Phase transition in the "superconducting glass" model

I. O. Kulik and A. G. Pedan

Low-temperature Physicotechnical Institute, Academy of Sciences of the Ukrainian SSR

(Submitted 4 April 1980)
Zh. Eksp. Teor. Fiz. **79**, 1469–1482 (October 1980)

We study the superconducting transition in a system described by the Hubbard Hamiltonian with negative U-centers (attraction between electrons with opposite spins on one site). We derive and solve in the self-consistent field approximation equations for the modulus of the order parameter and the chemical potential. We show that the superconducting transition is the result of Bose condensation of electron pairs. The formula for the transition temperature is $T_c = W(1-2\nu)/\ln(\nu^{-1}-1)$, where W is the band width and 2ν is the number of electrons per site. We calculate the thermodynamic quantities and the current. We write down equations for a disordered model ("superconducting glass"). In the simplest case of two ideal sublattices their solution gives a steep decrease in T_c when the single-site energy spread increases.

PACS numbers: 61.40.Df, 74.10. + v

1. INTRODUCTION

The superconductivity transition in the delocalized-pair model is not very sensitive to structural disorder. For instance, superconducting alloys with electron mean free paths less than the BCS coherence length $\xi \approx 0.2\hbar v_F/T_c$ have a critical temperature which differs little from the T_c of an ideal single crystal. In its simplest form this statement is known as the Anderson theorem.[1,2] At the same time there exist superconducting systems which are sensitive to their structural state so that the concept of a "superconducting glass"[3,4] may have a non-trivial meaning. Finely dispersed superconducting condensates,[5] superconducting compounds based upon transition metals (group A-15 compounds, "quasi-zero-dimensional" superconductors such as[6] $\mathrm{PbMo_6S_8}$) and some other systems may belong directly or indirectly to this kind of structure. Although for an explanation of the way T_c depends on the structural state in each of the above-mentioned systems one may propose concrete models (electrostatic energy of the granules,[7] one-dimensional chains in A-15,[8] and so on), the possibility of an alternatuve explanation is not excluded.

We shall analyze in the present paper a model of a superconducting transition which differs from the BCS model by the presence of localized electron pairs in the ground state and which leads to such a behavior. This model is close to the ideas of Bose-condensation of pairs[3,4,9,10], but it differs from it quantitatively. We conclude that a superconducting transition may exist in structurally disordered systems (such as amorphous semiconductors) with covalent centers of electron coupling, although with a very low ordering temperature.

As the basis of our model we take the Hubbard Hamiltonian with negative U-centers:

$$\hat{H}=-U\sum_{i}a^{+}_{i\uparrow}a_{i\uparrow}a^{+}_{i\downarrow}a_{i\downarrow}+\sum_{ij,\sigma}t_{ij}a_{i\sigma}{}^{+}a_{j\sigma}=\hat{H}_0+\hat{V}. \tag{1}$$

Here $U > 0$ and we assume that $t_{ij} \ll U$, $a^{+}_{i\sigma}$ is the creation operator for an electron with spin component σ $(=\uparrow, \downarrow)$ at the lattice site i and $t_{ij,\sigma}$ in the matrix element for the transition between nearest-neighbor centers at the sites i,j. Negative values of U can be obtained if we take into account the interaction of an electron with local displacements of a given site. In complete analogy with the usual electron-phonon mechanism of superconductivity, this leads to an attraction of two electrons with opposite values of the spin component at a single site.[11,12] We shall assume that the energy of such a coupling exceeds the usual Hubbard correlation energy, i.e., that the resulting interaction in (1) is negative. The analysis by Anderson[12] showed that such a model can explain several properties of amorphous semiconductors.

At low temperatures the Hamiltonian (1) leads, as will become clear from what follows, to the occurrence of a superconducting correlation between pairs. In terms of delocalized electrons the second term in the Hamiltonian (1) corresponds to the kinetic energy of the band motion (the width of the band $\propto |t_{ij}|$), and the first one to the interaction between electrons (interaction energy U). In the BCS model the band width is large and one can therefore consider the interaction to be a perturbation. The basic difference between the model studied here and the BCS model is that we shall assume the band width to be small compared to U, i.e., consider the second term to be a perturbation. In the superconducting glass model[3,4], i.e., in the case when U changes from site to site (or when the energy ε_i of the single-electron states on the sites is random; *vide infra*), the disorder affects the superconducting properties strongly, including T_c.

2. REGULAR MODEL

At $T=0$ and when there is no perturbation ($\hat{V}=0$) all electrons are bound in pairs that are localized on the lattice sites. We assume that the number of electrons (n) is smaller than twice the number of sites (N). When $T\neq 0$ the state of the system is a set of empty sites ($|0\rangle$), sites occupied by a single electron ($a^{+}_{i\uparrow}|0\rangle, a^{+}_{i\downarrow}|0\rangle$), and sites occupied by two electrons ($a^{+}_{i\uparrow}a^{+}_{i\downarrow}|0\rangle$). The number of sites occupied by a single electron is proportional to $n\exp(-U/T)$. At temperatures $T \ll U$ it is small compared to the number of pairs. Since we shall be interested just in such temperatures, we shall neglect the presence of single electrons on sites. We note that the ground state of the system is degenerate, and its energy when there is no perturbation is

$$E_0=-{}^1/_2 nU. \tag{2}$$

When the perturbation $\hat{V}$ is turned on, there occur in

0038-5646/80/100742-07$02.40

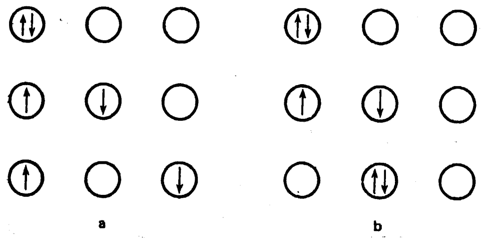

FIG. 1. Scheme of transition leading to the creation of single excitation (a) and scheme of transitions leading to the transfer of a pair from site to site (b).

