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THE METAL–DIELECTRIC DIVALENT CRYSTAL PHASE TRANSITION

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The effect of the correlational interband interaction of electrons in the form of Coulomb attraction between electrons and holes on the electron spectrum of a divalent crystal is investigated at arbitrary temperatures. It is shown that at temperatures below some value T_c the existence of bound electron-hole pairs of the Mott exciton type is possible. At T_c there occurs a second-order phase transition accompanied by a realignment of the $\mathcal{E}(\mathbf{p})$ spectrum from the metal or dielectric type into one of the superconducting type [cf. (9) and (10)]. When $\Delta\mathbf{p} \neq 0$, the system becomes superfluid; the superfluidity does not lead to superconductivity owing to the neutrality of the electron-hole pairs, possibly manifesting itself in "superthermal-conductivity." The dependence of the transition temperature and of $\Delta(\mathbf{p})$ on the relative position of the bands of the non-realigned spectrum is obtained. It is shown that when $\Delta(\mathbf{p}) \neq 0$ the system is antiferromagnetic if the pairing occurs in the triplet state, the period of the magnetic structure being determined by the distance between the extrema of the bands in reciprocal space.

In 1961 Mott[1] discussed the question of the occurrence of a metallic state in a univalent lattice when atoms are brought together from infinity. He indicated that the appearance of a conduction band can be delayed by the Coulomb interaction of the electrons and the holes, which leads to the formation of bound electron-hole pairs of the Mott exciton type. He considered also the case of a divalent crystal; at sufficiently large interatomic distances, such a crystal has a dielectric-type electron spectrum. With decreasing lattice constant, the valence and the conduction bands partially overlap. However, even in this case the pairing of the electrons with the holes can retard the transition to the metallic state. This question was subsequently considered by Arkhipov[2] and by Keldysh and Kopaev[3]. In the present work we consider also this simpler case, while the analysis of the univalent crystal will be the subject of a different paper.

1. FORMULATION OF THE PROBLEM

Assume that we have a divalent crystal with two close-lying bands. At high temperatures the interband correlation is not important and the spectrum is well described by the self-consistent-field approximation. We shall assume that this spectrum is known. With decreasing temperature, the correlation interaction between the different bands, which has the character of a Coulomb attraction of electrons and holes, can become sufficiently significant for the pairing of electrons and holes to become thermodynamically convenient. Here, obviously, a second-order phase transition takes place. We shall determine the character of the realignment of the spectrum and the temperature of the phase transition as a function of the pressure, and we shall also clarify the magnetic structure resulting from triplet pairing.

Assume that prior to the realignment (when the interband interaction is insignificant) the electron spectrum is $\mathcal{E}_1(\mathbf{p})$ in the lower band and $\mathcal{E}_2(\mathbf{p})$ in the upper band. In our problem the principal role is played by states with energies in the vicinity of $\max \mathcal{E}_1(\mathbf{p})$ and $\min \mathcal{E}_2(\mathbf{p})$. In this region, the spectrum can be regarded as quadratic. The extrema of the bands can be either at one point of the Brillouin zone, or at noncoinciding points. For example, a case is possible when the minimum of the conduction band is located at the center of the Brillouin zone, and the maximum of the valence band at its vertices. For a cubic crystal, in the region of interest to us, the dispersion law is then expressed as follows:

$$\begin{aligned} \mathcal{E}_1(\mathbf{p}) &= \max \mathcal{E}_1 - (\mathbf{p} - \mathbf{q})^2 / 2m_1, \\ \mathcal{E}_2(\mathbf{p}) &= \min \mathcal{E}_2 + p^2 / 2m_2, \end{aligned} \qquad (1)$$

where $\mathbf{p}$—quasimomentum, $\mathbf{q}$—half of the major diagonal of the Brilluoin zone (accurate to within the reciprocal-lattice vector, depending on the value of $\mathbf{p}$), and m_1 and m_2 are the effective masses.

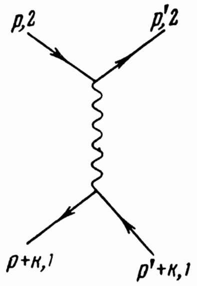

FIG. 1.

