

Hole superconductivity in Hubbard subbands

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(Received 14 July 1993; revised manuscript received 30 November 1993)

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 ϵ_k . It turns out to be a nearly linear function of ϵ_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 observed¹ also in heavy fermion superconductors with very low transition temperatures and cubic (fcc) alkali-metal doped fullerenes.

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 estimated⁴ 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 Hubbard⁵ and Hubbard and Jain⁶ 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 re-

sults 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}

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

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), μ 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 estimated⁵ 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 Margaglio papers,⁴ and the references therein).

Following the Hubbard work⁵ we introduce for the normal system in the intermediate region of interaction U the new operators $d_{i\sigma}^\alpha$ defined as

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

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

$$c_{i\sigma} = \sum_{\alpha} d_{i\sigma}^\alpha. \quad (3)$$

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-workers⁷ and Das and Das⁸ 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-workers⁷ 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

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

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,

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

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

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

Here we use the following abbreviations:

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

and

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

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

$$Y_{k\nu} = N_{k\nu} T_{k\nu} \left[1 + \frac{Kn}{2} \right] - \frac{2N_{k\nu}}{\varepsilon_k} K, \quad (12)$$

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

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 ,

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

In deriving Eqs. (9) and (13) we have assumed that for the large and positive U that we are interested in, the inter-subband 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 ε_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 Marsiglio⁴ 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 ε_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 ε_k , but it is roughly of

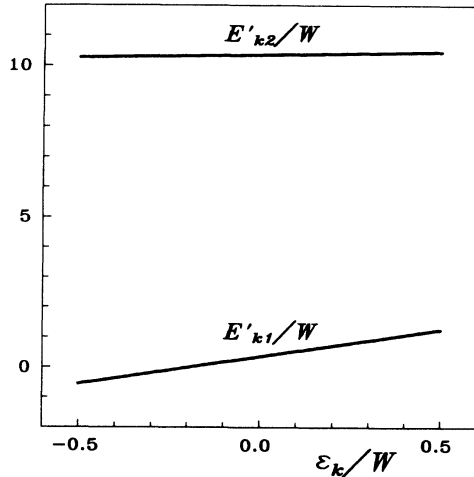


FIG. 1. The energy of the Hubbard subbands E'_{kv} [see Eqs. (11) and (4)] in the normal state with the “correlated term” taken into account. Both E'_{kv} and ϵ_k are expressed in the units of bandwidth W .

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 ϵ_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., $\mu(n, T=T_c)$.

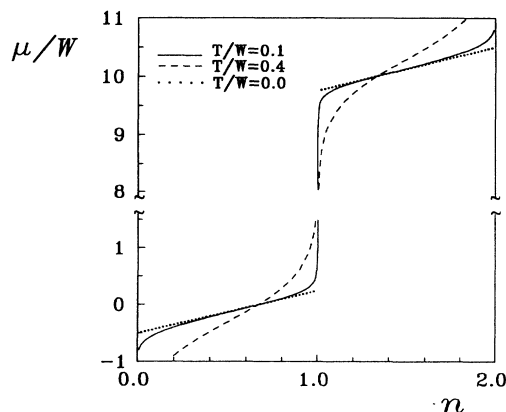


FIG. 2. The chemical potential as a function of concentration n for $T=0$ K (dotted line), $T=0.1W$ (solid line), and $T=0.4W$ (dashed line). Note the jump of μ at half filling $n=1$.

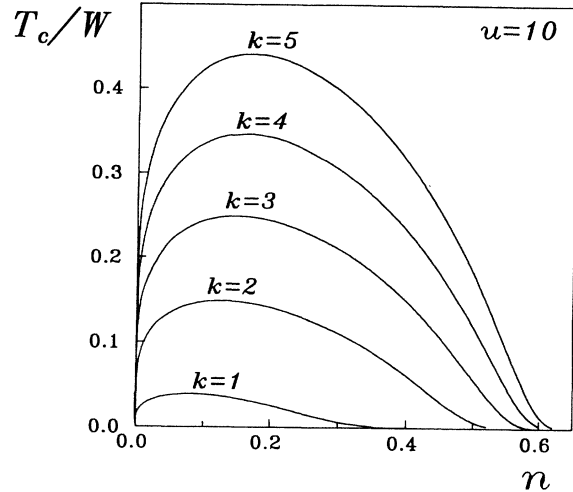


FIG. 3. The dependence of the transition temperature T_c on n for various values of the “correlated hopping” term k and $u=10$.