the system different excitations which can be divided into single-particle and two-particle (pair) excitations. Single-particle excitations lead to the transition of one of the electrons to a neighboring site. As a result of the pair breaking the energy increases by an amount U, i.e., a single-particle excited state is separated from the ground state by an energy gap (Fig. 1a). A two-particle excitation leads to the transition of a pair of electrons to a neighboring site without activation (Fig. 1b). One sees easily[3] that these kinds of transitions lead to a lowering of the energy of the ground state by an amount of the order of t^2/U.

For further studies it is necessary to isolate from the Hamiltonian thus describes all the possible excitations the part (H^{eff}) that describes the pair excitation. Since in our approximation there are only electron pairs in the ground state, while the kind of excitations which interest us leads to the transition of pairs from site to site (i.e., where one ground state goes over into another one), H^{eff} must be a Hamiltonian operating in the space of the ground-state wave functions. Introducing the operator P which projects onto the sub-space of the "ground" states $\Phi_n = a_{i\uparrow}^+ a_{i\downarrow}^+ \ldots a_{k\uparrow}^+ a_{k\downarrow}^+ |0\rangle$ with a given number of pairs, we get[13] when $|t_{ij}| \ll U$

$$H^{eff} = P\hat{H}_0 P - P\frac{\hat{V}^2}{U}P. \tag{3}$$

Accurate to terms of order $|t_{ij}|^2/U$, the Hamiltonian H^{eff} has the same transition matrix elements between the states l and m as H. In terms of the electron second quantization operators, H^{eff} has the form

$$H^{eff} = -U\sum_i a_{i\uparrow}{}^+ a_{i\uparrow} a_{i\downarrow}{}^+ a_{i\downarrow} - \sum_{ij,\sigma} \frac{|t_{ij}|^2}{U}(a_{i\sigma}{}^+ a_{j\sigma} a_{j\sigma}{}^+ a_{i\sigma} + a_{i\sigma}{}^+ a_{i\bar{\sigma}}{}^+ a_{j\bar{\sigma}} a_{j\sigma}). \tag{4}$$

The second term in the interaction term corresponds to a transfer of a pair from site to site, while the first term corresponds to the "virtual" transitions of one of the electrons of a pair to a neighboring site.

It will be more convenient in what follows to work not with the operators $a_{i\sigma}^+$ and $a_{i\sigma}$ but with the pair creation and annihilation operators: $A_i = a_{i\downarrow} a_{i\uparrow}$ and $A_i^+ = a_{i\uparrow}^+ a_{i\downarrow}^+$. The pair-number operator for a site is $N_i = A_i^+ A_i$. The operators introduced here have the following commutation rules:

$$A_l A_{l'}{}^+ - \eta_{ll'} A_{l'}{}^+ A_l = \delta_{ll'},$$
$$\delta_{ll'} = \begin{cases} 0, & l \neq l' \\ 1, & l = l', \end{cases} \quad \eta_{ll'} = 1 - 2\delta_{ll'}, \tag{5}$$

i.e., they are "fermion-like" ($\eta = -1$) for one site, and "boson-like" ($\eta = 1$) for different sites ($l \neq l'$).

Using the fact that in the sub-space of the "ground-state" wavefunctions Φ_n, in which there are only pairs, the following identity holds:

$$\hat{n}_{i\sigma}\Phi_n = \hat{n}_{i\sigma}\hat{n}_{i\bar{\sigma}}\Phi_n = \hat{N}_i\Phi_n,$$

where $\hat{n}_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$ we can rewrite the Hamiltonian H^{eff} in terms of the operators A_i and A_i^+ ($U \gg t^2/U$):

$$H^{eff} = \mathscr{H}_0 + \mathscr{H}'_{int} + \mathscr{H}''_{int},$$

$$\mathscr{H}_0 = -U\sum_i N_i, \quad \mathscr{H}'_{int} = 2\frac{t^2}{U}\sum_{ij} N_i N_j, \quad \mathscr{H}''_{int} = -2\frac{t^2}{U}\sum_{ij} A_i{}^+ A_j. \tag{6}$$

We have already noted that the operators A_l, A_l^+ satisfy fermion commutation relations forbidding two pairs to be on one site. The presence of the term $\mathscr{H}'_{int}$ in the Hamiltonian (6) is a consequence of this exclusion. For sufficiently high concentrations of pairs, $\nu = n/2N$ (n is the number of electrons, N is the number of lattice sites) the role of this term is important, and as a result the quasi-momentum k of the pairs will be a poor quantum number. However, when the concentration drops the Pauli interaction $\mathscr{H}'_{int}$ will play an ever smaller role. Finally, when $\nu \ll 1$ one may take the pairs to be almost ideal bosons and describe them by means of the delocalized wave functions[3,4]

$$A^+(\mathbf{k})|0\rangle = N^{-1/2}\sum_n e^{i\mathbf{k}\mathbf{n}} A_n{}^+|0\rangle. \tag{7}$$

One should note that the Hamiltonian $\mathscr{H}'_{int}$ is isomorphic with the antiferromagnetic Ising Hamiltonian which describes a system of spins in an external field (h). One can easily check this by expressing $\mathscr{H}'_{int}$ in terms of the spin variables $s_i = \frac{1}{2} - N_i$ ($N_i = 0, 1$). Up to a constant we get

$$\mathscr{H}'_{int} = h\sum_i s_i + V\sum_{ij} s_i s_j, \quad V = 2t^2/U. \tag{8}$$

Here $h = -Vz$, where z is the coordination number (number of nearest neighbors).

