# Hole superconductivity in Hubbard subbands

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We study the superconducting properties of the system described by the correlated-hopping model in the limit of intermediate and strong correlations. The main effect of the Hubbard term $U$ is reflected in the appearance of the separated Hubbard subbands. The other interaction term $K_{ij}$ in the Hamiltonian introduces the correlation between quasiparticles and for small number of holes in the system leads to the appearance of superconductivity. The superconducting transition temperature hardly changes with $U$ in the approximation we use. We have found the dependence of the superconducting energy gap on temperature $T$ and energy $\varepsilon_k$. It turns out to be a nearly linear function of $\varepsilon_k$. The temperature dependence of the two components of the gap slightly differ from the BCS $\Delta(T)$ function. The effective gap to the $T_c$ ratio strongly depends on the carrier concentration $n$ taking on large values for small $n$ ($n<0.1$) and being close to the BCS value of 1.76 at larger $n$.

## I. INTRODUCTION

There is growing evidence that high-$T_c$ superconducting (HTS) oxides possess a number of common characteristics.[1,2] They may be caused by some properties shared by all HTS's like the quasi-two-dimensional nature of the Cu-O planes, the short coherence length, low Fermi energy, etc. It is, however, not obvious which of these properties are really important as some universal features of HTS are observed[1] also in heavy fermion superconductors with very low transition temperatures and cubic (fcc) alkali-metal doped fullerides.

One of the models studied, with hopes of explaining the phenomenon of HTS, is the "correlated-hopping"[3] or "hole-superconductivity"[4] model. It belongs to the family of extended Hubbard models and has been argued to capture a lot of physics of high-temperature superconducting oxides.

In the previous works (see Refs. 3 and 4 and references therein) the model has been studied mainly in the Hartree-Fock-Bogolubov approximation. One expects this mean-field scheme not to be valid for the large values of $U$ (on-site correlation energy) used in those studies. On the other hand, the "correlated-hopping" parameter $K$ has been estimated[4] to be of the order of the bandwidth $W$ or larger, and seems to be unphysically large. The value of $U$ has been taken ten times larger than $W$, and has had a very destructive effect on $T_c$.

In the present work we shall study the "correlated-hopping" model by using the approximation developed previously by Hubbard[5] and Hubbard and Jain[6] and shown to lead to correct behavior of susceptibility in the weak and strong correlation limits. This scheme has already been extended to study the superconductivity in the Hubbard model with a positive and negative $U$ (Ref. 7) and also has been applied to the "correlated-hopping" model by Das and Das.[8] We extend the previous work and consider not only $T_c$ but also the energy gap, density of states, etc. In Sec. II we shall discuss the model and main points of its solution. In Sec. III we present the results of numerical calculations and compare them with the corresponding data obtained in the mean-field approximation.

## II. HAMILTONIAN AND THE SOLUTION

The Hubbard Hamiltonian with a correlated hopping term can be written as[3,4]

$$H=-\sum_{ij\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}-\mu\sum_{i\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}+\tfrac{1}{2}U\sum_{i\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}c_{i-\sigma}^{\dagger}c_{i-\sigma}$$
$$-\sum_{ij}K_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}(n_{i-\sigma}+n_{j-\sigma})\ , \tag{1}$$

where $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) is the electron annihilation (creation) operator, $t_{ij}$ is the hopping integral (for the clean system we take $t_{ii}=0$), $K_{ij}$ denotes the correlated-hopping term (hopping modulated by the presence or absence of electrons on sites $i$ and $j$), $\mu$ denotes the chemical potential, and $U$ represents the on-site electron-electron repulsion ($U>0$). For the nearest-neighbor hopping in two dimensions we have $t_{ij}=t$, $K_{ij}=Kt_{ij}$, and $W=8t$, where $W$ is the bandwidth.