The 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-

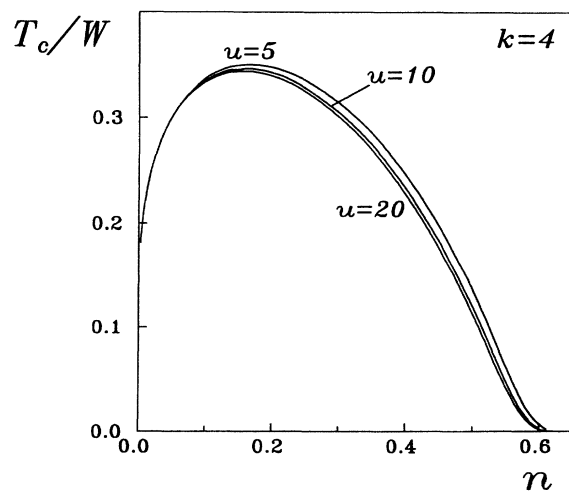


FIG. 4. The on-site Coulomb repulsion u has a little influence on $T_c(n)$. Here we show T_c in units of bandwidth W for $k=4$ and $u=5, 10, 20$.

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, observed³ 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 hole¹¹ and electron¹² 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 $\Delta_{k,\nu}$

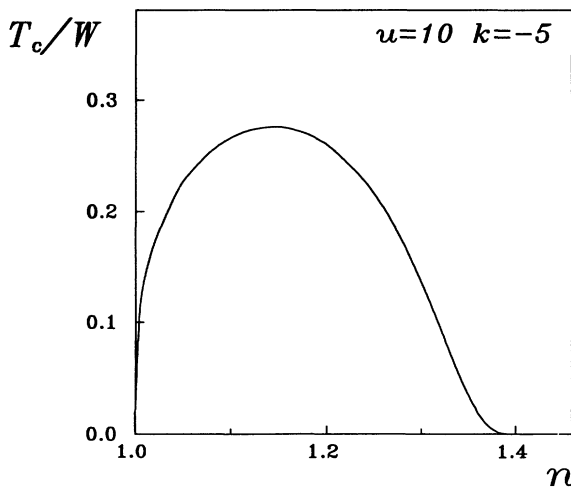


FIG. 5. For negative values of k the system undergoes the metal superconductor transition for $n > 1$. Here we plot the critical temperature in the upper Hubbard subband ($\nu=2$) for $u=10$, $k=-5$. Comparison with the $u=10$, $k=5$ case presented in Fig. 3 shows the differences between “hole” and “electron”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

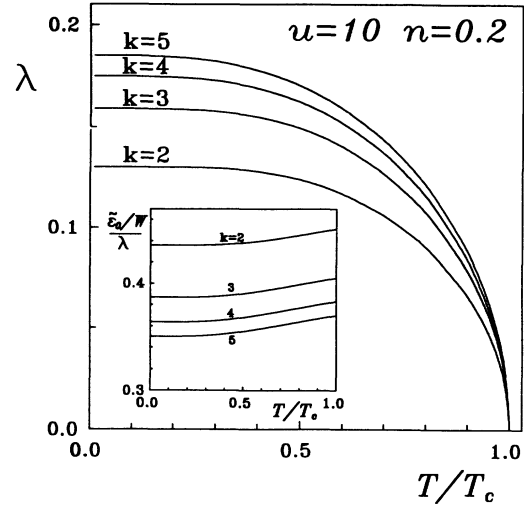


FIG. 6. The temperature dependence of λ (in inset we plot $\bar{\epsilon}_0/\lambda$) for $u=10$ and several values of k . The concentration $n=0.2$, corresponds to maximal values of T_c for the parameters studied.

depend in a complicated way on the wave vector \mathbf{k} (or rather energy ϵ_k). In general, we have two unknown parameters $\bar{\epsilon}_0$ and λ . Using the form (8) for $\Delta_{k,\nu}$ we have solved (9) numerically finding λ and $\bar{\epsilon}_0$ 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 λ and $\bar{\epsilon}_0$ we can calculate the (T, ϵ_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

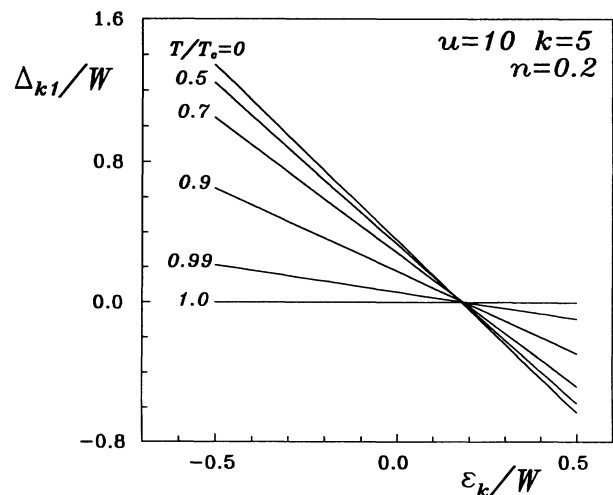
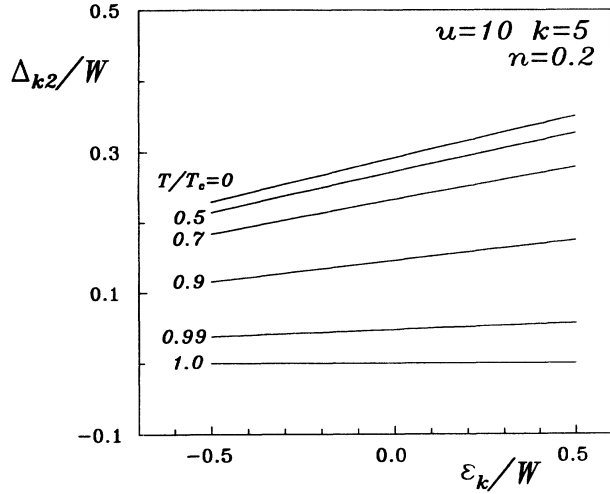


FIG. 7. The gap function Δ_{k1} vs energy ϵ_k (both measured in the bandwidth units W) for various temperatures, ranging from $T=T_c$ to $T=0$. The nearly linear dependence is observed. At one point (ϵ^*) the gap changes its sign.