In a system described by such a Hamiltonian, a phase transition is possible only if the term describing the field h vanishes. For this it is necessary that $\sum_i s_i = 0$, i.e., that the band be half-full ($\nu = \frac{1}{2}$). Since we are interested here mainly in small concentrations (or concentrations close to unity) we can conclude that there is no phase transition in the temperature range $T \sim t^2/U$ in a system with Hamiltonian $\mathscr{H}'_{int}$.

The term $\mathscr{H}'_{int}$ in the Hamiltonian (6) has another meaning. It corresponds to delocalization of pairs, i.e., to preference of plane-wave states such as (7) over states localized on sites $A_n^+|0\rangle$. At low temperatures $T \lesssim t^2/U$ such states have a tendency to Bose-condensation at $\mathbf{k} = 0$. We shall trace in what follows in more detail the assumption that the self-consistent field model is applicable.

We introduce the quantity (quasi-average)

$$\alpha_i = \langle A_i \rangle, \tag{9}$$

which has the meaning of an order parameter vanishing at the transition point T_c. In the limit of low concentrations we can neglect correlations between particles at neighboring sites and, using the self-consistent field approximation, make the following decoupling in the Hamiltonian

$$N_iN_j\to\langle N_i\rangle N_j+\langle N_j\rangle N_i,\quad A_i^+A_j\to\langle A_i^+\rangle A_j+\langle A_j\rangle A_i^+.$$

Using this the Hamiltonian (6) can be written in the form

$$\tilde{\mathscr{H}}=(-U-\mu)\sum_i N_i-2\frac{t^2}{U}\sum_{ij}(\alpha_jA_i^++\alpha_i^*A_j). \qquad (10)$$

Here μ is the chemical potential of the pairs.

According to (10) the problem was reduced to a single-center one, while in the uniform case the order parameter is independent of the site number ($\tilde{\mathscr{H}}=\sum_i\tilde{\mathscr{H}}_i$). The quantity α_i is found from the self-consistency condition

$$\alpha_i=\operatorname{Sp}A_i\exp(-\beta\tilde{\mathscr{H}}_i)/\operatorname{Sp}\exp(-\beta\tilde{\mathscr{H}}_i). \qquad (11)$$

In the single-site representation the Hamiltonian $\tilde{\mathscr{H}}_i$ is a (2×2) matrix in the basis of states realized on the site, $|0\rangle, A_i^+|0\rangle$:

$$\tilde{\mathscr{H}}_i=\begin{pmatrix}0 & -W\alpha^*\\ -W\alpha & -U-\mu\end{pmatrix}. \qquad (12)$$

We have introduced here the notation $W=2zt^2/U$. The quantity W has the meaning of a delocalization energy. It is assumed ot be much smaller than the binding energy U of the pairs.

Diagonalization of (12) leads to the energy eigenvalues

$$\varepsilon_{12}={}^1/_2\{-(U+\mu)\operatorname{sign}(U+\mu)\pm R\},\quad R=[(U+\mu)^2+4W^2|\alpha|^2]^{1/2}, \qquad (13)$$

corresponding to the eigenfunctions

$$\Phi_1=c\left\{|0\rangle-\frac{\varepsilon_1}{W\alpha^*}A_i^+|0\rangle\right\},\quad \Phi_2=-c^*\left\{\frac{\varepsilon_1}{W\alpha}|0\rangle+A_i^+|0\rangle\right\}, \qquad (14)$$

c is the normalization constant.

Knowing the eigenfunctions (14) and the eigenvalues (13) of the Hamiltonian $\tilde{\mathscr{H}}_i$ we easily get from (11) a self-consistency equation for the order parameter

$$\varepsilon_1^2+W^2|\alpha|^2=W\varepsilon_1\operatorname{th}{}^1/_2\beta R. \qquad (15)$$

Apart from the trivial solution $|\alpha|=0$ this equation also has a solution $|\alpha|\neq 0$ (when $T<T_c$, where T_c is the transition temperature, *vide infra*). The equation for the chemical potential μ as function of the pair concentration (ν) and the temperature ($\beta=1/T$) can be found in two equivalent ways. The first one consists in using the well known thermodynamic equation

$$\nu=-\partial\Omega/\partial\mu;\quad \Omega=-T\ln Z.$$

Here Ω is the thermodynamic potential per site and Z the single-site partition function which has the form

$$Z=e^{-\beta\varepsilon_1}+e^{-\beta\varepsilon_2}.$$

The second method is a direct evaluation of the average

$$\langle N_i\rangle=\nu=\operatorname{Sp}A_i^+A_i\exp(-\beta\tilde{\mathscr{H}}_i)/\operatorname{Sp}\exp(-\beta\tilde{\mathscr{H}}_i). \qquad (16)$$

In both cases we are led to the relation

$$\nu-\frac{1}{2}=\frac{U+\mu}{R}\operatorname{th}\frac{1}{2}\beta R. \qquad (17)$$

The set of two Eqs. (15) and (17) determines the modulus of the order parameter $|\alpha|$ and the chemical potential μ as functions of the temperature.