The term $K_{ij}$ has been estimated[5] to be an order of magnitude smaller than the diagonal Coulomb repulsion $U$. It is also smaller than other off-diagonal terms $V_{ij}$, previously considered in the same context.[7] The arguments for the importance of the $K_{ij}$ term have been extensively discussed in the literature (see Hirsch and Marsiglio papers,[4] and the references therein).

Following the Hubbard work[5] we introduce for the normal system in the intermediate region of interaction $U$ the new operators $d_{i\sigma}^{\alpha}$ defined as

$$d_{i\sigma}^{\alpha}=n_{i-\sigma}^{\alpha}c_{i\sigma}\quad\text{for }\alpha=1,2\ , \tag{2}$$

where $n_{i\sigma}^{1}=1-n_{i\sigma}$, $n_{i\sigma}^{2}=n_{i\sigma}$, and

$$c_{i\sigma}=\sum_{\alpha}d_{i\sigma}^{\alpha}\ . \tag{3}$$

Operator $d_{i\sigma}^{1}=(1-n_{i-\sigma})c_{i\sigma}$ acts on the Hilbert subspace of singly occupied states and $d_{i\sigma}^{2}=n_{i-\sigma}c_{i\sigma}$ on the

 

subspace of doubly occupied states. Their conjugate counterparts $d_{i\sigma}^{1+}, d_{i\sigma}^{2+}$ act in the subspaces of empty and singly occupied states, respectively. Such a division of the Hilbert subspace of the single site reflects some physics of the narrow band correlated systems where we do expect the appearance of subbands connected with singly and doubly occupied states.

Because our treatment of the Hamiltonian (1) nearly exactly traces the calculations of Jain and co-workers[7] and Das and Das[8] we shall skip all the details and merely discuss some salient features of the calculations and approximations.

One writes the equation of motion for the operators $d_{i\sigma}^{\alpha}$. The resulting highly nonlinear terms appearing on the right-hand side of the obtained equation are linearized in the spirit of the Hartree-Fock-Bogolubov approximation.[6-9] There is a difference, however, between our treatment of the $K_{ij}$ term and that of the work.[8] We have adopted an approach similar in spirit to one used by Jain and co-workers[7] in their study of superconductivity in the Hubbard model with the on-site $U$ and intersite $V_{ij}$ terms and have neglected the modifications of the normal-state spectrum by the "correlated-hopping" term. Our subband energies, therefore, are defined in the same way as in Ref. 5 and 7 and read

$$E_{k\nu}=\tfrac{1}{2}(U+\varepsilon_k)+\tfrac{1}{2}(-1)^{\nu}[(U-\varepsilon_k)^2+2nU]^{1/2} , \quad (4)$$

with carrier concentration $n\in[0,2]$. We then define, again following Refs. 6 and 7, the annihilation operators for electrons (holes) in subbands by

$$D_{k\sigma}^{\nu}=\varepsilon_k^{-1}N_{k\nu}\left[\frac{d_{k\sigma}^{1}}{(E_{k\nu}-U)}+\frac{d_{k\sigma}^{2}}{E_{k\nu}}\right] \quad (5)$$

where

$$N_{k\nu}^{-1}=\sum_{\alpha=1,2}\frac{n_\alpha}{(E_{k\nu}-\varepsilon_\alpha)^2} \quad (6)$$

and

$$\varepsilon_\alpha=\begin{cases}0 & \text{for } \alpha=1 ,\\ U & \text{for } \alpha=2 .\end{cases} \quad (7)$$

The BCS-like equations for the generalized gap functions,

$$\Delta_{k\nu}=X_{k\nu}\tilde{\varepsilon}_0+Y_{k\nu}\lambda , \quad (8)$$

for the upper and lower subbands ($\nu=1,2$), are derived in the standard way[7,8] and read

$$\Delta_{k\nu}=\frac{1}{2}\sum_q\sum_\alpha[X_{k\nu}\varepsilon_q-Y_{k\nu}]\times\frac{N_{q\alpha}\Delta_{q\alpha}}{\varepsilon_q^2\tilde{E}_{q\alpha}}[f(\tilde{E}_{q\alpha})-f(-\tilde{E}_{q\alpha})] . \quad (9)$$