The process responsible for the pairing is shown in Fig. 1. In this process the electron goes over from a state with quasimomentum **p** from zone 2 into a state **p**′, 2, while the hole goes from the state **p** + **k**, 1 into the state **p**′ + **k**, 1. With the aid of the diagram technique of field theory we can readily verify that this scattering is large in any order of perturbation theory, if the conduction and valence bands overlap. This was done by Keldysh and Kopaev[3] for the case when the extrema of the bands are located at one point.

The first correction to the vertex part, describing the interaction of the electron with the hole, is of the form

$$\Gamma^{12(1)}(p,p';k)=\frac{i}{(2\pi)^4}\int d^4p''\Gamma^{12(0)}(p,p'')G^{11(0)}(p''+k)$$
$$\times G^{22(0)}(p'')\Gamma^{12(0)}(p'',p), \qquad (2)$$

where $\Gamma^{12(0)}(p, p'')$ is a simple vertex, $p'' = (\mathbf{p}'', \epsilon'')$, $k = (\mathbf{k}, \omega)$, and $G^{11(0)}$ and $G^{22(0)}$ are the Green's functions of zeroth approximation in the lower and upper bands, respectively.

If the distance between the extrema of the bands in momentum space is **q**, then as $k \to (\mathbf{q}, 0)$ the poles of both Green's functions G^{11} and G^{22} come closer together on the Fermi surface, as a result of which the entire expression (2) becomes singular. Putting, for example, $k = (\mathbf{q}, \omega)$ and using the dispersion law (1), we obtain after integration with respect to ϵ''

$$\Gamma^{12(1)}(p, p'; \omega)$$
$$=\int \Gamma^{12(0)}(p, p'')\Gamma^{12(0)}(p'', p')\frac{\operatorname{sign}(p_F-|\mathbf{p}''|)}{(p_F^2-p''^2)/2\mu-\omega}\frac{d^3p''}{(2\pi)^3}, \qquad (3)$$

where p_F is the Fermi momentum and $\mu = m_1m_2/(m_1 + m_2)$. We set Planck's constant equal to unity. It is seen from (3) that $\Gamma^{(1)}(\omega)$ has a logarithmic singularity at the point $\omega = 0$. This circumstance points to a strong correlation between the state **p**, 2 and **p** + **q**, 1.

Summing the corrections obtained from (2) by iteration, we can obtain an integral equation for the vertex part, the solution of which has poles at values of **k** close to **q**. These poles offer evidence of instability of the ground state relative to pairing of the electrons with the holes. However, there is no need to investigate the vertex part. We can formulate a self-consistent problem, by introducing Green's functions G^{12} and G^{21} which are non-diagonal in the quasimomentum. These functions differ from zero if pairing takes place, and vanish when there is no pairing. We set up a system of equations of the type of the Dyson equations for the functions $G^{nn'}$, where $n, n' = 1, 2$, and pick out those solutions of this system which correspond to the minimum of the thermodynamic potential.

2. DERIVATION OF THE FUNDAMENTAL RELATIONS

It is clear from general considerations that the interband correlation should lead to the appearance of a new period $2\pi/\mathbf{q}$ in the crystal. In the case of the dispersion law (1), **q** is half the diagonal of the Brilluoin zone, so that the lattice is doubled. The requirement of translational symmetry imposes on the Green's function

$$G^{nn'}(\mathbf{p}, \mathbf{p}'; \omega)=\int G(\mathbf{r}, \mathbf{r}'; \omega)\,\psi_{\mathbf{p}}{}^{n*}(\mathbf{r})\,\psi_{\mathbf{p}'}{}^{n'}(\mathbf{r}')\,d^3r\,d^3r'$$

certain definite conditions. Namely,

$$G^{nn'}(\mathbf{p}, \mathbf{p}') = a\delta_{\mathbf{pp}'} + b\delta_{\mathbf{p+q},\,\mathbf{p}'}.$$

We can assume here that G^{11} and G^{12} are proportional to $\delta_{pp'}$, while G^{12} and G^{21} are proportional to $\delta_{p+q,p'}$ inasmuch as $G^{11}(\mathbf{p}+\mathbf{q},\mathbf{p})$, $G^{22}(\mathbf{p}+\mathbf{q},\mathbf{p})$, $G^{12}(\mathbf{p},\mathbf{p})$ and $G^{21}(\mathbf{p},\mathbf{p})$ correspond to transitions in which the energy change is of the order of the width of the band. We shall henceforth set $G^{12}(\mathbf{p} + \mathbf{q},\mathbf{p}) = G^{12}(\mathbf{p})$.