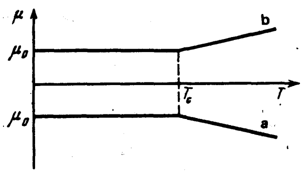

FIG. 2. Temperature dependence of the pair chemical potential: for a low electron concentration, $\nu\ll 1$(a) and for a low hole concentration $1-\nu\ll 1$ (b).

We turn to an analysis of the equations obtained. Putting in (17) $|\alpha|=0$ we get an equation for the chemical potential when $T>T_c$. Its solution is ($T\ll U$)

$$\mu=-U+T\ln\frac{\nu}{1-\nu}. \qquad (18)$$

Moreover, solving the set of Eqs. (15), (17) for $T<T_c$ we get

$$\mu=\mu_0=-U-(1-2\nu)W. \qquad (19)$$

The chemical potential is thus independent of the temperature below the transition temperature. This fact is a confirmation of the Bose-condensation assumption.

It is clear from Eqs. (18), (19) that the behavior of the chemical potential differs for $\nu<\frac{1}{2}$ and $\nu>\frac{1}{2}$ (Fig. 2). This is explained by the fact that the roles of holes (empty sites) and electron pairs change places when we pass through the point $\nu=\frac{1}{2}$, while for $\nu\gg 1-\nu$ we can talk about a hole condensate in contrast to a condensate of electron pairs when $\nu\ll 1$.

We must note that a condensation of pairs (holes) differs from the condensation of an ideal Bose gas. This difference is connected with the appearance of a gap in the pair energy spectrum[14] whereas the spectrum of the elementary excitations of ideal bosons is continuous. The appearance of a gap [like the presence of the term $\mathscr{H}'_{\text{int}}$ in the Hamiltonian (6)] is due to the existence of Pauli exclusion for electron pairs.

From the expressions (13) for the single-site energies of the effective Hamiltonian it follows that the quantity ε_1 plays the role of an energy gap ($\varepsilon_1=\Delta$). Substituting into the expression for Δ the values (18), (19) of the chemical potential we get for $\nu\ll 1$ ($\nu\gg 1-\nu$)

$$\Delta=W|\alpha|^2. \qquad (20)$$

Matching the values of the chemical potential above and below the transition point we find an expression for T_c

$$T_c=W\frac{1-2\nu}{\ln(\nu^{-1}-1)}. \qquad (21)$$

We thus found that the transition temperature is of the the order of the bandwidth W. This result is explained by the fact that in the given model pairs exist when there is no interaction ($W=0$), but their correlation appears as a result of taking into account the transition of pairs to neighboring sites ($W\neq 0$). In that sense all pairs are superconducting at $T=0$ (in contrast to the BCS model in which a small part of the electrons,

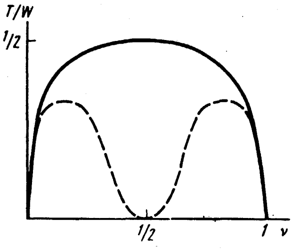

FIG. 3. Concentration dependence of T_c. Dashed line: assumed change in T_c when pair correlation are taken into account [term $H\,\mathscr{H}$ in (6)].

situated near the Fermi surface, is superconducting).

It is clear from Eq. (21) that, in the self-consistent field approximation, the plot of T_c as a function of the concentration has a maximum at $\nu=\frac{1}{2}$ and goes through zero when $\nu=0$ and when $\nu=1$ (Fig. 3).

However, taking the correlation of pairs on neighboring sites into account (going beyond the limits of the self-consistent field theory in the term $\mathscr{H}'_{\text{int}}$) changes this picture. This change will be especially important near the value $\nu=\frac{1}{2}$ when the term with the effective field h in (8) vanishes. The justification for assuming that is that strong correlations will suppress the superconducting transition and in the case of a half-filled band ($\nu=\frac{1}{2}$) lead to $T_c=0$. This is connected with the fact that, as we discussed earlier, the term $\mathscr{H}'_{\text{int}}$ in the Hamiltonian (6) by itself leads to a phase transition (different from the phase transition caused by $\mathscr{H}''_{\text{int}}$) if $\nu=\frac{1}{2}$.

The dependence of the order parameter on the temperature and concentration in the self-consistent field approximation is given by the equations

$$|\alpha|={}^1/_2[(\varepsilon/W)^2-(1-2\nu)^2]^{1/2},\quad \varepsilon=W\,\mathrm{th}(\varepsilon/2T). \tag{22}$$

Solving (22) we can draw the graph $|\alpha|=|\alpha(T)|$ (Fig. 4) and analytically continue the behavior of $|\alpha|$ near $T=T_c$ and $T=0$. When $\nu\ll 1$ we get

$$|\alpha|=\begin{cases}\nu^{1/2}-{}^1/_2\,\nu^{-1/2}e^{-W/T}, & T\ll T_c\\ 2^{1/2}|\alpha(0)|[W(T_c-T)/T_c^2]^{1/2}, & T_c-T\ll T_c\end{cases}. \tag{23}$$

Comparing (20) and (21) we see that when $\nu\ll 1$ the ratio of the gap at $T=0$ to the quantity T_c is equal to

$$\Delta(0)/T_c=\nu\ln\nu^{-1},$$

i.e., small compared to unity.

