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 $U>|V_{ij}|$. [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. 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. 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 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 and slave-boson methods.

We take the Hamiltonian in the following form:

$$
H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow} + \sum_{i,j} V_{ij} n_{i\uparrow} n_{j\downarrow},
$$

$$
-\mu \sum_{i,\sigma} n_{i\sigma},
$$

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., in both weak- ($U \ll t$) and strong-coupling ($U \gg t$) limits. It has also been qualitatively analyzed in the Hubbard-Jain approach. However, no explicit calculations have been performed so far. In all cases we assume $|V| \ll W$, ($W=\pi t$ 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:

$$
H_{\text{eff}} = -\sum_{i,j,\sigma} t_{ij} h_{i\sigma}^\dagger h_{j\sigma} + \sum_{i,j} J_{ij}(\delta_{i,j} - \frac{1}{4} N_i N_j)
$$

$$
+ \sum_{i,j} V_{ij} N_i N_j - \mu \sum_{i,\sigma} n_{i\sigma},
$$

where $h_{i\sigma} = c_{i\sigma}^\dagger (1-n_{i\sigma})$, $N_{i\sigma} = h_{i\sigma}^\dagger h_{i\sigma} = n_{i\sigma} (1-n_{i\sigma})$, $N_i = \sum_{\sigma} N_{i\sigma}$, $\delta_{i,j} = c_{i\uparrow}^\dagger c_{j\uparrow}$, $\delta_{i,j} = \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})$ and $J_{ij} = 2t_{ij}^2/U$. 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:

$$
\Delta_{k} = \frac{1}{N} \sum_{q} V_{kq} \frac{\Delta_{q}}{2E_{q}} \tanh \left( \frac{\beta E_{q}}{2} \right)
$$

with $E_{q} = \sqrt{\xi_{q}^2 + |\Delta_{q}|^2}$ and $\xi_{q} = \delta \cdot \epsilon_{q} - \mu$ 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 $\delta$. 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 boson field ($b_{i}$) operators. The require-
FIG. 1. Plot of the $N_{k_1}T_{k_1}/\varepsilon_{k_1}$ function (a) and the normalized $N_{k_1}/\varepsilon_{k_1}^2$ function (b) versus single-particle energy $\varepsilon_{k_1}$ for several values of $U$.

renormalization of interaction 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

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

Here $n_i = \sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma}$, and $\lambda_i$ denotes the Lagrange multiplier. The mean field for slave bosons means replacement of all bosonic fields by their classic values $b_i = b_i^0 = r$ and $\lambda_i = \lambda$. Parameters $\lambda$ 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 $\lambda = -\varepsilon_0 n V / \varepsilon_k$.

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

The Hubbard subband operator approach relies on the introduction of new operators $d_{i\sigma}^\dagger = n_i^\dagger - c_{i\sigma}$ and their conjugate counterparts $d_{i\sigma} = (d_{i\sigma}^\dagger)^\dagger$, where $n_i^\dagger = 1 - n_{i\sigma}$ 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

$$\omega d_{k\sigma} = \left( \varepsilon_{\sigma} - \overline{\mu} \right) d_{k\sigma} + n_{\varepsilon_k} c_{k\sigma}$$

$$+ e_{k'} \sum_{k'} \left[ (1)^{\sigma} (\varepsilon_{k'} + 2 \varepsilon_{k'}) + 2n \sum_{k'} V_{k-k'} \right] c_{-k'} + \sum_{\sigma} c_{k\sigma}$$

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

$$E_{k\sigma} = \frac{-1}{2} \left[ U + \varepsilon + (1)^{\sigma} \sqrt{(U - \varepsilon_k)^2 + 2nU\varepsilon_k} \right]$$

and

$$N_{k\sigma} = \left[ \frac{n/2}{(E_{k\sigma} - U)^2} + \frac{1 - n/2}{E_{k\sigma}^2} \right]^{-1}.$$
FIG. 3. Critical temperature for the $s$-wave superconducting state (a) and $d$-wave superconducting state (b) as a function of total carrier concentration $n = (n_{\uparrow\uparrow}) + (n_{\downarrow\downarrow})$. 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.

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

Neglecting nondiagonal correlation functions, we arrive at the gap equation

$$\Delta_{k\nu} = \sum_{k'} \left[ T_{k\nu} N_{k\nu}(e_k + 2e_{k'}) + \frac{N_{k\nu}}{e_k} 2V_{k-k'} \right] \langle D^{\nu}_{-k'-\sigma} D^{\sigma}_{k\sigma} \rangle,$$  \hfill (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 ($U \to \infty$) the on-site pairing is prohibited. So we neglect all the terms which would lead to the formation of such pairs. Finally, for $n \leq 1$ and for $U \to \infty$, we obtain that $\Delta_{k\nu}$ is expressed by Eq. (3) with $V_{k-q} = (1-n/2)^2 V_{k-q} \xi_q = e_q(1-n/2) - \tilde{\mu}$.

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

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

where $f(x) = 1/\{e^{Rx} + 1\}$ 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 $k$-dependent gap function takes then the following form:

$$\Delta_{k\nu} = \frac{T_{k\nu} N_{k\nu}}{e_k} \Delta^{(0)}_{\nu} + \frac{N_{k\nu}}{e_k} \Delta^{(s)}_{\nu} e_k + \frac{N_{k\nu}}{e_k} \Delta^{(d)}_{\nu} \eta_k,$$  \hfill (11)

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

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 the BCS approximation according to canonical transformation method$^6$ and dotted ones to the slave-boson approach.
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 $\mu$. The dependence of $\mu$ on $n$ is shown in Fig. 2(a). The thick lines denote edges of the lower subband, the dashed line shows $\mu$ for $T = 0$ K and the dotted line at $T = 0.1W$. Figure 2(b) shows $\mu_{SB} = \mu - 2nV$. 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 ($n \approx 1$) there appears 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 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 $\delta \approx 0.15$ to $\delta = 0.6$. 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 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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