing $|W|/D$. The d-wave pairing is the most stable one, as it gives the highest T_c for any given $|W|/D$.

In Fig. 1 we present the numerical solution for T_c of s-, p-, and d-wave pairings. The necessary lattice sums were performed by direct numerical integration or with the use of the exact DOS [Eq. (3.1)].

In Fig. 2 we give a preliminary ground-state phase diagram for the extended Hubbard model in two dimensions for $n=1$, based on the analysis of critical temperatures for pure phases. For $U>0$ and $W>0$ there are only two phases possible: the charge-density wave (CDW) and the SDW which are separated by the line $U=4W$. For $U<0$, the CDW and singlet-superconducting state (SS) (on-site pairing) meet at $W=0$. For $W<0$ and $U<0$ one has the SS (on-site) pairing and the d-wave pairing, whereas the SDW and the d-wave pairing are possible for $W<0$ and $U>0$. We would like to point out that Fig. 2 only indicates the main-pure phases and it does not contain a possible mixed superconducting state (d-s), mixed superconducting-SDW state, nor a condensation transition.

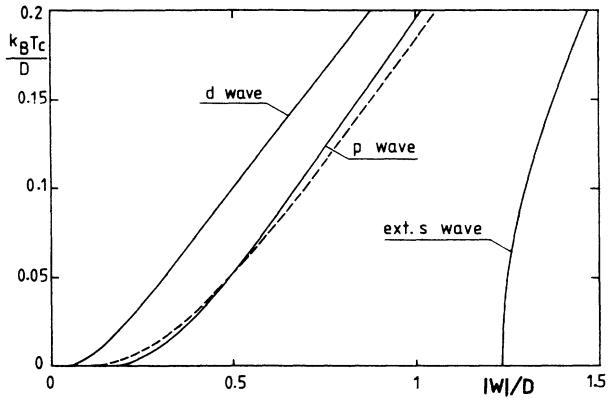

FIG. 1. T_c for d-, p-, and extended s-wave pairings for the square lattice and half-filled band. The dashed line indicates T_c for both on-site (s) pairing vs $-U/D$ and SDW vs U/D.

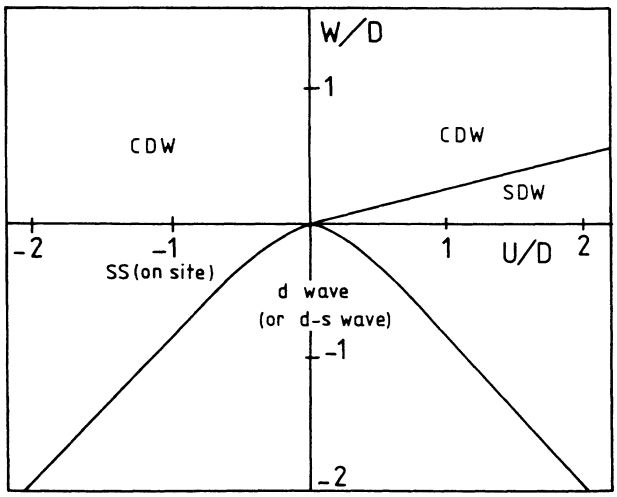

FIG. 2. A preliminary ground-state phase diagram of the extended Hubbard model in two dimensions and square lattice for $n=1$. CDW denotes charge-density waves; SDW denotes spin-density waves; SS denotes singlet pairing (on-site). d-s means a possible mixed superconducting state of d-wave and s-wave admixture.

For the half-filled-band case we have also checked the sensitivity of T_c for the s-wave pairing with respect to the different choices of the DOS. For the $U<0$ Hubbard model the on-site s-wave pairing is strongly enhanced by Van Hove's singularity in comparison to the square DOS. On the other hand, the extended s-wave pairing for $W<0$ is overestimated by the square DOS in comparison to the exact one.

Let us now come to the case of arbitrary band filling. For $n\neq 1$ one has to solve the equations for T_c (2.19)–(2.21) and (2.25) together with the equation fixing the chemical potential, which is given by

$$n-1=-\frac{2}{N}\sum_{\mathbf{q}}\bar{\varepsilon}_{\mathbf{q}}F_{\mathbf{q}}(T_c)\ , \tag{3.7}$$

with $\bar{\varepsilon}_{\mathbf{q}}=\varepsilon_{\mathbf{q}}-\bar{\mu}$, and $F_{\mathbf{q}}(T_c)$ given by Eq. (2.20).

Consider first of all the s-wave pairing. Equation (2.19) can be analyzed analytically for arbitrary electron density upon making use of the approximated square DOS

$$\rho(\varepsilon)=\begin{cases}1/2D, & |\varepsilon|\leq D\ ,\\ 0, & \text{otherwise}\ .\end{cases} \tag{3.8}$$

Although this DOS neglects the logarithmic singularity it is useful for qualitative analysis. One obtains in the weak-coupling limit (low T_c)

$$k_BT_c=1.14D\sqrt{n(2-n)}\exp\left[-\frac{1+\lambda[3(n-1)^2-1]+\alpha\lambda(n-1)^2}{2\lambda\{(n-1)^2-\alpha/4\lambda+(\alpha/4)[1+(n-1)^2]\}}\right]\ , \tag{3.9}$$

where $\alpha=U/D$ and $\lambda=|W|/D$. To derive (3.9) we have used $\bar{\mu}\approx D(n-1)$ at low T. Equation (3.9) shows, among others, that the s pairing takes place in the whole Brillouin zone with the half-bandwidth playing the role of the energy scale. Moreover Eq. (3.9) indicates that for $U>0$ there exists some limiting value for U and $|W|$ and given density n in order for s-wave pairing to exist. The behavior of T_c vs n is nonmonotonous.