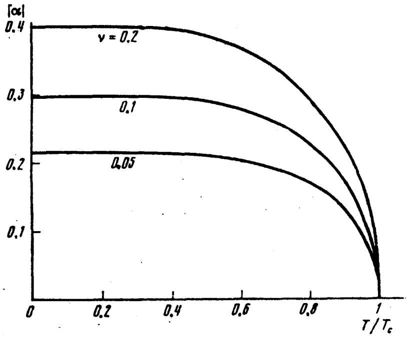

FIG. 4. Temperature dependence of the order parameter.

It is clear from (23) that the quantity $|\alpha(0)|=\nu^{1/2}$ when $\nu\ll 1$. This result corresponds to the picture of Bose condensation. Indeed, the Bose condensation phenomenon presupposes the occupation by a macroscopic number of particles (N_0) of a single quantum state. We can then neglect the fact that the creation and annihilation operators of particles in that state do not commute and consider them as c-numbers (equal to $N_0^{1/2}e^{\pm i\chi}$, where χ is a phase). Indeed, if the pairs condense at $\nu\ll 1$ into the level $\mathbf{k}=0$, we must at $T=0$ find $\langle A(\mathbf{k}=0)\rangle=(n/2)^{1/2}$ (n is the number of electrons).

Averaging $A(0)$ we have in the uniform case

$$\langle A(0)\rangle=N^{-1/2}\sum_n\langle A_n\rangle=N^{-1/2}\sum_n\alpha_n=N^{1/2}|\alpha(0)|.$$

Substituting here $|\alpha(0)|=\nu^{1/2}$ we get, as required, $\langle A(0)\rangle=(n/2)^{1/2}$.

3. THERMODYNAMICS OF THE REGULAR MODEL. CURRENT

We consider the problem of the behavior of the basic thermodynamic quantities in the present model. We use the formula for the derivative of the thermodynamic potential with respect to the interaction constant:[15]

$$\delta\Omega/\delta W=\langle H_{\text{int}}\rangle/W. \tag{24}$$

Integrating this relation we get an expression for the difference of the thermodynamic potential in the normal and the superconducting phases

$$\Omega_s-\Omega_n=-2N\int_0^W|\alpha|^2\,dW. \tag{25}$$

Hence, by using well known thermodynamic formula we can obtain the analogous differences for other thermodynamic quantities. In particular, the temperature dependence of the specific heat for $\nu\ll 1$ is given by the following formula:

$$C=\frac{NT}{\nu-|\alpha|^2}\left(2|\alpha|^2\frac{d|\alpha|^2}{dT}+\frac{T\nu}{\nu-|\alpha|^2}\left(\frac{d|\alpha|^2}{dT}\right)^2+T|\alpha|^2\frac{d^2|\alpha|^2}{dT^2}\right). \tag{26}$$

Hence we get the asymptotic behavior

$$C=\begin{cases}2N(W/T)^2e^{-W/T}, & T\ll T_c\\ 4N\nu\left(\dfrac{TW}{T_c^2}\right)^2-8N\nu\dfrac{T_c-T}{T_c}\dfrac{TW^2}{T_c^3}, & T_c-T\ll T_c\end{cases}.$$

It is clear from (27) that the specific heat undergoes a jump (Fig. 5) in the phase transition point. The magnitude of this jump differs, however, from the value given by the BCS theory.[15]

The specific heat of the normal state in the framework of the approximations made turned out to be equal to zero. This is connected with the above-mentioned neg-

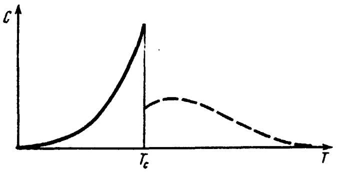

FIG. 5. Temperature dependence of the specific heat (full-drawn curve). Dashed line: qualitative behavior of the specific heat of the normal state.

lect of pair correlations in neighboring sites. Taking the corrections into account lifts the degeneracy (2) and leads to a finite value of C. Using the formula

$$C=\partial\langle H\rangle/\partial T, \tag{28}$$

we get for $T>T_c$

$$C=\frac{W}{z}\sum_{ij}\frac{\partial\langle N_iN_j\rangle}{\partial T}. \tag{29}$$

In the one-dimensional case ($z=2$) the correlator $\langle N_iN_j\rangle$ can be calculated exactly (see the Appendix). For $\nu\ll 1$ we have

$$\langle N_iN_j\rangle=\nu^2e^{-W/2T}.$$

Hence, we get for the specific heat the following expression:

$$C={}^1/_2N\nu^2(W/T)^2e^{-W/2T}. \tag{30}$$

We show in Fig. 5 by a dashed line the dependence of C on T for $|\alpha|=0$. As there is no phase transition in the system with Hamiltonian $\mathscr{H}_0+\mathscr{H}'_{\text{int}}$ (when $\nu\neq\frac{1}{2}$) for any spatial dimensionality, this curve gives qualitatively the behavior also of the specific heat of the normal phase in the three-dimensional case.