The physical meaning of the function $G^{12}(\mathbf{p}, -0)$ is clear. It is the wave function of the pair in momentum space, and in the case of singlet pairing $G^{12} \sim 1$, while in the case of triplet pairing $G^{12} \sim \mathbf{n} \cdot \boldsymbol{\sigma}$. Here **n** is a unit vector which generally speaking depends on **p**, while $\boldsymbol{\sigma}$ is a vector whose components are Pauli matrices.

We shall carry out the analysis for arbitrary temperatures, using the temperature Green's functions $\mathfrak{G}^{nn'}(\mathbf{p},\omega_n)$. In the general case, the equations for the Green's functions are shown in Fig. 2. This figure corresponds to the following expressions:

$$(i\omega_n - \mathscr{E}_2(\mathbf{p}) + \mu)\mathfrak{G}^{22}(\mathbf{p}, \omega_n) = 1 + \Sigma^{12+}(\mathbf{p}, \omega_n)\mathfrak{G}^{12}(\mathbf{p}, \omega_n),$$
$$(i\omega_n - \mathscr{E}_1(\mathbf{p}) + \mu)\mathfrak{G}^{12}(\mathbf{p}, \omega_n) = \Sigma^{12}(\mathbf{p}, \omega_n)\mathfrak{G}^{22}(\mathbf{p}, \omega_n), \quad (4)$$

where μ is the chemical potential,

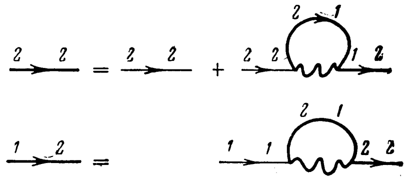

FIG. 2.

$$\Sigma^{12}(\mathbf{p}, \omega_n) = -T\sum_m \int \frac{d^3p'}{(2\pi)^3}\Gamma^{12}(\mathbf{p}, \mathbf{p}';\ \omega_n - \omega_m)\mathfrak{G}^{12}(\mathbf{p}', \omega_m), \tag{5}$$

and $\Gamma^{12}(\mathbf{p}, \mathbf{p}'; \omega_n - \omega_m)$ is the vertex describing the Coulomb interaction of the electrons with the holes and corresponding to the processes shown in Fig. 1. The use of only this type of vertex has the following physical meaning: in accordance with the pairing notion, we neglect the processes in which the number of electrons and holes changes, since such processes are accompanied by pair annihilation or production; the scattering of electrons by electrons, corresponding to the vertices Γ^{11} and Γ^{22}, is assumed to be taken into account in the non-realigned spectrum $\mathcal{E}_n(\mathbf{p})$.

We shall assume for simplicity that the dispersion law (1) is symmetrical, that is, we put $m_1 = m_2$. Let, in addition $\mathcal{E}_1(\mathbf{p})$ and $\mathcal{E}_2(\mathbf{p})$ be measured from the Fermi level. Then

$$\mathcal{E}_2(\mathbf{p}) = -\mathcal{E}_1(\mathbf{p} - \mathbf{q}) = \mathcal{E}(\mathbf{p}). \tag{6}$$

The solution of (4) is of the form

$$\mathfrak{G}^{22}(\mathbf{p}, \omega_n) = -\frac{i\omega_n + \mathcal{E}(\mathbf{p})}{\omega_n^2 + \mathcal{E}^2(\mathbf{p}) + |\Sigma^{12}(\mathbf{p}, \omega_n)|^2}$$

$$\mathfrak{G}^{12}(\mathbf{p}, \omega_n) = \frac{-\Sigma^{12}(\mathbf{p}, \omega_n)}{\omega_n^2 + \mathcal{E}^2(\mathbf{p}) + |\Sigma^{12}(\mathbf{p}, \omega_n)|^2}. \tag{7}$$