Here we use the following abbreviations:

$$\tilde{E}_{k\nu}=\sqrt{(E'_{k\nu}-\mu)^2+\Delta_{k\nu}^2} \quad (10)$$

and

$$E'_{k\nu}=E_{k\nu}+\frac{N_{k\nu}nK}{\varepsilon_k} . \quad (11)$$

The parameter $K$ is determined by the relation $K_k=K\varepsilon_k$ and the coefficients $Y_{k\nu},X_{k\nu}$ denote respectively

$$Y_{k\nu}=N_{k\nu}T_{k\nu}\left[1+\frac{Kn}{2}\right]-\frac{2N_{k\nu}}{\varepsilon_k}K ,$$

$$X_{k\nu}=N_{k\nu}T_{k\nu}\left[\frac{2}{\varepsilon_k}+\frac{3Kn}{2\varepsilon_k}\right]+\frac{2N_{k\nu}}{\varepsilon_k^2}K , \quad (12)$$

and

$$T_{k\nu}=\frac{U}{E_{k\nu}(E_{k\nu}-U)} .$$

The equation (9) for the gap is supplemented by the equation for the carrier concentration $n$,

$$n=\sum_k\sum_\nu\frac{N_{k\nu}}{\varepsilon_k^2}\left[\left[1+\frac{E'_{k\nu}-\mu}{\tilde{E}_{k\nu}}\right]f(\tilde{E}_{k\nu})+\left[1-\frac{E'_{k\nu}-\mu}{\tilde{E}_{k\nu}}\right]f(-\tilde{E}_{k\nu})\right] . \quad (13)$$

In deriving Eqs. (9) and (13) we have assumed that for the large and positive $U$ that we are interested in, the intersubband pairing can be neglected.

Our neglect of the effect of $K_{ij}$ on subband energies has the virtue that subsequent expressions for parameters $N_{k\nu}$ and $T_{k\nu}$ are exact. Taking this correction into account leads to expressions more complicated than those used in previous treatments of the model.[8] As already mentioned, the importance of the "correlated-hopping" term is connected with the special correlations it introduces between the holes in the band. These lead to the superconducting instabilities in the system. In our case it is the $U$ term in the Hamiltonian which is mainly responsible for the modifications of the normal-state spectrum.

## III. RESULTS

We start the discussion of the results with some details on the normal-state spectrum of the model. As previously discussed, the main effect of the large Hubbard $U$ term is connected with the appearance of Hubbard subbands of singly and doubly occupied states. The gap which appears in the spectrum is of the order of $U$, and it is a well-known drawback of this approximation that it gives a gap for any value of $U$. In Fig. 1 we plot the Hubbard energies $E'_{k\nu}$ defined in Eq. (11) as a function of single particle energies $\varepsilon_k$, both measured in units of the bandwidth. The parameters used for this and most of the other figures are $U=10W$ and $K=5$, and correspond to those taken by Hirsch and Marsiglio[4] in their mean-field study of the model.

A few features can be noted. The dependence of both subband energies $E'_{k\nu}$, $\nu=1,2$, on $\varepsilon_k$ is nearly linear. The lower band (in our notation $\nu=1$) has the larger slope and width while the upper one is very narrow. Their separation depends on the value of $\varepsilon_k$, but it is roughly of

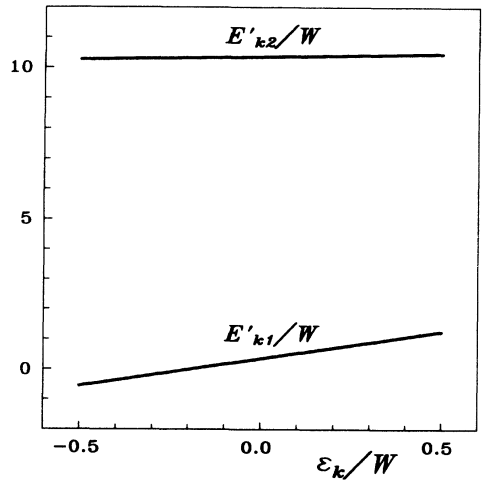


FIG. 1. The energy of the Hubbard subbands $E'_{kv}$ [see Eqs. (11) and (4)] in the normal state with the "correlated term" taken into account. Both $E'_{kv}$ and $\varepsilon_k$ are expressed in the units of bandwidth $W$.