For other types of pairing the above approximation based on DOS (3.8) is no longer useful. In general, one can perform the high-T_c expansion for arbitrary value of n to determine T_c for s-, p-, and d-wave pairing in the strong-coupling regime. The weak-coupling formulas for the different pairings with the use of exact DOS or logarithmic approximation and exploring the idea of averaging the pairing potential over the Fermi surface are not accurate, since in our model we essentially allow for pairing in the whole Brillouin zone and there is no cutoff wave vector (except for a reciprocal vector).

The coupled equations for T_c and μ were solved by direct numerical integration, thus properly taking into account the Van Hove singularity. In evaluating T_c for d-wave pairing the following exact relation has been used:

$$\phi_\eta=16(\phi_1-\phi_p)-\phi_\gamma\ , \tag{3.10}$$

where

$$\phi_p=\frac{1}{N}\sum_{\mathbf{q}}\sin^2(q_x)F_{\mathbf{q}}(T_c)\ , \tag{3.11}$$

$$\phi_\eta=\frac{1}{N}\sum_{\mathbf{q}}\eta_{\mathbf{q}}^2F_{\mathbf{q}}(T_c)\ , \tag{3.12}$$

which holds for the square lattice, and $\phi_1(T_c)$ and $\phi_\gamma(T_c)$ are given by Eqs. (2.19b) and (2.19d), respectively.

Figures 3–6 gives T_c vs n for different values of U/D and $|W|/D$. These plots are symmetric with respect to $n\rightarrow 2-n$, due to the electron-hole symmetry. For small

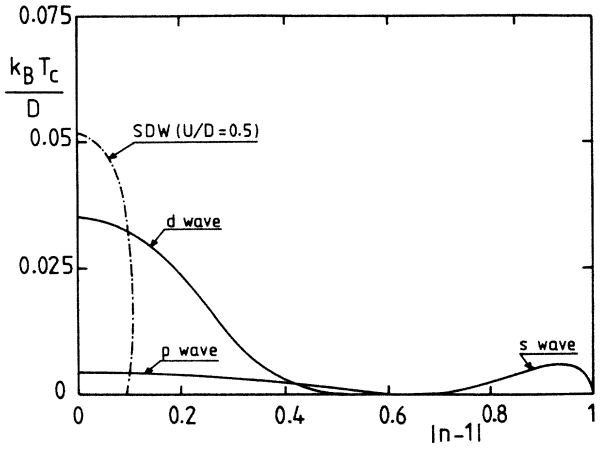

FIG. 3. T_c for s-, p-, and d-wave pairings for the square lattice vs electron density for $|W|/D=0.25$, $u=0$. T_c for SDW is marked by the dashed-dot line.

$|W|/D$ the d-wave pairing gives high transition temperatures in comparison with the p-wave or the extended-s-wave pairing. This is related to the fact of a very fast increase of T_c for d-wave pairing for small $|W|/D$ (compare Fig. 1). Figure 3 shows the phase diagram for $|W|/D=0.25$. With increasing $|W|/D$ the other pairings develop and extend their stability regions (Figs. 4–6). For the nearly-half-filled band the d-wave pairing always yields the highest T_c, while upon decreasing n the p-wave and the s-wave pairings become more stable. T_c for both d and p pairings monotonously decreases with n deviating from $n=1$. T_c for the s-wave pairing exhibits strong nonmonotonic behavior with increasing band filling. It rises rapidly for small n, goes through a maximum, and then vanishes asymptotically below some values of n (Figs. 4 and 5). For $U>0$, s pairing is reduced and the maximum of T_c is shifted towards higher values of $|n-1|$ with increasing U. Let us point out that such a behavior of T_c for the extended s-wave pairing is obtained for any $U>0$ as long as $|W| < |W|_{\text{crit}}=(\pi^2/8)D$. For $|W| > |W|_{\text{crit}}$,

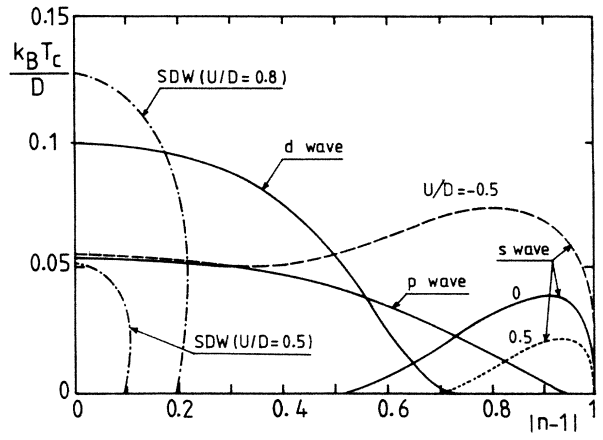

FIG. 4. As in Fig. 3 for $|W|/D=0.5$ and for different values of U/D.

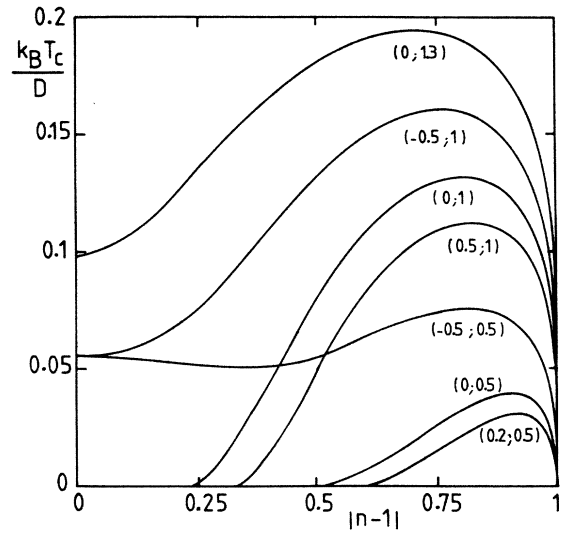

FIG. 5. T_c for s-wave pairing vs electron density for different values of $|W|/D$ and U/D. Numbers next to curves are $(U/D;|W|/D)$.