Substituting (7) in (5) we arrive at an equation for $\Sigma^{12}(\mathbf{p}, \omega_n)$:

$$\Sigma^{12}(\mathbf{p}, \omega_n) = T\sum_m \int \frac{d^3p'}{(2\pi)^3}\Gamma^{12}(\mathbf{p}, \mathbf{p}'; \omega_n - \omega_m)$$

$$\times \frac{\Sigma^{12}(\mathbf{p}', \omega_m)}{\omega_m^2 + \mathcal{E}^2(\mathbf{p}') + |\Sigma^{12}(\mathbf{p}', \omega_m)|^2}. \tag{8}$$

This equation always has a trivial solution $\Sigma^{12}(\mathbf{p}, \omega_n) \equiv 0$, corresponding to the non-realigned spectrum. We wish to find a nontrivial solution.

We neglect retardation, that is, we assume that $\Gamma^{12}(\mathbf{p}, \mathbf{p}')$ does not depend on the frequency. Then $\Sigma^{12}(\mathbf{p})$ likewise does not depend on the frequency, and the quantity

$$\pm\varepsilon(\mathbf{p}) = \pm\left[\mathcal{E}^2(\mathbf{p}) + \left|\overset{12}{\Sigma}(\mathbf{p})\right|^2\right]^{1/2} \tag{9}$$

determines two branches of the elementary-excitation spectrum, with a gap

$$\Delta(\mathbf{p}) = |\Sigma^{12}(\mathbf{p})|. \tag{10}$$

In the right side of (8) we can now sum over the frequencies, and we obtain an equation for the gap:

$$\Delta(\mathbf{p}) = \int \frac{d^3p'}{(2\pi)^3}\Gamma^{12}(\mathbf{p}, \mathbf{p}')\frac{\Delta(\mathbf{p}')}{2\varepsilon(\mathbf{p}')}\operatorname{th}\frac{\varepsilon(\mathbf{p}')}{2T}, \tag{11}^*$$

Equation (11) has been written out for the case of singlet pairing. If the pairs are triplet, then we obtain in lieu of (11)

$$\Delta(\mathbf{p}) = \int \frac{d^3p'}{(2\pi)^3}\Gamma^{12}(\mathbf{p}, \mathbf{p}')\frac{\Delta(\mathbf{p}')}{2\varepsilon(\mathbf{p}')}\operatorname{th}\frac{\varepsilon(\mathbf{p}')}{2T}(\mathbf{n}_\mathbf{p}\mathbf{n}_{\mathbf{p}'}). \tag{12}$$

We see from this equation that the maximum value of the gap (which is most convenient thermodynamically) corresponds to the function $\mathbf{n}(\mathbf{p}) = \text{const}$. Thus, the magnitude of the gap does not depend on the total spin of the pair.

The thermodynamic potential Ω can be calculated from the formula[4]

$$\lambda\frac{\partial\Omega}{\partial\lambda} = \langle\hat{H}_{int}\rangle, \tag{13}$$

where λ is the interaction parameter. In our problem

$$\lambda\frac{\partial\Omega}{\partial\lambda} = -\sum_{\mathbf{p},\mathbf{p}'}\Gamma^{12}(\mathbf{p}, \mathbf{p}')\operatorname{Sp}\{\mathfrak{G}^{12}(\mathbf{p}, -0)\mathfrak{G}^{12+}(\mathbf{p}', -0)\}$$

$$= -\sum_{\mathbf{p},\mathbf{p}'}\Gamma^{12}(\mathbf{p}, \mathbf{p}')\frac{\Delta(\mathbf{p})\Delta^*(\mathbf{p}')}{2\varepsilon(\mathbf{p})\varepsilon(\mathbf{p}')}\operatorname{th}\frac{\varepsilon(\mathbf{p})}{2T}\operatorname{th}\frac{\varepsilon(\mathbf{p}')}{2T}. \tag{14}$$

We see that the minimum of the thermodynamic potential corresponds, as should be the case, to the maximum value of the gap.