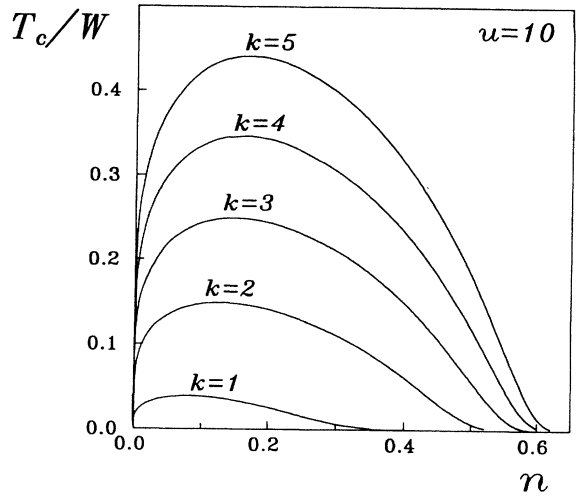


FIG. 3. The dependence of the transition temperature $T_c$ on $n$ for various values of the "correlated hopping" term $k$ and $u=10$.

the order of $U$. Another important feature is the dependence of the Fermi level on carrier density $n$. It is a functional of the host metal density of states (DOS). In this paper we assume the constant DOS to describe the band $\varepsilon_k$. This is correct for a free two-dimensional electron gas and serves as a good approximation for square lattice and low densities. The corresponding $\mu(n)$ functions for three different temperatures $T=0$, $0.1W$, and $0.4W$ are plotted in Fig. 2. The zero-temperature $\mu(n)$ function shows nearly linear dependence on the concentration $n$ in both subbands with a discontinuity at $n=1$. At higher temperatures, $T>0$, the departures from linearity near the edges of subbands are easily visible. Our calculations of $T_c$ have all been carried on self-consistently, that means that for each concentration $n$ we have obtained $T_c$ using the actual chemical potential value, i.e., $\mu(n, T=T_c)$.

The obtained dependence of $T_c$ on $n$ for $u \equiv U/W=10$ and a number of $k \equiv K$ values is plotted in Fig. 3. It is seen that the transition temperature reaches very high values in the range from $0.1W$ to $0.5W$ despite the large value of the repulsive term $U$. The range of concentrations for which $T_c$ is different from zero quite strongly depends on the value of the "correlated-hopping" term $K$.

On the other hand neither the value of $T_c$ nor the range of concentrations for which the material is superconducting at low temperatures appreciably depend on $U/W$. As shown in Fig. 4, for $k=4$ both $T_c$ and $n_{\max}$ (defined as maximal concentration for which $T_c \neq 0$) hardly change with changing $u$ (ranging from 5 to 20). This result nicely agrees with the corresponding calcula-

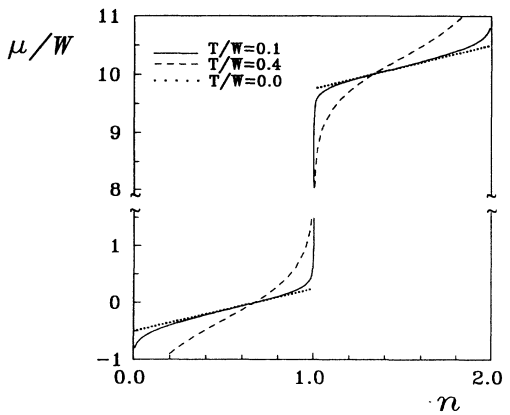


FIG. 2. The chemical potential as a function of concentration $n$ for $T=0$ K (dotted line), $T=0.1W$ (solid line), and $T=0.4W$ (dashed line). Note the jump of $\mu$ at half filling $n=1$.