T_c tends to a finite value for $n=1$ (Fig. 5). Moreover, for $U<0$, the s-wave pairing can always be the most stable one for sufficiently large values of negative U. The boundary between the p- and d-wave pairing states (Fig. 6) is located at $0.2<n<0.52$ for $0<|W|/D\leq 2$. The numerical analysis also indicates that the effect of Van Hove's singularity in DOS is less pronounced with n going toward lower densities, i.e., higher values of $|n-1|$. This is, in particular, observed for on-site s pairing and large

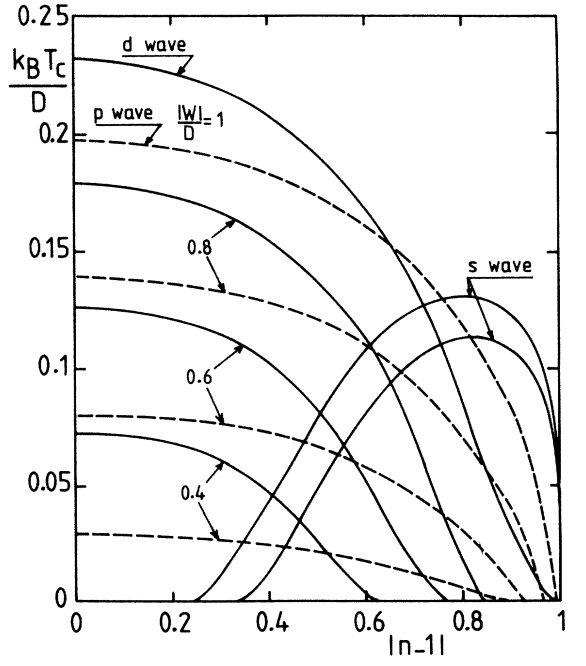

FIG. 6. T_c for d- and p-wave pairings for several values of $|W|/D$. T_c for s-wave pairing: upper curve, $|W|/D=1.0$ and $U/D=0$; lower curve, $|W|/D=1$ and $U/D=0.5$.

negative U.

One therefore expects the sequence of transitions with decreasing electron density: $d \rightarrow p \rightarrow s$ for $U > 0$ or small negative U. For $U < 0$, a $d \rightarrow s$ transition is possible or only the s-wave state is most stable for any n. We need to point out that the choice of parameters W/D and U/D in the plots for $k_B T_c/D$ was made for the purpose of presentation only. These plots reflect a general behavior of the model, as long as the Hartree-Fock approximation is reasonable. It is also interesting to look at the large-U, $|W|$, limit of the Hartree-Fock solutions, mainly for the sake of continuity in the variation of T_c ($|W|/D, U/D$). One obtains the somewhat surprising result that the s-wave pairing is only weakly affected by increasing U for large $|W|$.

A very interesting situation occurs for small electron densities. In this regime of concentration the Cooper pairs (considered here) may become local, real intersite pairs, and a sort of Bose-condensation is possible. This important problem, which unfortunately cannot be fully studied within the present mean-field approach, requires a more elaborate treatment.

Contrary to the local on-site pair formation, where the problem can be reduced to that of the hard-core charged Bose gas on a lattice in the $|U| \gg t$ limit,[7] it is not quite clear whether a similar limit is approached for the intersite local pairs.

In this respect we should mention that the Hartree-Fock–type theory can interpolate between the BCS limit and the local pair limit for the $U < 0$ Hubbard model, but at the ground state only.[21] A study of finite temperatures still remains to be done.[22] Moreover, for $W < 0$, the strong nonmonotonic behavior of s-wave pairing versus electron density differs from the smooth behavior of T_c vs n for the $U < 0$ Hubbard model.[7,21]

Let us now consider the SDW ordering. T_N for the onset of SDW can be readily obtained for the half-filled-band case from the negative-U Hubbard model (the repulsion-attraction transformation) [see Eqs. (3.4)–(3.6) and Fig. 1].

For $n \neq 1$ we observe that the SDW ordering can be rather quickly destroyed by deviating from the $n = 1$ case due to the spoiling of the Fermi-surface nesting. At $T = 0$ K, the stability boundary using a square DOS is given by $|n-1| = \exp(-2D/U)$. Within the logarithmic approximation for the DOS [Eq. (3.2)] the onset of SDW occurs for

$$|\bar{\mu}| = 4D \exp\{[-\pi^2 D/UC' + (\ln 4)^2]^{1/2}\} \tag{3.13}$$

and μ is given by

$$n - 1 = \frac{\bar{\mu}}{D} - \frac{\bar{\mu}}{D} \ln \left| \frac{\bar{\mu}}{D} \right| \Big/ (\ln 4 + 1). \tag{3.14}$$

To obtain these results we normalized the DOS in the logarithmic approximation to 1, i.e.,

$$\rho(\varepsilon) = \frac{2C'}{D\pi^2} \ln \left(\frac{4D}{|\varepsilon|} \right), \quad C' = \frac{\pi^2}{4} \frac{1}{\ln 4 + 1} = 1.0339.$$

A simple analysis shows that the stability region of SDW with respect to the paramagnetic state at $T = 0$ K is expanded in comparison to approximations based on the square DOS, but still the onset of SDW occurs for rather small deviations from the half-filling even for U/D as large as 1.

T_N for different values of U is given in Figs. 3 and 4. Thus the SDW state can dominate near half-filling for sufficiently large U. We also observe a reentrant behavior in T_N vs $|n-1|$. We perhaps have to stress again that the mean-field solutions for T_N in our $d = 2$ model merely indicates the importance of spin fluctuations and by no means a phase transition. In order to have a true phase transition the interlayer coupling has to be consistently taken into account.