It is easy to obtain the value of the critical magnetic field which destroys the superconductivity. In the case of a cylinder with its axis along H

$$H_c(T)=\begin{cases} H_c(0)\,(1-T/2T_c), & T\ll T_c \\ H_c(0)\,(W/T_c)^{1/2}[\,(T_c-T)/T_c], & T_c-T\ll T_c \end{cases}. \tag{31}$$

Here $H_c(0)=(8\pi N\nu W)^{1/2}$.

An important characteristic of the superconducting phase is the presence of a dissipationless current I. The current operator in the model with Hamiltonian (4) has in the one-dimensional case the form ($W=4t^2/U$)

$$\hat{I}=\frac{ieW}{2N}\sum_n(A_{n+1}^+A_n-A_n^+A_{n+1}). \tag{32}$$

The average of the operator $\hat{I}$ in the self-consistent field approximation in the case where the phase of the order parameter grows uniformly along the chain is equal to

$$I=eW|\alpha|^2\sin k. \tag{33}$$

Here k is the difference of the phases at neighboring sites.

We find k-dependence of the modulus of the order parameter by substituting the quantity $\alpha_n=|\alpha|e^{ikn}$ into the Hamiltonian (10). As a result we get the equation

$$\varepsilon=W\,\text{th}\left(\frac{\varepsilon}{2T}\cos k\right),\quad |\alpha|=\frac{1}{2}\left[\left(\frac{\varepsilon}{W}\right)^2-(1-2\nu)^2\right]^{1/2}. \tag{34}$$

Equations (33),(34) thus determine the k-dependence of the dissipationless current. In particular, the magnitude of the critical current at temperatures close to T_c equals

$$I_c=2e\nu\left(\frac{W}{T_c}\right)^2\frac{T_c-T}{T_c}.$$

4. DISORDERED LATTICE

We now turn to a study of a disordered system (i.e., a "glass"). We shall produce the disorder by including in the Hamiltonian random independent single-site energies $\varepsilon_i\ll U$ (in the model studied the introduction of the ε_i is equivalent to the introduction of random correlation energies U_i):

$$H=\sum_i(-U-\mu+\varepsilon_i)N_i+\sum_{ij}\frac{|t_{ij}|^2}{U}(N_iN_j-A_i^+A_j). \tag{35}$$

We can now write Eqs. (15),(17) in the form (for simplicity we assume that $t_{ij}=t$)

$$\begin{aligned} \alpha_i&=\frac{W\bar{\alpha}_i}{E_i^2+W^2|\bar{\alpha}_i|^2}\,\text{th}\frac{1}{2}\beta R_i,\\ 2N_i-1&=\frac{\mu_i}{R_i}\,\text{th}\frac{1}{2}\beta R_i,\qquad R_i=[\mu_i^2+4W^2|\bar{\alpha}_i|^2]^{1/2}. \end{aligned} \tag{36}$$

Here $E_i=\frac{1}{2}\{-\mu_i\,\text{sign}\,\mu_i+R_i\}$, $\mu_i=U+\mu-\varepsilon_i+W\bar{N}_i$, N_i is the pair occupation number of the i-th site. The quantities $\bar{\alpha}_i$ and $\bar{N}_i$ are defined as averages over the nearest neighbors of the i-th site, i.e.,

$$\bar{\alpha}_i=\frac{1}{z}\sum_j\alpha_j,\quad \bar{N}_i=\frac{1}{z}\sum_jN_j.$$

We must look for a solution of Eqs. (36) by first specifying the distribution function of the single-site energies ε_i. These equations are rather complicated. However, some conclusions can be drawn without solving them. For instance, it is clear from (36) that the order parameter on a given site is essentially determined by the order parameters on neighboring sites and if $\bar{\alpha}_i=0$, then α_i also vanishes automatically.

If we consider the case of a uniform distribution (in an interval ω) of the single-site energies ε_i all states are, according to Anderson,[16] localized for values of ω/W larger than some critical value. In that case there will not be a transition to a superconducting state. When the critical value (ω_c) is reached delocalized states appear, first in the center of the band, i.e., a superconducting transition becomes possible. When the parameter ω/N decreases further the region of delocalized states broadens until it occupies almost the whole band. One must assume that then in the formula for T_c not the total concentration ν but the concentration of delocalized pairs should occur.

If we leave the problem of the localization alone Eqs. (36) allow us to find a solution for the simplest models which, however, may be helpful for explaining the superconducting transition in completely disordered substances. We consider, for instance, a one-dimensional system consisting of two ideal sublattices with a difference between single-site energies equal to ε ($\varepsilon=\omega$) (Fig. 6). The solution of Eq. (36) in this case gives the transition temperature

$$T_c=W/[\ln\nu_1\ln(2\nu-\nu_1)]^{1/2}. \tag{37}$$

Here ν_1 is the electron concentration in the sublattice with the larger single-site energy at $T=T_c$.

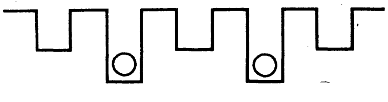

FIG. 6. Model describing qualitatively the effect of disorder on T_c.

When $\varepsilon \gg W$ we get easily from (37)

$$T_c \approx W^2/\varepsilon \ln \nu.$$

Thus, T_c decreases with increasing ω already in a model consisting of two sublattices. One must apparently expect that in a completely disordered model T_c will also depend strongly on the degree the single-site energies are spread.

