Superconductivity in a strongly correlated one-band system

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We study superconductivity in the extended Hubbard model with a strong on-site repulsion U and weak attractive density-density interaction V_{ij}. The electron correlation effects, beyond the weak-coupling regime of U, are included approximately by employing Hubbard decoupling approximations. The formulas for superconducting transition temperature T_c of the present approach are compared to those obtained with the strong-coupling expansion and slave-boson techniques. The methods share some common features. We discuss behavior of T_c for superconducting phases with s- and d-wave symmetry of the superconducting order parameter. In contrast to the mean-field treatment of U, we find that the strong on-site repulsion does not destroy superconductivity induced by $V_{ij}<0$ even when $U\gg|V_{ij}|$. [S0163-1829(96)02929-3]

Study of superconductivity in strongly correlated electron systems in narrow energy bands has been pursued with renewed interest since the discovery of high-T_c cuprate oxides.[1] Most of these studies are based on the premise that a single band or extended Hubbard-type models can be used to capture the physics of high-T_c cuprate superconductors.[2] The methods employed range from broken symmetry mean-field approximations through various decoupling approximation schemes, canonical transformations, $1/N$ expansions, to slave-fermion or slave-boson techniques. Still, there is no unambiguous proof that superconducting correlations strong enough to lead to high-T_c's arise from strong on-site repulsion in a single band Hubbard model. It is now well accepted that Coulomb interaction on the Cu sites in high-T_c cuprate oxides is strong enough to split-off the uncorrelated Cu-d band into Hubbard subbands and that superconducting pairing occurs in the less than half-filled Hubbard subband. A theoretical study of superconducting pairing in the Hubbard subbands is, then, of considerable interest. In this paper, we present such an investigation employing an extended Hubbard model with strong on-site repulsive and weak attractive intersite interactions (U and V_{ij}, respectively). We employ the Hubbard subband operator approach[3–5] to include the many-body correlations arising from the strong on-site repulsive interaction U. We will also compare our results with those obtained using strong-coupling canonical expansion[6] and slave-boson[7,8] methods.

We take the Hamiltonian in the following form:

$$H=-\sum_{i,j,\sigma} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_{i} n_{i\downarrow}n_{i\uparrow}+\sum_{i,j}\sum_{\sigma,\sigma'} V_{ij}n_{i\sigma}n_{j\sigma'} -\mu\sum_{i,\sigma} n_{i\sigma}. \tag{1}$$

Further on the V_{ij} term is assumed to be at least an order of magnitude smaller than U. This model has been previously studied by Micnas *et al.*[6] in both weak- ($U\ll t$) and strong-coupling ($U\gg t$) limits. It has also been qualitatively analyzed in the Hubbard-Jain approach.[4,5] However, no explicit calculations have been performed so far. In all cases we assume $|V|\ll W$, ($W=8t$ and V is interaction between the nearest sites in $2d$ square lattice) so that the Hartree-Fock-Bogoliubov factorization for that part of Hamiltonian is legitimate.

To start let us recall the strong-coupling limit of the Hamiltonian (1). To leading order in $1/U$ it reads[6,9]

$$H_{\rm eff}=-\sum_{i,j,\sigma} t_{ij}h^{\dagger}_{i\sigma}h_{j\sigma}+\sum_{i,j} J_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}N_iN_j\right) +\sum_{i,j} V_{ij}N_iN_j-\mu\sum_{i,\sigma} n_{i\sigma}, \tag{2}$$

where $h_{i\sigma}=c_{i\sigma}(1-n_{i-\sigma})$, $N_{i\sigma}=h^{\dagger}_{i\sigma}h_{i\sigma}=n_{i\sigma}(1-n_{i-\sigma})$, $N_i=\Sigma_\sigma N_{i\sigma}$, $S^{+}_i=c^{\dagger}_{i\uparrow}c_{i\downarrow}$, $S^{z}_i=\frac{1}{2}(n_{i\uparrow}-n_{i\downarrow})$ and $J_{ij}=2t^2_{ij}/U$. Terms corresponding to hopping of nearest-neighbor electron pairs are not taken into account.