Let us point out now that from the present analysis it follows that the high superconducting transition temperatures can be achieved even if $U \gg |W|$. It is an interesting question how the spin fluctuations can influence the superconducting state. For example, we can readily incorporate within the present mean-field theory the effect of effective spin exchange of the form $\sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j$, where $S_i^{\dagger} = c_{i\uparrow}^{\dagger} c_{i\downarrow}$, $S_i^z = \frac{1}{2}(c_{i\uparrow}^{\dagger} c_{i\uparrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow})$. J_{ij} will enter the equations for extended s-wave and d-wave pairings as $|W| + \frac{3}{2} J$, the equation for p-wave pairing as $|W| - \frac{1}{2} J$, and the equation for SDW as $U + J\gamma_0$, respectively. Thus, $J > 0$ destabilizes p-wave pairing with respect to s- and d-wave pairings as well as the SDW state. J will also influence the phase boundary between the s- and d-wave pairings ($T_c^s = T_c^d$). However, consistent treatment of competition between antiferromagnetism and superconductivity requires analysis of mixed solutions SDW-anisotropic superconductivity which is beyond the scope of this paper. Another problem is an extension of present RPA treatment to include the spin fluctuations within the paramagnon theory which possibly could enhance the d-wave pairing close to $n = 1$ due to antiferromagnetic spin fluctuations.[15,23,24]

IV. EFFECTS OF NEXT-NEAREST-NEIGHBOR HOPPING

For the next-nearest-neighbor hopping and the square lattice,

$$\varepsilon_k = -2t(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y \ .$$

The perfect nesting condition $\varepsilon_{k+Q} = -\varepsilon_k$ is not satisfied any longer and there is no electron-hole symmetry. Consequently, the Van Hove singularity does not coincide with the Fermi energy for $n = 1$ and the maximum of T_c for d- and p-wave pairing is shifted due to the fact that the logarithmic singularity moves to $n \neq 1$. We have performed detailed numerical analysis of T_c for s-, p-, and d-wave pairing, and the results for given ratio $|W|/D$ and t_2/t and the band filling are given in Figs. 7–11. Figure 7 shows the effect of t_2 on the phase diagram for $n = 1$, and $t_2/t = 0.3$. In Figs. 8 and 9(a)–9(c) we show T_c for s-, p-, and d-wave pairings versus the band filling for different t_2/t. We stress that there exists the following relation for T_c:

$$T_c(n, t_2/t) = T_c(2-n, -t_2/t) \ ,$$

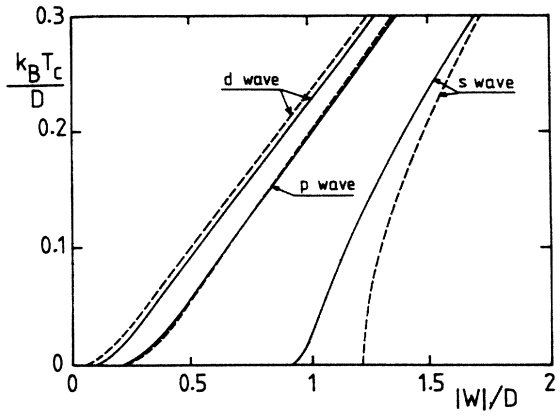

FIG. 7. T_c for d-, p-, and s-wave pairings for $n=1$ for the square lattice with nearest- and next-nearest-neighbor hopping. $t_2/t=0.3$. The dashed lines indicate T_c for $t_2=0$. T_c for p-wave pairing is almost unaltered for this value of t_2/t.

which links the cases of $t_2>0$ and $t_2<0$. In Fig. 8 we compare T_c vs n for $t_2/t=0.3$ with that for $t_2=0$.

The evolution of T_c with increasing t_2/t ratio is clearly indicated by plots in Figs. 8 and 9(a)–9(c). Upon increasing t_2/t the s-wave pairing is enhanced in the regime $1<n<2$ and spread over a wider region of densities. The nonmonotonic variation of T_c with electron density is smoothened upon increasing t_2, and the maximum of T_c moves toward the half-filled band. For $0<n<1$, the s-wave pairing is much reduced upon increasing t_2, but it can still be stable for small n. The effect of $U>0$ on s-wave pairing is illustrated in Fig. 9(a), which shows a reduction of T_c and the movement of the maximum towards lower densities.

The plots for the d-wave pairing are particularly interesting. A maximum of T_c decreases and moves from $n=1$ towards lower densities, and the strong nonmonoton-

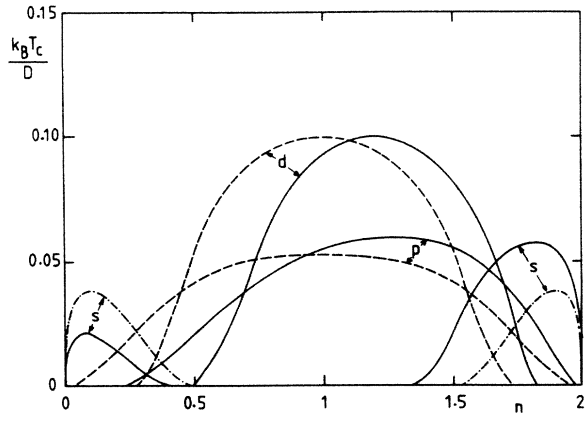

FIG. 8. Comparison of critical temperatures for different types of pairings for the square lattice (for $|W|/D=0.5$, $U=0$) vs electron density with nearest- and next-nearest-neighbor hopping. The solid lines are plotted for $t_2/t=0.3$; the dashed and dashed-dot lines are for $t_2=0$.