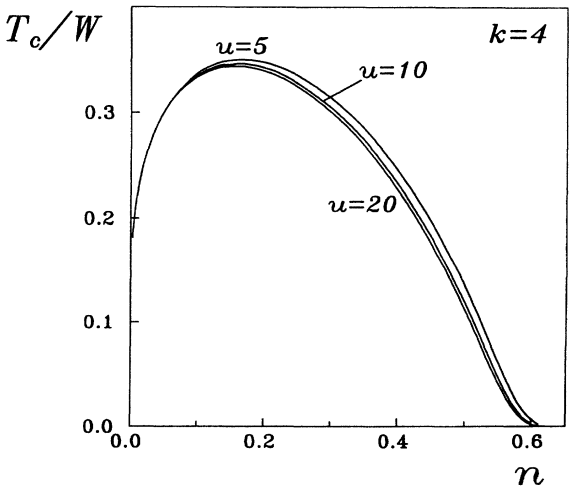


FIG. 4. The on-site Coulomb repulsion $u$ has a little influence on $T_c(n)$. Here we show $T_c$ in units of bandwidth $W$ for $k=4$ and $u=5, 10, 20$.

tions via the slave-boson technique.[10]

Our interpretation of this result which is in strong contrast to the mean-field calculations[3,4] is the following. In the first order, the presence of the large $U$ results in the appearance of two subbands accompanied by the corresponding mass renormalizations visible in their relative narrowness. The term $K_{ij}$ introduces (in the off-diagonal terms) superconducting correlations between carriers and this explains why $T_c$ does not (in the first order) depend on $U$.

In this context it is important to remark that the "particle-hole" symmetry, observed[3] in the mean-field treatment of the present model $T_c(n,K)=T_c(2-n,-K)$ is violated in this case. We have calculated $T_c$ for $u=10$ and $k=-5$ and found that the system is superconducting for the upper subband being partially occupied. The value of $T_c$ (see Fig. 5) is, however, smaller (approximately by the factor of 2). At present we do not know whether this "particle-hole" asymmetry can serve as an explanation of the experimentally observed asymmetry between hole[11] and electron[12] superconductors.

The special version of the model with $K_{ij}=0$, and also supplemented by the $V_{ij}$ term, has been previously studied analytically by Jain, Ramakumar, and Chancey.[7] Our explicit numerical calculations nicely agree with the conclusion obtained by these authors that "large $U$ values may not preclude the appearance of the superconductivity in the system".[7,13]

We believe that the approximations adopted here have to be modified when dealing with the negative-$U$ Hubbard model so we cannot directly compare with the previous work on that model. Recently the same method has been used to study two band model with interlayer coupling, but no numerical results have been presented.[14]

Inspection of Eqs. (8) and (12) shows that the gaps $\Delta_{k,\nu}$ depend in a complicated way on the wave vector $\mathbf{k}$ (or rather energy $\varepsilon_k$). In general, we have two unknown parameters $\tilde{\varepsilon}_0$ and $\lambda$. Using the form (8) for $\Delta_{k\nu}$ we have solved (9) numerically finding $\lambda$ and $\tilde{\varepsilon}_0$ for various temperatures. The $T$ dependence of both parameters has been plotted in Fig. 6 for $u=10$ and $n=0.2$. The inset shows the ratio of both parameters. Over a large temperature range the ratio is constant. Its value depends on the Hamiltonian parameters. Here we show it for $u=10$ and $k=5,4,3,2$.