Gorkov-type factorization leads to the BCS-like equation for the gap function[6]

$$\Delta_k=\frac{1}{N}\sum_{q} V_{kq}\frac{\Delta_q}{2E_q}\tanh\left(\frac{\beta E_q}{2}\right) \tag{3}$$

with $E_q=\sqrt{\xi^2_q+|\Delta_q|^2}$ and $\xi_q=\delta\cdot\varepsilon_q-\overline{\mu}$ and $\delta=1-n$ (n is the electron concentration). An important point of this approach is the renormalization of charge-charge interaction $V_{kq}=V\delta\gamma_{k-q}$ through the factor δ. Such a term, as we shall see, is absent in the mean-field approximation to the slave-boson method.

The use of the slave-boson method is particularly simple in the $U=\infty$ limit. Electron configurations of a system (for $n<1$) can under such circumstances consist only of singly occupied and empty sites. No double occupancy is allowed. One replaces the electron operators ($c_{i\sigma}$) via new fermion ($f_{i\sigma}$) and auxiliary bose field (b_i) operators. The require-

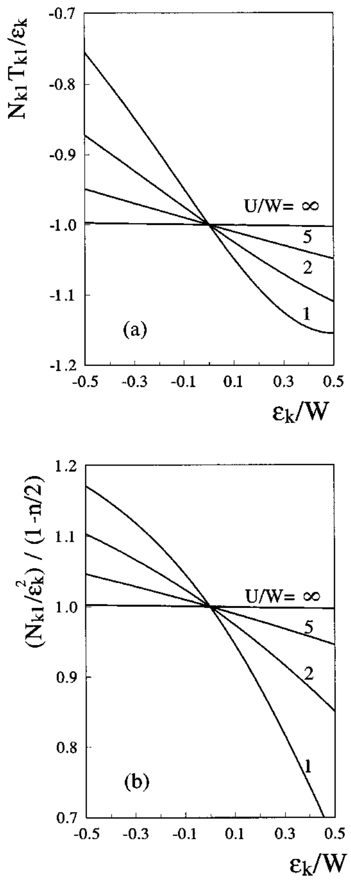

FIG. 1. Plot of the $N_{k1}T_{k1}/\varepsilon_k$ function (a) and the normalized N_{k1}/ε_k^2 function (b) versus single-particle energy ε_k for several values of U.

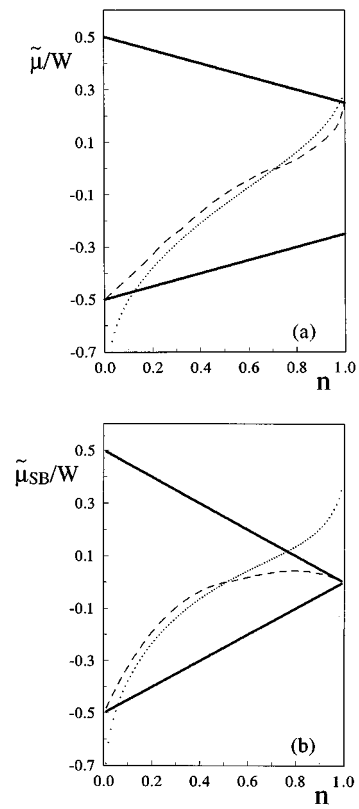

FIG. 2. Position of a chemical potential $\widetilde{\mu}$ in the effective lower Hubbard subband obtained by the Hubbard-Jain method (a) and in the effective band by the slave-boson method (b). The dashed lines correspond to zero temperature while dotted ones to $T=0.1W$.

ment of no double occupation in this limit is fulfilled with the introduction of a term into the Hamiltonian which constrains the allowed states. One gets a Hamiltonian in the form

$$H^{\mathrm{SB}}=-\sum_{i,j,\sigma} t_{ij}f_{i\sigma}^{\dagger}f_{j\sigma}b_i b_j^{\dagger}-\mu\sum_{i\sigma} f_{i\sigma}^{\dagger}f_{i\sigma}+\sum_{i,j} V_{ij}n_in_j +\sum_i \lambda_i\left(\sum_{\sigma} f_{i\sigma}^{\dagger}f_{i\sigma}+b_i^{\dagger}b_i-1\right). \tag{4}$$

Here $n_i=\Sigma_\sigma f_{i\sigma}^{\dagger}f_{i\sigma}$, and λ_i denotes the Lagrange multiplier. The mean field for slave bosons means[10] replacement of all bosonic fields by their classic values $b_i=b_i^{\dagger}=r$ and $\lambda_i=\lambda$. Parameters λ and r are determined by minimization of the ground-state energy ($E=\langle H\rangle$) of the system. This leads to $r^2=1-n$ and $\lambda=-\Sigma_k n_{k\sigma}\varepsilon_k$.