If we take into account the exchange interaction of the electrons from different bands, $\Gamma^{12}_{\text{exch}}$, then there will appear in the right side of (14) a term of the form

$$\sum_{\mathbf{p},\mathbf{p}'}\Gamma_{\text{exch}}{}^{12}(\mathbf{p}, \mathbf{p}')\operatorname{Sp}\mathfrak{G}^{12}(\mathbf{p}, -0)\cdot\operatorname{Sp}\mathfrak{G}^{12+}(\mathbf{p}', -0).$$

This term differs from zero only in the case of singlet pairing and is equal to

$$\sum_{\mathbf{p},\mathbf{p}'}\Gamma_{\text{exch}}{}^{12}(\mathbf{p}, \mathbf{p}')\frac{\Delta(\mathbf{p})\Delta^*(\mathbf{p}')}{\varepsilon(\mathbf{p})\varepsilon(\mathbf{p}')}\operatorname{th}\frac{\varepsilon(\mathbf{p})}{2T}\operatorname{th}\frac{\varepsilon(\mathbf{p}')}{2T}.$$

If $\Gamma^{12}_{\text{exc}} > 0$, then pairing in the triplet state is easier.

The behavior of the function $\Gamma^{12}(\mathbf{p}, \mathbf{p}')$ in the region of small momentum transfers depends strongly on the character of the spectrum. In the metallic phase Γ^{12} tends to a finite value as $|\mathbf{p} - \mathbf{p}'| \to 0$, and in the dielectric phase it behaves like $|\mathbf{p} - \mathbf{p}'|^{-2}$. We can calculate Γ^{12} in the usual

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*th = tanh.

manner, by threading electron and hole loops on the principal interaction line and summing the resultant chains. Here, in view of the foregoing, the result can depend essentially on whether exact or zero Green's functions are used. Therefore, generally speaking, it is necessary to solve a self-consistent problem in which the interaction Γ^{12}, which determines the energy gap, depends itself on this gap.

Carrying out the indicated summation with allowance for four different loops, we obtain

$$\Gamma^{12}(\mathbf{k}, \omega_n) = \frac{4\pi e^2}{k^2 + 4\pi e^2 \Pi(\mathbf{k}, \omega_n)};$$

$$\Pi(\mathbf{k}, \omega_n) = -T\sum_m \int \frac{d^3q}{(2\pi)^3} \mathrm{Sp}\{\mathfrak{G}^{11}(\mathbf{q}, \omega_n)\mathfrak{G}^{11}(\mathbf{q}+\mathbf{k}, \omega_m + \omega_n)$$
$$+ \mathfrak{G}^{22}(\mathbf{q}, \omega_n)\mathfrak{G}^{22}(\mathbf{q}+\mathbf{k}, \omega_m + \omega_n)$$
$$+ 2\mathfrak{G}^{12}(\mathbf{q}, \omega)\mathfrak{G}^{21}(\mathbf{q}+\mathbf{k}, \omega_m + \omega_n)\},$$

where the functions $\mathfrak{G}^{nn'}$ are determined by formulas (7), and e is the effective charge.

Summing the latter expression over m and neglecting retardation, we obtain

$$\Pi(\mathbf{k})$$
$$= 2\int \frac{d^3q}{(2\pi)^3} \frac{\varepsilon(\mathbf{q}+\mathbf{k})\varepsilon(\mathbf{q}) - \mathscr{E}(\mathbf{q}+\mathbf{k})\mathscr{E}(\mathbf{q}) - \Delta(\mathbf{q}+\mathbf{k})\Delta(\mathbf{q})}{\varepsilon(\mathbf{q}+\mathbf{k})\varepsilon(\mathbf{q})}$$
$$\times \frac{n(\mathbf{q}+\mathbf{k}) + n(\mathbf{q}) - 1}{\varepsilon(\mathbf{q}+\mathbf{k}) + \varepsilon(\mathbf{q})}$$
$$- 2\int \frac{d^3q}{(2\pi)^3} \frac{\varepsilon(\mathbf{q}+\mathbf{k})\varepsilon(\mathbf{q}) + \mathscr{E}(\mathbf{q}+\mathbf{k})\mathscr{E}(\mathbf{q}) + \Delta(\mathbf{q}+\mathbf{k})\Delta(\mathbf{q})}{\varepsilon(\mathbf{q}+\mathbf{k})\varepsilon(\mathbf{q})}$$
$$\times \frac{n(\mathbf{q}+\mathbf{k}) - n(\mathbf{q})}{\varepsilon(\mathbf{q}+\mathbf{k}) - \varepsilon(\mathbf{q})}$$
$$n(\mathbf{q}) = \left(\exp\frac{\varepsilon(\mathbf{q})}{T} + 1\right)^{-1}.$$