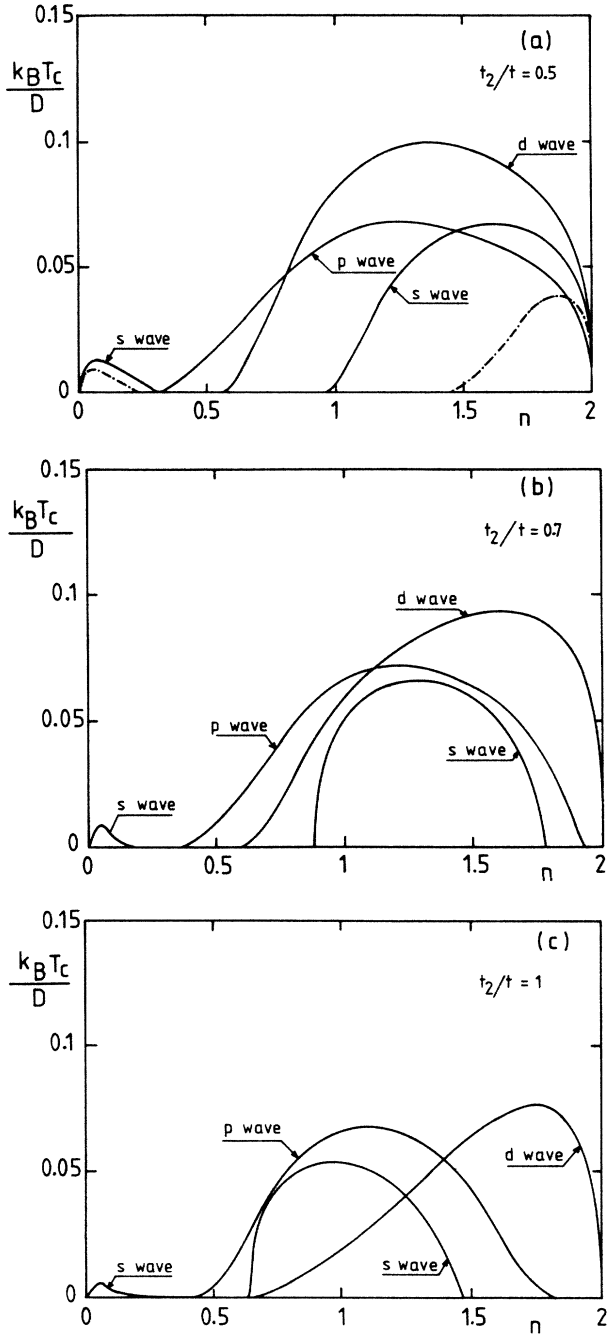

FIG. 9. T_c for d-, p-, and s-wave pairing for the square lattice vs electron density and different ratio t_2/t, for $|W|/D=0.5$, $U=0$. (a) $t_2/t=0.5$; (b) $t_2/t=0.7$; (c) $t_2/t=1.0$. In (a) dashed-dot lines mark T_c for s-wave pairing for $|W|/D=0.5$ and $U/D=0.5$.

ic variation of T_c vs n is observed for a larger t_2/t ratio. As far as the p-wave is concerned, T_c first increases for small t_2/t then its stability range shrinks and the maximum of T_c goes to $n\cong 1$.

From comparison of T_c we give the diagram of relative stability of s-, p-, and d-wave pairings in Fig. 10. One then concludes that the d-wave pairing is the one which is most stable for $1<n<2$ with increasing t_2/t, followed by

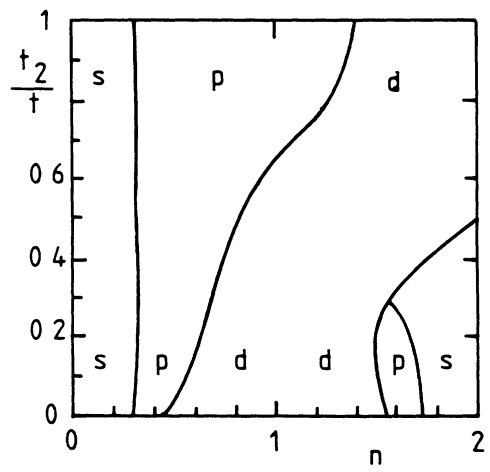

FIG. 10. Diagram of relative stability of s-, p-, and d-wave pairings for the square lattice with nearest- and next-nearest-neighbor hopping in t_2/t-n plane. ($|W|/D=0.5, U=0$).

the p wave which is most stable for $n \approx 1$ and large t_2/t. For $0<n<1$ the p-wave pairing can be stabilized by increasing the t_2/t ratio and the s wave is restricted to smaller densities. This overall variation of T_c with the t_2/t ratio obtained for the case of intersite attraction is interesting to compare with the T_c for purely on-site attraction ($U<0$ Hubbard model with next-nearest-neighbor hopping). Figure 11 shows T_c for the $U<0$ case and $t_2/t=0.3$, from which we see the effect of moving the Van Hove singularity and strong enhancement of T_c for on-site pairing.

Let us also comment on the effects of next-nearest-neighbor hopping on the SDW state.[25] As it was shown in the past due to a lack of perfect nesting, there can be a critical value of t_2/t to realize SDW for $n=1$ and the possibility of first-order phase transitions at $T=0$ K. Moreover, the numerical simulations of the Hubbard model in $d=2$ point out that the SDW state is not stable with respect to the paramagnetic state[25] for large deviations from the half-filled band; therefore, we conclude that the next-nearest-neighbor hopping does not favor the SDW state at least for moderate values of U.

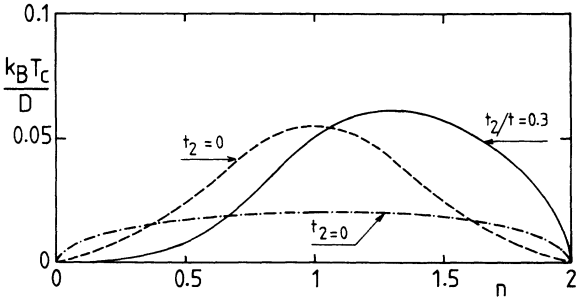

FIG. 11. Effects of next-nearest-neighbor hopping on T_c for the $U<0$ Hubbard model for the square lattice, $U/D=-0.5$. The solid line is for $t_2/t=0.3$; the dashed line for $t_2/t=0$. The dashed-dot line indicates T_c vs n for the square density of states and nearest-neighbor hopping.