A standard Gorkov-type procedure allows a derivation of the formula (3) with $V_{k-q}=V\gamma_{k-q}$ and $\xi_k=r^2\varepsilon_k-\mu+\lambda+2nV$. Thus the two approaches differ with respect to renormalization of interaction V_{kq} and additional shift λ of the spectrum. In the slave-boson approach the renormalization of interaction does not appear while in the canonical transformation method the term δ is introduced in order to get the correct $\delta\rightarrow 0$ limit.

The Hubbard subband operator approach[3,4] relies on the introduction of new operators $d_{i\sigma}^{\alpha}=n_{i-\sigma}^{\alpha}c_{i\sigma}$ and their conjugate counterparts $d_{i\sigma}^{\alpha\dagger}=(d_{i\sigma}^{\alpha})^{\dagger}$, where $n_{i\sigma}^{1}=1-n_{i\sigma}$ and $n_{i\sigma}^{2}=n_{i\sigma}$. One writes then the equation of motion for these new operators. Using again Gorkov-type decoupling and Fourier transformation one gets[5]

$$\omega d_{k\sigma}^{\alpha}=(\varepsilon_\alpha-\widetilde{\mu})d_{k\sigma}^{\alpha}+n^{\alpha}\varepsilon_k c_{k\sigma} +c_{-k-\sigma}^{\dagger}\sum_{k'}\left[(-1)^{\alpha}(\varepsilon_k+2\varepsilon_{k'})+2n^{\alpha}\sum_{k'} V_{k-k'}\right] \times\langle c_{-k'-\sigma}c_{k'\sigma}\rangle \tag{5}$$

with $\widetilde{\mu}=\mu-8nV$. At this step it is convenient to introduce the ''Hubbard subband'' operators $D_{k\sigma}^{\nu}=(N_{k\nu}/\varepsilon_k)[d_{k\sigma}^{1}/E_{k\nu}+d_{k\sigma}^{2}/(E_{k\nu}-U)]$ where $E_{k\nu}$ are solutions of the Hubbard I problem

$$E_{k\nu}=\tfrac{1}{2}[U+\varepsilon+(-1)^{\nu}\sqrt{(U-\varepsilon_k)^2+2nU\varepsilon_k}] \tag{6}$$

and

$$N_{k\nu}=\left[\frac{n/2}{(E_{k\nu}-U)^2}+\frac{1-n/2}{E_{k\nu}^2}\right]^{-1}. \tag{7}$$

The subband operators obey the following equation of motion:

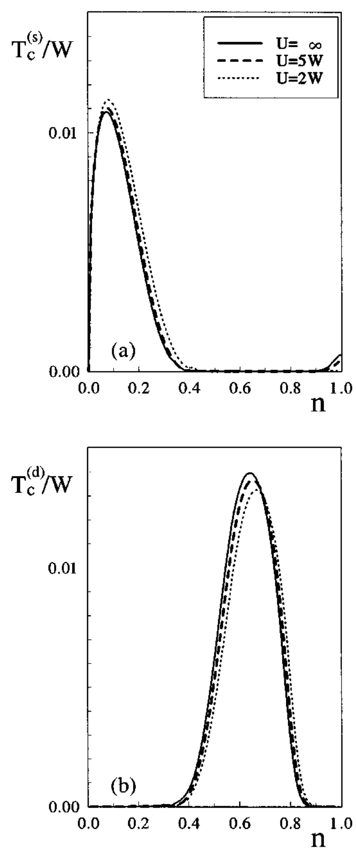

FIG. 3. Critical temperature for the s-wave superconducting state (a) and d-wave superconducting state (b) as a function of total carrier concentration $n=\langle n_{i\sigma}\rangle+\langle n_{i-\sigma}\rangle$. Strength of intersite attraction is in all cases the same and equal $V=-0.1W$. Values of U for particular curves are shown in the legend.