FIG. 8. The same as in Fig. 7 but for Δ_{k2} .

range of parameter values the dependence is nearly linear,

$$\Delta_{k\nu} \approx \Delta_{0\nu} + \Delta_{1\nu} \varepsilon_k, \quad (14)$$

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 work⁸ 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 ε^* at which Δ_{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

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

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 $\rho(\varepsilon)$,

$$\rho(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k). \quad (16)$$

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.

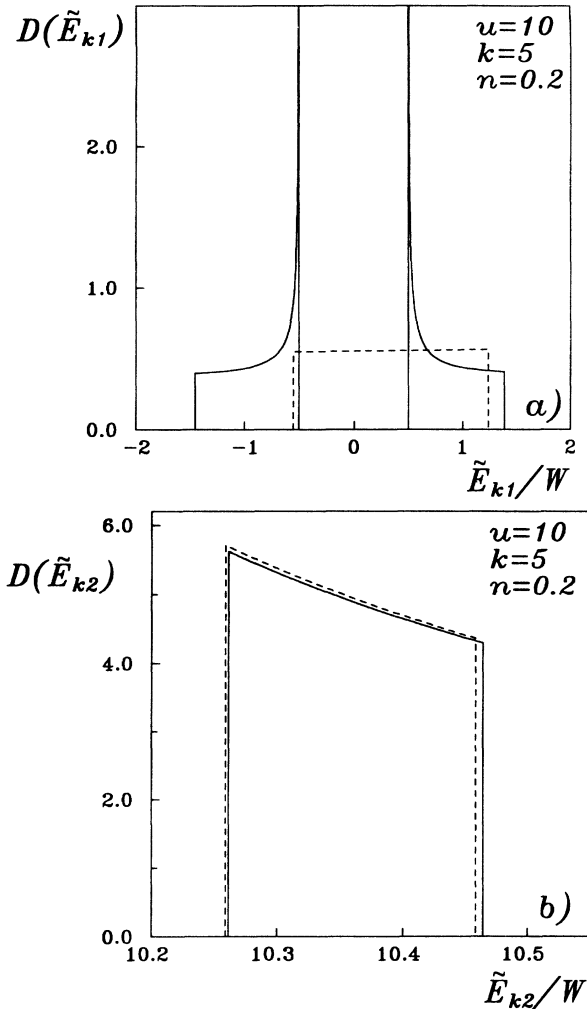


FIG. 9. The superconducting density of states (solid line) in (a) the lower and (b) the upper subbands for $u=10$, $k=5$, and $n=0.2$. The dashed curves describe the corresponding densities of states of the normal material, i.e., $D(E'_k - \mu)$. Note the difference of the used scales.

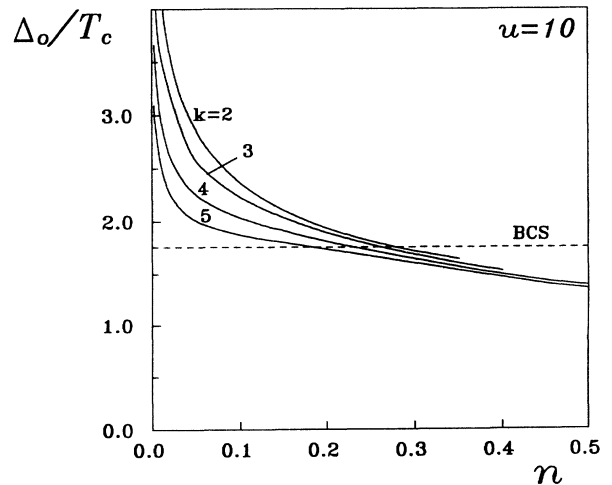


FIG. 10. The ratio of the effective energy gap Δ_0 at zero temperature [as shown in Fig. 9(a)] and the transition temperature T_c as a function of concentration n . The BCS theory prediction is plotted in the figure by the dashed line.

The value of the gap seen in the lower subband is (like T_c) concentration dependent and we denote it by Δ_0 (subscript 0 referring to the zero temperature). The n dependence of the ratio Δ_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-Jain⁶ 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

The work has been partially supported by a grant from State Committee for Scientific Research (KBN). We acknowledge the fruitful discussions with Professors R. Micnas, S. Robaszkiewicz, and J. Spałek.

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