The above analysis clearly indicates the importance of the next-nearest-neighbor hopping on the stability of superconducting states and the variation of superconducting T_c with electron density. For a definite range of n, T_c can be substantially altered even for small t_2 and both cases $t_2>0$ and $t_2<0$ are important. This is an interesting effect since it can be responsible for the pressure dependence of T_c.

V. THE LIMIT OF STRONG CORRELATIONS

In the bulk of this paper we discussed a mean-field approach for the superconductive properties of the extended Hubbard model with attractive intersite intercation. We find for the half-filled band d- and p-wave pairings which may be destabilized by SDW's for large enough U. Clearly, we would expect that for strong correlations no superconducting state exists for the half-filled-band case (the Mott insulator limit). Consequently, an important problem is to study whether the superconducting state can be established in the strong correlation limit away from the half-filled-band case. This is best studied by applying to our starting Hamiltonian (1.1) the canonical transformation method.[26-29]

Assuming $U \gg t, W$, one obtains an effective Hamiltonian acting only in the subspace of singly occupied sites of the following form:

$$H_{\text{eff}}=\sum_{ij\sigma} t_{ij} h_{i\sigma}^{\dagger} h_{j\sigma} + \sum_{ij} J_{ij}(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} N_i N_j) + \tfrac{1}{2} \sum_{ij} W_{ij} N_i N_j - \mu \sum_{i\sigma} n_{i\sigma} , \tag{5.1}$$

where

$$h_{i\sigma}=c_{i\sigma}(1-n_{i-\sigma}),\ N_i=N_{i\uparrow}+N_{i\downarrow} ,$$

$$N_{i\sigma}=h_{i\sigma}^{\dagger} h_{i\sigma}=n_{i\sigma}(1-n_{i-\sigma}) ,$$

$$S_i^{\dagger}=c_{i\uparrow}^{\dagger} c_{i\downarrow},\ S_i^z=\tfrac{1}{2}(n_{i\uparrow}-n_{i\downarrow}),\ J_{ij}=2t_{ij}^2/U .$$

In (5.1) we retain only the leading terms. The pair hopping terms that are generated by the canonical transformation are omitted. If $n=1$ (the Mott insulator), $N_i=1$ and (5.1) reduces to the well-known Anderson kinetic exchange term

$$H_{\text{eff}}=\sum_{ij} J_{ij}(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4}) + \text{const} , \tag{5.2}$$

where const $=\frac{1}{2} WzN$, and z is the number of nearest neighbors. H_{eff} of the form of (5.1) is the generalization of the kinetic exchange Hamiltonian for the non-half-filled band. In two dimensions the nature of the ground state of (5.2) is at present not established, i.e., whether the ground state is the Néel state corrected by the zero-point fluctuations or is a sort of spin liquid state (the resonating-valence-bond state),[30,31] but in any case superconductivity is excluded. The superconducting state can only be possible for the non-half-filled-band case. There are two sources of superconducting pairing in (5.1). One is due to $W<0$ and the other comes from the exchange term. Any potential superconducting state has to compete with a possible magnetic ground state. The great difficulty in constructing a sensible mean-field theory is due to the fact that (5.1) is defined only in the subspace of singly occupied sites. Such a condition is not easy to han-

dle and several proposals have recently appeared.[10,18,32-35] A rather simplified picture of the superconductivity is obtained upon relaxing the doubly occupancy condition by linearization of the kinetic-energy term $t_{ij}h_{i\sigma}^{\dagger}h_{j\sigma}$ $\rightarrow \delta t_{ij}c_{i\sigma}^{\dagger}c_{i\sigma}$, where $\delta=1-n$ means the fractional occupation. Such a procedure requires a supplementary projection operation which excludes the doubly occupied sites. We notice that all the mean-field schemes so far proposed in the literature[18,32-35] are internally inconsistent in the limit $\delta=0$. In this section we propose a simplified but internally consistent mean-field treatment by scaling the spin and charge couplings in the following way, replacing (5.1) by

$$H\cong\sum_{ij\sigma}t_{ij}\delta c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{ij}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j+\sum_{ij}\delta W'_{ij}n_in_j -\mu\sum_{i\sigma}n_{i\sigma}+\text{const} , \tag{5.3}$$

where

$$W'_{ij}=-\tfrac{1}{4}J_{ij}+\tfrac{1}{2}W_{ij},\quad n_i=n_{i\uparrow}+n_{i\downarrow} .$$

Upon making the Gorkov-type factorizations, we obtain the following gap equation for the singlet pairing (neglecting the Fock averages):

$$\Delta_k=\frac{1}{N}\sum_{\mathbf{q}}V_{\mathbf{kq}}\Delta_{\mathbf{q}}F_{\mathbf{q}} , \tag{5.4}$$

where

$$F_{\mathbf{q}}=(2E_{\mathbf{q}})^{-1}\tanh(\beta E_{\mathbf{q}}/2) , \tag{5.5}$$

$$E_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+|\Delta_{\mathbf{k}}|^2} , \tag{5.6}$$

where

$$\xi_{\mathbf{k}}=-t\delta\gamma_{\mathbf{k}}-\mu \text{ and } \gamma_{\mathbf{k}}=2(\cos k_x+\cos k_y) ,$$
$$V_{\mathbf{kq}}=\tfrac{3}{2}J\gamma_{\mathbf{k}-\mathbf{q}}+\tfrac{1}{2}J\delta\gamma_{\mathbf{k}-\mathbf{q}}-W\delta\gamma_{\mathbf{k}-\mathbf{q}} . \tag{5.7}$$

Upon using the decomposition $\Delta_{\mathbf{k}}=\Delta_\gamma\gamma_{\mathbf{k}}+\Delta_\eta\eta_{\mathbf{k}}$ we have respectively for the extended s-wave pairing

$$\Delta_\gamma=\frac{1}{N}\sum_{\mathbf{q}}\tfrac{1}{4}[\tfrac{3}{2}J(1+\delta/3)-W\delta]\gamma_{\mathbf{q}}^2\Delta_{\mathbf{q}}F_{\mathbf{q}} , \tag{5.8a}$$

and for the d-wave pairing

$$\Delta_\eta=\frac{1}{N}\sum_{\mathbf{q}}\tfrac{1}{4}[\tfrac{3}{2}J(1+\delta/3)-W\delta]\eta_{\mathbf{q}}^2\Delta_{\mathbf{q}}F_{\mathbf{q}} . \tag{5.8b}$$