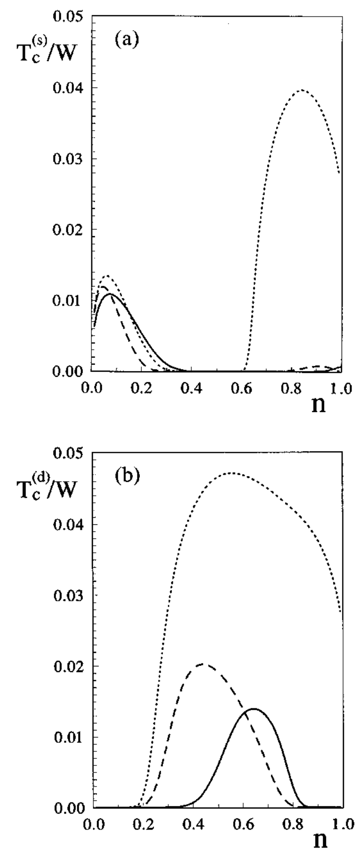

FIG. 4. Comparison of transition temperatures of s-wave (a) and d-wave (b) superconducting phases for the extended Hubbard model with $U=\infty$ and $V=-0.1W$. Solid lines refer to the Hubbard-Jain approximation, dashed ones to those obtained according to canonical transformation method[6] and dotted ones to the slave-boson approach.

$$\omega D^{\nu}_{k\sigma}=(E_{k\nu}-\tilde{\mu})D^{\nu}_{k\sigma}+\Delta_{k\nu}\sum_{\nu'=1,2}D^{\nu'\dagger}_{-k-\sigma}. \qquad (8)$$

Neglecting nondiagonal correlation functions, we arrive at the gap equation

$$\Delta_{k\nu}=\sum_{k'}\left[\frac{T_{k\nu}N_{k\nu}}{\varepsilon_k}(\varepsilon_k+2\varepsilon_{k'})+\frac{N_{k\nu}}{\varepsilon_k^2}2V_{k-k'}\right]\langle D^{\nu}_{-k'-\sigma}D^{\nu}_{k'\sigma}\rangle, \qquad (9)$$

where $T_{k\nu}=U/[E_{k\nu}(E_{k\nu}-U)]$. The gap equation (9) looks a little bit more complicated than that given previously (3). For comparison with the previous formulas let us evaluate it in the leading order with respect to $1/U$. In doing so we have to take into account that in the large-U limit ($U\rightarrow\infty$) the on-site pairing is prohibited. So we neglect all the terms which would lead to the formation of such pairs. Finally, for $n<1$ and for $U\rightarrow\infty$, we obtain that Δ_{k1} is expressed by Eq. (3) with $V_{kq}=(1-n/2)^2V\gamma_{k-q}$ and $\xi_q=\varepsilon_q(1-n/2)-\tilde{\mu}$.

Thus the Hubbard-subband-operator method leads in a natural way to renormalization of both: the single-particle energies and interactions. Renormalization of energies, however, does not lead to vanishing of the bandwidth at $n=1$. Further analytical comparison is a little bit complicated because in each case a position of the Fermi level has to be calculated for a given carrier concentration. For example, for $U\gg W$, the position of the Fermi level in the lower Hubbard subband ($n<1$) is given by the formula

$$\frac{n}{2}=\left(1-\frac{n}{2}\right)\sum_k f[(1-n/2)\varepsilon_k-\tilde{\mu}], \qquad (10)$$

where $f(x)=1/(e^{\beta x}+1)$ is the Fermi-Dirac distribution function.

For a numerical illustration of our results for the model (1) with arbitrary U, we use the general form of the gap equation (9). The $\vec{k}$-dependent gap function takes then the following form:

$$\Delta_{k\nu}=\frac{T_{k\nu}N_{k\nu}}{\varepsilon_k}\Delta_{\nu}^{(0)}+\frac{N_{k\nu}}{\varepsilon_k^2}\Delta_{\nu}^{(s)}\varepsilon_k+\frac{N_{k\nu}}{\varepsilon_k^2}\Delta_{\nu}^{(d)}\eta_k, \qquad (11)$$

where $\varepsilon_k=-2t(\cos k_x+\cos k_y)$, $\eta_k=-2t(\cos k_x-\cos k_x)$. Here $\Delta_{\nu}^{(0)}$, $\Delta_{\nu}^{(s)}$, and $\Delta_{\nu}^{(d)}$ refer to isotropic and extended s-wave or d-wave symmetry gap functions, respectively. The additional factors in front of them depend on $\vec{k}$ through ε_k only, and for $U>W$ are relatively slowly varying functions. Their dependence on ε_k for various values of U is shown in Fig. 1. With increasing U, both factors tend to their asymptotic values $[(T_{k1}N_{k1}/\varepsilon_k)\overset{U\rightarrow\infty}{=}-1,\ (N_{k1}/\varepsilon_k^2)\overset{U\rightarrow\infty}{=}1-n/2]$.