When T = 0 we have

$$\Pi(\mathbf{k}) = 2\int \frac{d^3q}{(2\pi)^3}$$
$$\times \frac{\varepsilon(\mathbf{q}+\mathbf{k})\varepsilon(\mathbf{q}) - \mathscr{E}(\mathbf{q}+\mathbf{k})\mathscr{E}(\mathbf{q}) - \Delta(\mathbf{q}+\mathbf{k})\Delta(\mathbf{q})}{\varepsilon(\mathbf{q}+\mathbf{k})\varepsilon(\mathbf{q})[\varepsilon(\mathbf{q}+\mathbf{k}) + \varepsilon(\mathbf{q})]}. \tag{15}$$

3. SOLUTION OF THE EQUATION FOR THE GAP

In this section it will be convenient to use an atomic system of units, in which $\hbar = m = e = 1$. The equation for the gap when T = 0 is of the form

$$\Delta(\mathbf{p}) = \int \frac{d^3p'}{(2\pi)^3} \Gamma^{12}(\mathbf{p}, \mathbf{p}') \frac{\Delta(\mathbf{p}')}{2\varepsilon(\mathbf{p}')}. \tag{16}$$

We consider three different cases of relative positions of the bands of the non-realigned spectrum.

Case A. $\mathscr{E}(\mathbf{p}) = p^2/2 + d$. The bands do not overlap, and the width of the forbidden band is large compared with $\Delta(\mathbf{p})$. We rewrite (16) in the form

$$2\varepsilon(\mathbf{p})\psi(\mathbf{p}) = \int \frac{d^3p'}{(2\pi)^3} \Gamma^{12}(\mathbf{p}, \mathbf{p}')\psi(\mathbf{p}'), \tag{17}$$

where $\psi = \Delta/2\epsilon$, and the renormalization of the vertex can certainly be neglected. The left side of this equation can be rewritten approximately in the form

$$(p^2 + 2d + \Delta^2(0)/d)\psi(\mathbf{p}), \tag{18}$$

and (17) takes the form of the Schrödinger equation in the momentum representation for two oppositely charged particles with reduced mass 1/2, the quantity $2d + \Delta^2(0)/d$ playing the role of the binding energy. The latter, as is well known,[5] is equal to one-quarter of the atomic energy unit. Hence

$$\Delta(0) = d_k(2(1 - d/d_k))^{1/2}, \tag{19}$$

where $2d_k = 1/4$ is the maximum width of the forbidden band, at which pairing takes place. In the usual units

$$d_k = 3.4\frac{me^4}{m_0 e_0^4}, \text{eV},$$

where m_0 and e_0 are the mass and charge of the free electron.

Case B. $\mathscr{E}(\mathbf{p}) = p^2/2$. The vertices of the bands touch the Fermi level. From the form of (17) it follows that $\psi(\mathbf{p})$ decreases rapidly when $p > p_1 = [2\Delta(0)]^{1/2}$. Therefore we can put under the integral sign in (17)

$$\psi(\mathbf{p}) = \begin{cases} \psi(0), & p < p_1 \\ 0, & p > p_1 \end{cases}. \tag{20}$$

The vertex $\Gamma^{12}(\mathbf{k})$, calculated with the aid of (15), has for $k \ll p_1$ the form

$$\Gamma^{12}(\mathbf{k}) = 4\pi/k^2[1 + 0.25(d_k/\Delta(0))^{1/2}].$$

As will be shown below, $\Delta(0)$ is of the order of d_k, so that we can put $\Gamma^{12}(\mathbf{k}) = 4\pi/k^2$. Substituting now (20) in (17), we obtain

$$\psi(\mathbf{p}) = \frac{\psi(0)}{8\pi\varepsilon(\mathbf{p})}\left(\frac{p_1^2 - p^2}{p}\ln\left|\frac{p + p_1}{p - p_1}\right| + 2p_1\right). \tag{21}$$

Comparison of (21) and (20) shows that the latter formula gives a good approximation for the solution of equation (17).