It is well known that the presence of non-magnetic impurities (structural disorder) has in the BCS model no great effect on the critical temperature.[1,2]. This is explained by the fact that in a dirty metal Cooper pairing occurs not between electrons with opposite spins and quasi-momenta k (since **k** is no longer a good quantum number) but between electrons described by wavefunctions of states which change into one another under time reversal. When there are nonmagnetic impurities present, these functions correspond to the same energy of the paired electrons and the BCS calculation is not altered.

The situation is different in the superconducting glass model. Here the electron pairing is not directly connected with the superconducting transition. Generally speaking, pairs exist at any temperature as the pairing process is determined by the interaction of two electrons with opposite spins on one site. The phase transition occurs as the result of the Bose condensation of pairs. The Bose condensation is very sensitive to structural disorder and this explains the steep decrease in T_c when the disorder increases.

5. CONCLUSION

We have shown in the present paper that in a system described by the Hubbard Hamiltonian with negative U-centers a phase transition to a superconducting state must take place. We obtained the transition temperature T_c, derived equations for the order parameter, and constructed the thermodynamics of the model. However, all calculations were performed in the framework of the self-consistent-field approximation so that the theory contains the defects inherent in that approximation. In particular, we neglected the interaction between electron pairs on neighboring sites (both the Pauli and the Coulomb interaction). The next step should be a consistent account of such correlations. Preliminary calculations show that the correlations will suppress the phase transition and lead to its disappearance at $\nu = \frac{1}{2}$, i.e., at a pair concentration equal to half the lattice site concentration. For small ν and for ν close to unity the role played by such correlations is apparently unimportant.

Another deficiency of the self-consistent field approximation is the fact that the results are independent of the spatial dimensionality n. However, it is well known that Bose condensation is very sensitive to the dimensionality. In this connection it is of interest to study such a system by other, more rigorous methods, for instance, the renormalization group method.

In this paper we considered also a disordered model (a superconducting glass). We concluded that the transition temperature in such a model is very sensitive to the magnitude of the single-site energy spread. The superconducting glass model can thus be adduced for an explanation of the steep decrease in T_c in some superconductors when the disorder increases.

It follows from the results of Sec. 4 that a very large spread in the single-site energies (ε) leads to the critical temperature T_c decreasing, but all the same remaining finite, having a magnitude of order $T_c \sim T_{c0}^2/\varepsilon$ [Eq. (38)]. If we take $T_{c0} \sim 10$ K and $\varepsilon \sim 10^5$ K ~ 10 eV, we get $T_c \sim 10^{-3}$ K. Such low temperatures for a superconducting transition could, in principle, be found for amorphous semiconductors; Anderson[12] has discussed the applicability of the model of negative U-centers to them. However, one cannot consider this conclusion to be rigorous as we neglected many effects such as the Coulomb correlations of electrons on neighboring sites.

The basic conclusion of the study made here must be regarded to be the conclusion that it is possible to construct an alternative model for a superconducting transition in which pairs do not appear at the transition point, but exist already for $T > T_c$. At high temperatures we are, in fact, dealing with a semi-conductor rather than with a metal and, in particular, the conductivity has an activation character. We assume that qualitatively this corresponds to the semiconductor-superconductor transition observed by McLean *et al.*[5]

The present paper arose as a continuation of a study performed by one of the authors with E. Abrahams. As several ideas and conclusions of the present paper are connected with the earlier study we feel it a pleasant duty to express our gratitude to E. Abrahams for many discussions. We are also grateful to W. L. McLean for sending us a preprint of Ref. 5 prior to publication.

APPENDIX

We evaluate the correlator $\langle N_i N_j \rangle$ in a one-dimensional system described by the Hamiltonian

$$H = -U \sum_i N_i + V \sum_{ij} N_i N_j. \tag{A.1}$$

To do this we use the transfer matrix method.[17,18] We impose periodic boundary conditions

$$N_{N+1} = N_1 \tag{A.2}$$

and determine the (2×2) matrix P by its matrix elements

$$P(N_k, N_{k+1}) = \exp\{\beta[{}^1/_2 U(N_k + N_{k+1}) - V N_k N_{k+1}]\}, \tag{A.3}$$

where N_k and N_{k+1} independently can take the values (0, 1). The matrix elements of P are equal to

$$P(0, 0) = 1, \quad P(0. 1) = P(1. 0) = e^{\beta U/2} = x, \quad P(1. 1) = e^{\beta(U-V)} = x^2\omega.$$

Hence, we can write the matrix P in the form

$$P = \begin{vmatrix} 1 & x \\ x & x^2\omega \end{vmatrix}. \tag{A.4}$$

On the basis of these definitions we can write down the partition function Z_0 corresponding to the Hamiltonian (A.1) in the form

$$Z_0=\sum_{N_1}\sum_{N_2}\cdots\sum_{N_N}\exp\left\{\beta\sum_{k=1}^{N}(UN_k-VN_kN_{k+1})\right\}$$
$$=\sum_{N_1}\cdots\sum_{N_N}P(N_1,N_2)P(N_2,N_3)\ldots P(N_N,N_1)$$
$$=\sum_{N_1}P^N(N_1,N_1)=\mathrm{Sp}\,P^N=\sum_j\lambda_j^N. \qquad (\mathrm{A}.5)$$

Here λ_j are the eigenvalues of the matrix P. For large N (number of sites) it is necessary only to use the largest eigenvalue λ_M.