The chemical potential is determined by

$$\delta=\frac{1}{N}\sum_{\mathbf{q}}2\xi_{\mathbf{q}}F_{\mathbf{q}} . \tag{5.9}$$

We stress that in the present treatment there is no electron-hole symmetry (due to the fact that we work in the lower Hubbard subband) in contrast to the case of the weak electron correlations considered in Sec. III. The transition temperatures for the onset of s- and d-wave pairings is given by

$$\frac{1}{G}=\frac{1}{N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}^2\frac{\tanh(\beta_c\xi_{\mathbf{q}}/2)}{2\xi_{\mathbf{q}}}=\phi_\gamma(T_c) , \tag{5.10a}$$

$$\frac{1}{G}=\frac{1}{N}\sum_{\mathbf{q}}\eta_{\mathbf{q}}^2\frac{\tanh(\beta_c\xi_{\mathbf{q}}/2)}{2\xi_{\mathbf{q}}}=\phi_\eta(T_c) , \tag{5.10b}$$

$$G=\tfrac{3}{8}J(1+\delta/3)-\tfrac{1}{4}W\delta , \tag{5.10c}$$

and μ is given by Eq. (5.9) for $\Delta\rightarrow 0$. Had we worked with the Hamiltonian (5.3) without rescaling W' [by setting $\delta=1$ in Eqs. (5.7) and (5.10c)] we would have obtained a T_c dependent on W even in the half-filled-band case where we have no charge coupling in (5.1). With our proposed scaling of this term we find for $\delta\rightarrow 0$, $k_BT_c=\frac{3}{8}J$ for both types of couplings and hence no inconsistencies at least on this level of a mean-field approach. The fact that one obtains a finite T_c for $n=1$ is an artifact of the mean-field result (i) due to the neglect of phase fluctuations and (ii) due to not projecting out the doubly occupied states (see, however, Refs. 10 and 35). It is expected that a proper mean-field treatment should lead to the physical order parameter $\tilde{\Delta}=\Delta\delta$ which naturally vanishes for $n=1$.

It is interesting to observe that for small deviations from $n=1$, the d-wave state gives the highest T_c. This can be shown by making use of strong-coupling expansion (high T_c) of ϕ_γ and ϕ_η. One has for $d=2$,

$$\phi_\gamma(T_c)=\beta_c\left[1-\frac{(\beta_c\mu)^2}{12}-\tfrac{3}{4}(\beta_ct\delta)^2+\cdots\right] , \tag{5.11a}$$

$$\phi_\eta(T_c)=\beta_c\left[1-\frac{(\beta_c\mu)^2}{12}-\frac{(\beta_ct\delta)^2}{12}+\cdots\right] . \tag{5.11b}$$

Since in the lowest order $\beta_c\mu\approx 2\delta$ one gets for T_c^s and T_c^d, respectively,

$$k_BT_c^s=G\left[1-\frac{\delta^2}{3}-\frac{3t^2\delta^2}{4G^2}+\cdots\right] , \tag{5.12a}$$

$$k_BT_c^d=G\left[1-\frac{\delta^2}{3}-\frac{t^2\delta^2}{12G^2}+\cdots\right] , \tag{5.12b}$$

which shows that the T_c for s-wave pairing is always less than for the d-wave pairing, and indeed any $W<0$ strongly stabilizes the superconducting state.

As far as the p-wave (equal spin) pairing is concerned, it can only result from the W term, since the equal spin contribution precisely cancels in the second term of (5.1). The gap equation is formally given by our previous equation (2.22) with that difference that now the pairing potential is $V_{kq}^{\dagger}=\frac{1}{2}(W_{k+q}-W_{k-q})$. δ and $\bar{\varepsilon}_q=\xi_q=-t\delta\gamma_q-\mu$. T_c for the p-wave pairing is then given by [compare Eq. (2.25)]

$$1=\frac{2|W|\delta}{N}\sum_{\mathbf{q}}\sin^2q_x\frac{\tanh(\beta_c\xi_{\mathbf{q}}/2)}{2\xi_{\mathbf{q}}}=2|W|\delta\phi_p(T_c) . \tag{5.13}$$

Upon making the high-temperature expansion we obtain for $d=2$,

$$\phi_p(T_c)=\frac{\beta_c}{8}\left[1-\frac{(\beta_c\mu)^2}{12}-\frac{(\beta_ct\delta)^2}{4}+\cdots\right] , \tag{5.14}$$

which in lowest order of approximation yields

$$k_BT_c^p\cong\frac{|W|\delta}{4}\left[1-\frac{\delta^2}{3}-4t^2/W^2+\cdots\right] . \tag{5.15}$$

This shows that T_c^p starts from the origin as a function of doping. If we had not scaled the pairing potential by δ then the result would have been

$$k_B T_c^p \cong \frac{|W|}{4}\left(1-\frac{\delta^2}{3}-\frac{4t^2\delta^2}{W^2}+\cdots\right), \quad (5.16)$$

giving finite T_c for $\delta=0$.

A detailed discussion of the phase diagram in the $U\gg t$ limit for anisotropic superconductivity would require numerical work on the above set of equations. Moreover, the inclusion of pair hopping terms (not considered here) will stabilize the extended s-wave pairing. An entirely different approach to the strong correlations ($U\gg t$) problem close to the half-filled-band case is to consider the possibility of the formation and condensation of charged bosons—either local pairs of holes or bosons resulting from the RVB state.[10,12,32,35] These challenging problems are presently under investigation.