Putting p = 0 in (21), we find

$$\Delta(0) = \frac{2}{\pi^2} = 5.5\frac{me^4}{m_0 e_0^4}, \text{eV}. \tag{22}$$

Case C. $\mathscr{E}(\mathbf{p}) = (p^2 - p_F^2)/2$. Let $\Delta(\mathbf{p})$ be small compared with the Fermi energy $\mathscr{E}_F$. In this case in the region $k \ll p_1 = [2\Delta(p_F)]^{1/2}$ the vertex $\Gamma^{12}(k)$, calculated from formula (15), is of the form

$$\Gamma^{12}(\mathbf{k}) = 4\pi / k^2(1 + \alpha\Delta^{-2}(p_F)), \qquad \alpha = (d_k \mathscr{E}_F{}^3)^{1/2}.$$

When k are larger compared with p_1, the gap does not play any role and

$$\Gamma^{(12)}(\mathbf{k}) = 4\pi / (k^2 + \varkappa^2),$$

where κ is the reciprocal Debye radius:

$$\varkappa^2 = 8p_F / \pi = 2.5\, p_F. \tag{23}$$

We put

$$\Gamma^{12}(\mathbf{k}) = \begin{cases} \dfrac{4\pi}{k^2(1 + \alpha\Delta^{-2}(p_F))}, & k < p_1 \\ \dfrac{4\pi}{k^2 + \varkappa^2}, & k > p_1 \end{cases}$$

and break up the integral (16) into two parts

$$\Delta(\mathbf{p}) = \frac{1}{4\pi^2} \int\limits_{|\mathbf{p}-\mathbf{p}'|<p_1} \frac{d^3p'}{(\mathbf{p}-\mathbf{p}')^2(1 + \alpha\Delta^{-2}(p_F))} \frac{\Delta\mathbf{p}'}{\varepsilon(\mathbf{p}')}$$

$$+ \frac{1}{4\pi^2} \int\limits_{|\mathbf{p}-\mathbf{p}'|>p_1} \frac{d^3p'}{(\mathbf{p}-\mathbf{p}')^2 + \varkappa^2} \frac{\Delta(\mathbf{p}')}{\varepsilon(\mathbf{p}')}. \tag{24}$$

We have found above that in the case when the overlap of the bands is small compared with the gap, the latter is of the order of d_k. If we take $\mathscr{E}_F$ to be of the order of d_k, then all three momenta p_F, p_1, and κ become of the same order. The two terms on the right side of (24) will then also be of the same order. With further increase of the overlap, the first term in (24) becomes small compared with the second, and the equation takes the form

$$\Delta(p) = \frac{1}{4\pi p} \int p'\,dp' \frac{\Delta(p')}{\varepsilon(p')} \ln \frac{(p+p')^2 + \varkappa^2}{(p-p')^2 + \varkappa^2}. \tag{25}$$

The latter is valid when the condition $p_F \gg p_1$ is satisfied. The inequality $p_F \gg \kappa$ is simultaneously satisfied.

It is physically clear that $\Delta(p)$ reaches a maximum on the Fermi surface. We substitute in the right side of (25) $\Delta(p)$ in the form

$$\Delta(p) = \begin{cases} \Delta_0, & |p - p_F| < p_2 \\ 0, & |p - p_F| > p_2 \end{cases}; \tag{26}$$

Δ_0 and p_2 should be determined in a self-consistent manner. Integrating (25) after substitution of (26), we obtain

$$\Delta(p) = \frac{1}{2\pi v_F} \ln \frac{(p+p_F)^2 + \varkappa^2}{(p-p_F)^2 + \varkappa^2} \Delta_0 \ln \frac{2p_F p_2}{\Delta_0}. \tag{27}$$

Formulas (26) and (27) can be reconciled if the following condition is satisfied

$$\Delta(p_F \pm p_2) = {}^1\!/_2\Delta(p_F)$$

This condition yields

$$p_2 = (2\varkappa p_F)^{1/2} = 2\left(\frac{2}{\pi}\right)^{1/4} p_F{}^{3/4} = 1.8 p_F{}^{3/4},$$

$$\Delta_0 = 4\left(\frac{2}{\pi}\right)^{1/4} p_F{}^{7/4} \exp\left(-\frac{2\pi p_F}{\ln(\pi p_F/2)}\right). \tag{28}$$

The analysis carried out in this section shows that the dependence of the interaction Γ^{12} on $\Delta(p)$ is significant only in the case of overlap, when the Fermi energy is of the order of d_k.