For the further calculations it is necessary to introduce a unitary matrix S which diagonalizes P, i.e.,

$$S^+PS=\begin{vmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{vmatrix}=D_{ij}=\lambda_i\delta_{ij}.$$

We now write down an equation for $\langle N_i\rangle$ and the correlator $\langle N_iN_j\rangle$ (the number of sites $N\to\infty$)

$$\langle N_i\rangle=\nu=\frac{1}{Z_0}\mathrm{Sp}(P^i\tilde{N}_iP^{N-i})=\frac{1}{Z_0}\mathrm{Sp}(S^+P^i\tilde{N}_iP^{N-i}S)$$
$$=\frac{1}{Z_0}\mathrm{Sp}(D^iS^+\tilde{N}_iSD^{N-i})=\frac{1}{Z_0}\mathrm{Sp}(D^NS^+\tilde{N}S)$$
$$=\frac{1}{Z_0}\sum_i\lambda_i^N\left(\sum_m S_{mi}{}^2\tilde{N}_m\right)\approx\frac{\lambda_M{}^N}{Z_0}\sum_m S_{mM}{}^2\tilde{N}_m=\sum_m S_{mM}{}^2\tilde{N}_n. \qquad (\mathrm{A}.7)$$

Here

$$\tilde{N}_i=\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}.$$

For the correlator we get ($N\gg k$)

$$\langle N_iN_{i+k}\rangle=\frac{1}{Z_0}\mathrm{Sp}(D^{N-k}S^+\tilde{N}SD^kS^+\tilde{N}S)$$
$$=\frac{1}{Z_0}\sum_{i,m,p,q}\lambda_i{}^{N-k}\lambda_m{}^kS_{qi}S_{pi}S_{qm}S_{pm}\tilde{N}_q\tilde{N}_p\simeq\frac{1}{\lambda_M{}^k}\sum_m\lambda_m{}^k\left(\sum_p S_{pM}S_{pm}\tilde{N}_p\right)^2. \qquad (\mathrm{A}.8)$$

We find from Eq. (A.7) the matrix elements of the matrix S and substituting them into (A.8) we find the correlator $\langle N_iN_{i+k}\rangle$. Since we are interested in correlations between neighboring sites we get as a result, putting $k=1$, at $\nu\ll1$ the formula

$$\langle N_iN_{i+1}\rangle=\nu^2e^{-\nu/\tau}.$$

[1] P. W. Anderson, J. Phys. Chem. Solids **11**, 26 (1959).
[2] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **33**, 319 (1959) [Soviet Phys. JETP **6**, 250 (1960)].
[3] E. Abrahams and I. O. Kulik, Normal state conductivity, screening, and possible transition to the pair-correlated state in "superconducting glasses," preprint, 1977.
[4] I. O. Kulik and A. G. Fedan, Abstracts of Contributions to the XXth All-Union Meeting on Low-Temperature Physics, NT-20, M 1978, Chs. 3, 87.
[5] W. L. McLean, P. Lindefeld, and T. Worthington, Hopping conduction and superconductivity in granular aluminium, preprint, 1977.
[6] O. Fisher, M. Decroux, S. Roth, R. Chevrel, and M. Sergent, J. Phys. **A8**, L474 (1975).
[7] I. O. Kulik and R. I. Shekhter, Fiz. Nizk. Temp. **2**, 21 (1976)[Sov. J. Low Temp. Phys. **2**, 9 (1976)].
[8] L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **65**, 1658 (1973) [Sov. Phys. JETP 38, 830 (1974)].
[9] I. M. Dmitrenko and I. O. Kulik, Phys. Status Solidi B **64**, k 13 (1974).
[10] R. Pincus, P. Chaikin, and C. F. Coll, Solid State Commun. **12**, 1265 (1973)
[11] R. A. Bari, Phys. Rev. B3, 2662 (1971).
[12] P. W. Anderson, Phys. Rev. Lett. **34**, 953 (1975).
[13] V. J. Emery, Phys. Rev. **B14**, 2989 (1976).
[14] H. J. Lipkin, Quantum Mechanics, North Holland Publ. Co., Amsterdam, 1973.
[15] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polya v statisticheskoĭ fizike (Quantum Field Theoretic Methods in Statistical Physics) 1962 [English translation published by Pergamon Press, Oxford].
[16] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[17] G. F. Newell and E. W. Montroll, Rev. Mod. Phys. **25**, 353 (1953).
[18] G. Beni and P. Pincus, Phys. Rev. B9, 2963 (1974).

Translated by D. ter Haar

Parameters of an electron beam in a free-electron laser under strong saturation conditions

M. I. D'yakonov and M. É. Raĭkh

A. F. Ioffe Physicotechnical Institute, Academy of Sciences USSR
(Submitted 9 April 1980)
Zh. Eksp. Teor. Fiz. **79**, 1483–1490 (October 1980)

Bunching of the electron beam in a free-electron laser under strong saturation conditions is considered in the given-field approximation. The electron phase and the velocity distribution functions, and also the total energy transferred to the electromagnetic wave by the beam, are found.

PACS numbers: 42.55. – f, 41.80.Dd

1. The first experiments on the amplification and generation of light by means of a relativistic electron beam passing through a region with a transverse magnetic field that was varying periodically in space were carried out recently.[1-3] A linear theory of such an amplifier or generator, known as a free-electron laser, was developed in a number of works (see, for example, Refs. 4–6). Nonlinear phenomena in similar apparatus are due to the change in the parameters of the electron beam under the action of the electromag-