Having $\lambda$ and $\tilde{\varepsilon}_0$ we can calculate the $(T,\varepsilon_k)$ dependence of the gaps $\Delta_{k\nu}$, $\nu=1,2$. These results are shown in Figs. 7 and 8. For all practical purposes and in a broad

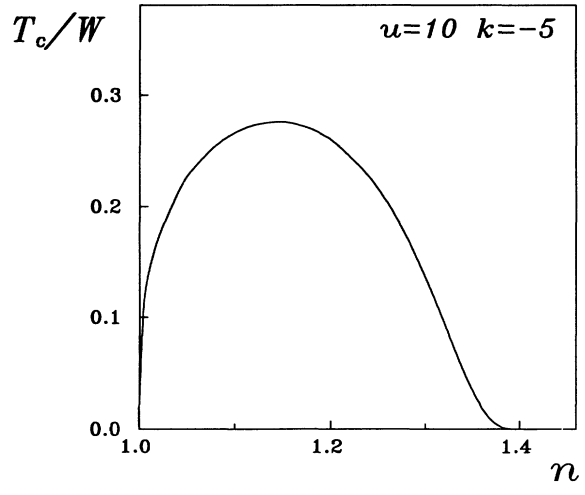


FIG. 5. For negative values of $k$ the system undergoes the metal superconductor transition for $n>1$. Here we plot the critical temperature in the upper Hubbard subband ($\nu=2$) for $u=10$, $k=-5$. Comparison with the $u=10$, $k=5$ case presented in Fig. 3 shows the differences between "hole" and "electron" superconductivity.

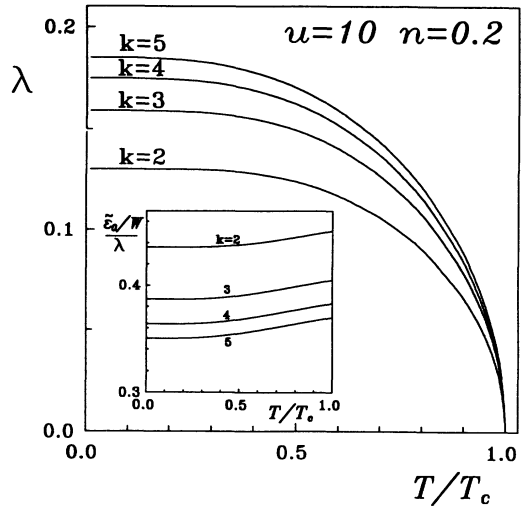


FIG. 6. The temperature dependence of $\lambda$ (in inset we plot $\tilde{\varepsilon}_0/\lambda$) for $u=10$ and several values of $k$. The concentration $n=0.2$, corresponds to maximal values of $T_c$ for the parameters studied.

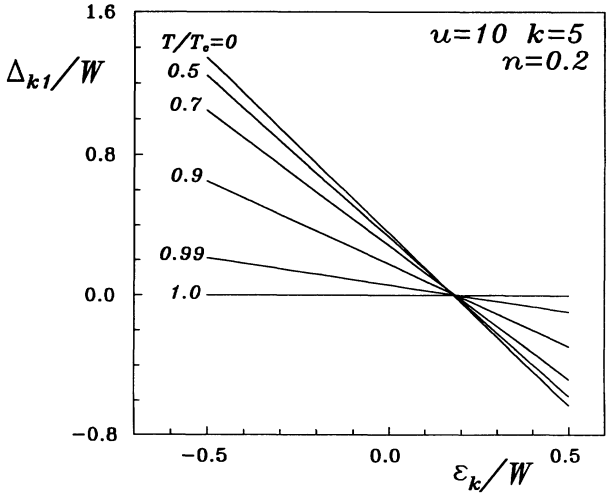


FIG. 7. The gap function $\Delta_{k1}$ vs energy $\varepsilon_k$ (both measured in the bandwidth units $W$) for various temperatures, ranging from $T=T_c$ to $T=0$. The *nearly* linear dependence is observed. At one point ($\varepsilon^*$) the gap changes its sign.