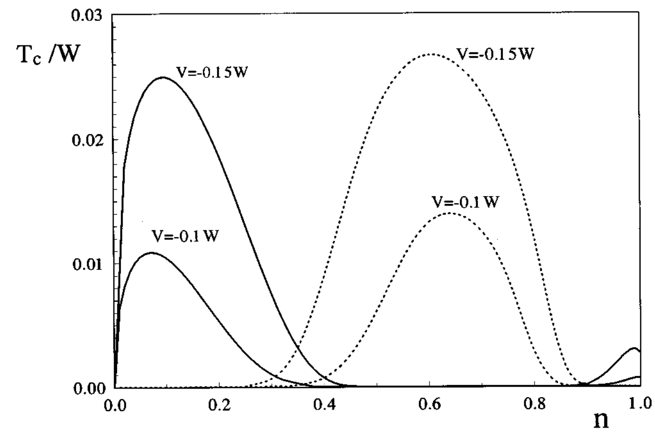

FIG. 5. Influence of the pairing potential V on the carrier dependence of $T_c^{(s)}$ (solid lines) and $T_c^{(d)}$ (dotted lines). The on-site interaction is in this case $U=10W$.

To get carrier concentration dependence of the transition temperature it is necessary to solve the gap equation self-consistently with the equation for chemical potential $\tilde{\mu}$. The dependence of $\tilde{\mu}$ on n is shown in Fig. 2(a). The thick lines denote edges of the lower subband, the dashed line shows $\tilde{\mu}$ for $T=0$ K and the dotted line at $T=0.1W$. Figure 2(b) shows $\tilde{\mu}_{\mathrm{SB}}=\mu-\lambda-2nV$. Note, that for $n=1$, the bandwidth vanishes in the slave-boson method.

The concentration dependences of $T_c^{(s)}$ and $T_c^{(d)}$ are plotted in Figs. 3(a) and 3(b), respectively, for a number of U values. Coulomb repulsion U has a small detrimental effect on the s-wave superconducting phase at low concentrations but $T_c^{(s)}$ remains finite (nonzero) even for $U=\infty$ (solid line). At low hole concentrations ($n\sim1$) there appears also another s-wave superconducting phase with very small $T_c^{(s)}$, which is relatively stable against U values. In fact, transition temperatures in that region increase with increasing U. The main effect of U on the d phase is a slight shift of maximal $T_c^{(d)}$ towards the lower concentrations n. The maximal value of $T_c^{(d)}$ surprisingly increases with increasing U.

Figure 4(a) shows the comparison of $T_c^{(s)}(n)$ calculated in the Hubbard-Jain approximation (solid line), strong-coupling expansion method (dashed line), and slave-boson approach (dotted line). Figure 4(b) presents similar data for $T_c^{(d)}(n)$.

It is important to note that in our approach the superconducting phase appears only for attractive interaction V. It is in contrast to slave-boson treatment of the present system[7] which, for finite U, leads to superconductivity even with repulsive V. Influence of the V strength on the magnitude of T_c is shown in Fig. 5. As is seen, values of critical temperatures considerably increase with increasing intersite attraction.

In conclusion, we have presented a study of the many-body effects of strong on-site repulsion U on BCS pairing in the extended Hubbard model. Contrary to the results in a Hartree-Fock treatment of U, we find that the strong U does not destroy the superconducting state produced by the weak intersite attractive interaction V. The s-wave superconductivity appears in the dilute regions (at small electron and small hole concentrations), while the d-wave phase arises around $\delta=0.33$, and for $V=-0.1W$ extends from $\delta\approx0.15$ to $\delta\approx0.6$. The maximal value of $T_c^{(d)}$ surprisingly increases with increasing U. It follows from this study as well as previous treatments of the correlated hopping model[11,12] by the same technique, that the main effect of on-site interaction U is a formation of Hubbard subbands and the BCS pairing occurs between the quasiparticles in the Hubbard subbands.

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