VI. DISCUSSION

In this paper we have carried out the mean-field analyses of the superconductivity in a narrow-band system with local short-range attractive interactions for two dimensions and arbitrary band filling. Based on the extended Hubbard model with nearest-neighbor attractive interaction we determined the superconducting transition temperatures for singlet pairings of d and s type and for equal-spin, triplet pairing which is of p type, as well as the SDW state. Our analysis in the case of nearest-neighbor hopping shows that close to the half-filled band d-wave pairing is most stable, while the p wave is stabilized for intermediate densities. T_c for s-wave pairing showing a strong nonmonotonous behavior as a function of electron densities is essentially realized for small densities, and is most affected by the on-site repulsion. In principle, one then expects the following order of transitions with increasing electron density: $s\rightarrow p\rightarrow d$ wave. This has to be compared, however, on the mean-field level with the SDW state which is realized close to $n=1$ and can be always most stable for sufficiently large $U>0$. It is interesting to compare the superconducting phases for $W<0$ with that of a purely attractive Hubbard model. For the $U<0$ Hubbard model, T_c for on-site pairing shows smooth behavior versus electron density and is always enhanced by the Van Hove singularity in $d=2$ for the square lattice. This pairing exists for any $U<0$ and arbitrary n. In the case of intersite attraction, we observe for s-wave pairing a sharp rise of T_c for small densities, then a maximum, and finally T_c vanishing asymptotically below some density. Moreover, for the $U<0$ Hubbard model one can go continuously to the large attraction limit, i.e., from the Cooper pairs to the local pairs.[7,21,22] For $W<0$ it is an open question of whether one can reach the limit of local intersite pairs by continuing from the Hartree-Fock limit.

In the case of next-nearest-neighbor hopping we observed essential changes in the phase diagrams with varying electron densities. This can be of importance as far as the T_c dependence on pressure is concerned. We did not consider the role of the Fock terms, which we believe changes only quantitatively the picture with the mean-field theory and leads essentially to temperature renormalization of the bandwidth. We discussed the SDW instability, which for the strictly $d=2$ system indicates only the presence of spin fluctuations but not a real phase transition. A coexistence of the SDW and anisotropic superconductivity is an interesting problem which is left for a future study.

The question of condensation transition for attractive interaction should also be addressed as far as the thermodynamic properties of the extended Hubbard model is concerned. In this respect we should only mention that for real systems long-range Coulomb interactions will have to be taken into account, which always will lead to the suppression of the condensed state. The applicability of the mean-field theory for strictly two-dimensional systems cannot be resolved unless the fluctuations are considered. This certainty calls for theories beyond RPA or renormalization-group studies.

For $U\gg t$, we demonstrated that our model is close to recent proposals for mechanism for high T_c superconductivity, with that difference that in our model superconductivity is an intrinsic consequence of the attractive intersite interaction. We should also stress the difference between the limits of weak and strong correlations. In the limit of weak correlations the anisotropic superconductivity can be readily established even for $n\approx 1$. In contrast for $U\gg t$ limit, the localization effects are important, and for $n=1$, certainly any superconductivity is absent. It is a very interesting question whether one can have the formation of real-space pairs for small electron densities and intersite attractive interaction. Our previous studies of the local-pair superconductivity restricted to effective on-site pairs indicate that a system of tightly bound pairs can undergo the Bose-condensation and this may lead to a superconductivity of a hard-core charged Bose-gas on a lattice. Such superconductivity differs form the BCS picture in many aspects. This concerns the thermodynamics electromagnetic properties as well as influence of structural disorder.[4,7,9]

Finally, let us relate the present study with the new high-T_c materials. It is now well established that these compounds exhibit quasi-two-dimensional characteristics. This comes from the transport measurements and the band-structure calculations. Our model which is in the present form rather simplified seems to capture some of experimental findings. First of all, superconducting T_c can be high due to the fact that the electron pairing takes place in the whole Brillouin zone contrary to the BCS model. The short coherence length observed in these materials is consistent with the model assuming local short range attractive interaction. The phase diagram derived in this paper containing the SDW ordering and superconductivity is reminisescent of the one observed experimentally in $(La_{1-x}M_x)_2CuO_{4-\delta}$,[36] $M=$Sr,Ba. A fast disappearance of antiferromagnetism in $La_2CuO_{4-\delta}$ (Ref. 37) with changing the oxygen vacancies can be interpreted within our model as a consequence of spoiling the Fermi surface nesting. The observed isotope effect in $La_{2-x}Sr_xCuO_{4-\delta}$ (Ref. 38) indicates that superconduc-

tivity is somehow related to electron-lattice couplings and tends to support the short-range pairing due to a polaronic mechanism. The linear T behavior of the resistivity in the a-b plane in the normal state can be accounted by the low carrier (holes) concentration.[39]

All these qualitative conclusions can be derived within the weak correlation limit. Recent spectroscopic measurements show that the real situation in these materials is perhaps the intermediate correlation regime ($U \sim 2D$).[40] Within the present model one can approach such a situation from the insulating side assuming $U \gg t$. The superconductivity then would result from the cooperation of polaronic and superexchange mechanism.[41] The experimentally observed low density of carriers, the small DOS at the Fermi level, and the fact that superconductivity exists even in very poor samples can be taken as an indication for the formation and condensation of charged bosons (for example, the real-space pairs instead of Cooper pairs). Such a possibility is contained in the present model when the electron density is small. The above considerations pointed out the role of polaronic effects and magnetic correlations. Another possibility is that the model essentially describes the holes in the oxygen valence band and the intersite pairing is due to either a purely electronic mechanism such as possible virtual peroxide states (chemical bonding)[42] or due to the coupling of oxygen holes to local spin configurations on the Cu sites.[12,43]

In conclusion, we have studied a simple model which incorporates magnetic correlations and superconducting pairing for narrow-band systems with short coherence length (nearest-neighbor real-space pairing). Although this model is extremely simplified as compared to the complex properties of the high-T_c oxides, some of our findings might be relevant in interpreting these materials.

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