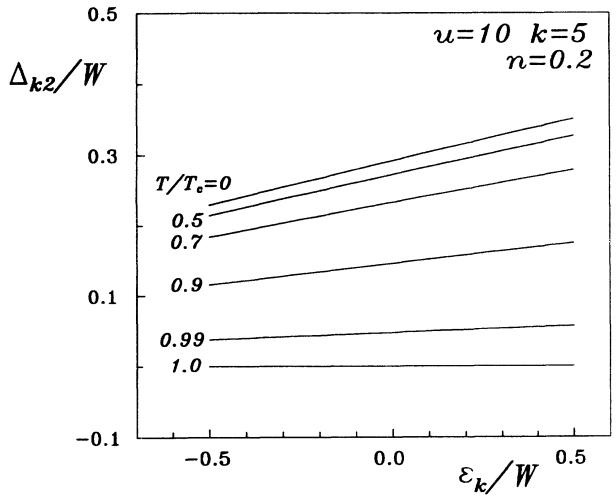


FIG. 8. The same as in Fig. 7 but for $\Delta_{k2}$.

range of parameter values the dependence is nearly linear,

$$\Delta_{k\nu} \approx \Delta_{0\nu} + \Delta_{1\nu}\varepsilon_k \ , \tag{14}$$

with $T$ dependent $\Delta_{0\nu}$ and $\Delta_{1\nu}$, $\nu=1,2$. Note the appreciable concentration and temperature dependence of the first term. In a previous work[8] the form (14) of the gap without the first term has been assumed at the outset. This is incorrect and leads to changes in all calculated characteristics.

We also note the very high maximal values of the gap in the lower band (Fig. 7) and smaller values in the upper one (Fig. 8). The slope of the $\Delta_{k\nu}$ is positive in the upper subband and negative in lower one, where it also changes its sign. The point $\varepsilon^*$ at which $\Delta_{k2}$ changes the sign does not depend on temperature. In a sense such a change of sign does not lead to physical effects as the modulus of the gap enters the various formulas.

To see the structure of spectrum of material in the superconducting state we have shown in Fig. 9 the density of states $D(\tilde{E})$ defined via

$$D(\tilde{E}) \equiv \frac{\partial \varepsilon}{\partial \tilde{E}} \tag{15}$$

where $\tilde{E}$ is, for each $\mathbf{k}$, defined in Eq. (10). In fact, such $D(\tilde{E})$ is the superconducting state DOS divided by the normal-metal density of states $\rho(\varepsilon)$,

$$\rho(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k) \ . \tag{16}$$

In this work the normal-metal DOS $\rho(\varepsilon)$ is assumed to be constant and is shown in Fig. 9 by the dashed lines, which formally represent $D(E-\mu)$ functions. At $T=0$ we see the typical (but asymmetric due to energy dependence of $\Delta_{k\nu}$) DOS of the BCS type in the lower subband and very narrow, slightly modified in the superconducting state as compared to the normal state DOS in the upper subband.

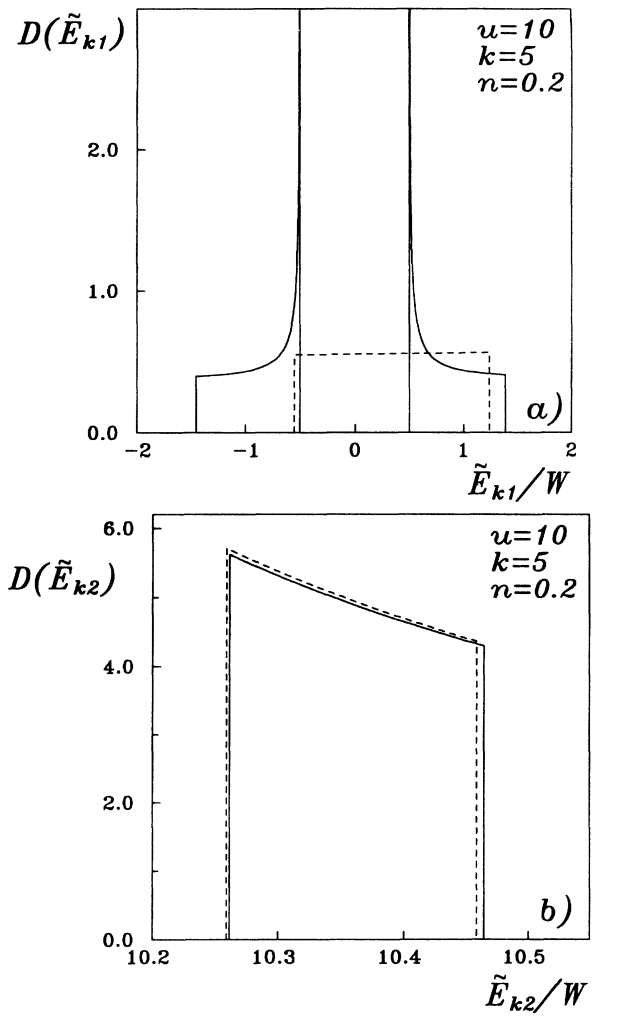


FIG. 9. The superconducting density of states (solid line) in (a) the lower and (b) the upper subbands for $u=10$, $k=5$, and $n=0.2$. The dashed curves describe the corresponding densities of states of the normal material, i.e., $D(E'_{k\nu}-\mu)$. Note the difference of the used scales.

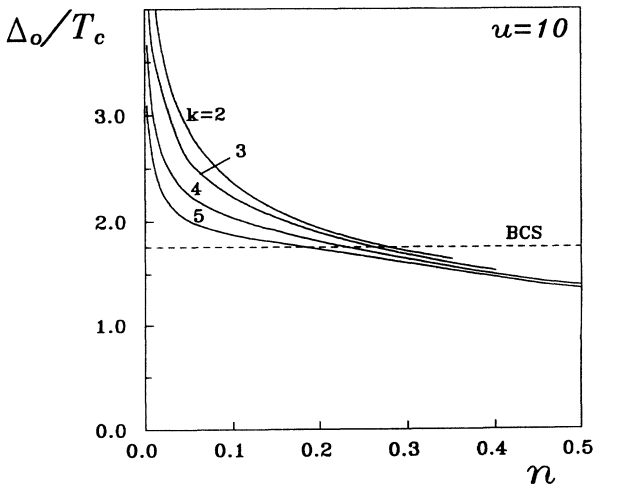


FIG. 10. The ratio of the effective energy gap $\Delta_0$ at zero temperature [as shown in Fig. 9(a)] and the transition temperature $T_c$ as a function of concentration $n$. The BCS theory prediction is plotted in the figure by the dashed line.

The value of the gap seen in the lower subband is (like $T_c$) concentration dependent and we denote it by $\Delta_0$ (subscript 0 referring to the zero temperature). The $n$ dependence of the ratio $\Delta_0/T_c$ is plotted in Fig. 10 for $u=10$ and several values of $k$. Instead of the BCS value 1.76 we have a strongly varying function with large values at low concentrations and smaller values of order 1.5 at higher concentrations. These trends are similar to what has been found in mean-field theory.[4]

## IV. CONCLUSIONS

We have studied the properties of the "correlated-hopping" model of superconductivity employing the Hubbard-Jain[6] approximation to treat the correlation problem in the normal-state and Hartree-Fock type of approximations in the superconducting sector of the theory.

The properties of the system in various aspects resemble those obtained in the mean-field treatment. The transition temperature $T_c$ is different from zero in a relatively narrow range of concentrations, the gap is a nearly linear function of energy, the effective gap to $T_c$ ratio diminishes with increasing concentration.

The approximation we use has the virtue that it describes better the normal-state properties in the intermediate and strong correlation limit. In the superconducting state it leads to nearly $U$ independent $T_c$ and $n_{\max}$—the concentration of carriers at which the system ceases to undergo metal-superconductor transition. Our results can explain why even very strongly correlated (large $U$) systems can become superconducting. We believe the present approximation improves previous mean-field calculations.[3,4]

## ACKNOWLEDGMENTS

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