4. MAGNETIC STRUCTURE

We have already seen that in the case of positive exchange interaction the total spin of the pair is equal to unity, and the Green's function $\mathfrak{G}^{12}$ is of the form

$$\mathfrak{G}^{12}(\mathbf{p}, -0) = -\frac{\Delta(\mathbf{p})}{2\varepsilon(p)}(\mathbf{n}\sigma). \tag{29}$$

In this case the average spin density $\mathbf{S}(\mathbf{r})$ differs from zero and is equal to

$$\mathrm{S}(\mathbf{r}) = \mathrm{Re\,Sp}(\sigma\mathfrak{G}^{12}(\mathbf{r}, -0))$$

$$= -\mathbf{n}f(\mathbf{r}) \cos\frac{\pi x}{a} \cos\frac{\pi y}{a} \cos\frac{\pi z}{a},$$

$$f(\mathbf{r}) = 8\,\mathrm{Re} \sum_{\mathbf{p}} u_{\mathbf{p}}^{2*}(\mathbf{r})\, u_{\mathbf{p}+\mathbf{q}}^{1}(\mathbf{r}) \frac{\Delta(\mathbf{p})}{\varepsilon(\mathbf{p})}, \tag{30}$$

where $u_{\mathbf{p}}^{n}(\mathbf{r})$ is the periodic part of the Bloch function $\psi_{\mathbf{p}}^{n}(\mathbf{r})$ and a is the lattice constant.

Inasmuch as f(r) is a periodic function with period a, according to expression (30) the magnetic moment reverses sign on being displaced by the vector **a**. Thus, in the case of triplet pairing the system is antiferromagnetic.

In the case when the extrema of the bands are at the same point of the Brillouin zone ($\mathbf{q} = 0$), there is no doubling of the lattice. However, in the case of triplet pairing an antiferromagnetic spin structure is produced here, too, with a period equal to the initial period a. The magnetic moments at all the sites will have the same direction, although the total magnetic moment is equal to zero.

5. GENERAL REMARKS

In Sec. 3 we determined the dependence of the character of the realignment of the spectrum and of the value of Δ_0 on the mutual placement of the bands of the non-realigned spectrum when T = 0. These results are shown in Fig. 3, which shows the dependence of Δ_0 on the parameter d, which is positive and equal to the half-width of the forbidden band in the absence of overlap, and which assumes negative values $-\mathscr{E}_F$ in the presence of overlap.

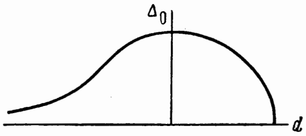

FIG. 3.

At large negative values of d, the gap is exponentially small. In the vicinity of d = 0, the gap Δ_0 is of the order of magnitude d_k and as $d \to d_k$ it vanishes like $(d_k - d)^{1/2}$. When $d > d_k$ the gap Δ_0 is equal to zero.

As will be seen from the formulas of Sec. 2, our model is analogous in its thermodynamic properties to a superconductor. In the case when $\mathscr{E}_F \gg \Delta(p)$, all the thermodynamic quantities can be calculated from the superconductivity-theory formulas (see, for example,[6]) in which we substitute Δ_0 for Δ and $v_F\sqrt{2\kappa p_F}$ in place of the Debye frequency ω_D. In particular, the temperature of the transition T_c is equal to $\gamma\Delta_0/\pi$, where $\ln\gamma = 0.577$. In the case of weak overlap ($\mathscr{E}_F \ll \Delta_0$), the order of magnitude of T_c is also Δ_0.

At values of d close to d_k and for $T \neq 0$, equation (11) takes on the form of the Schrödinger equation (17), in which the role of the effective potential energy is played by the product Γ^{12} $\tanh(\epsilon/2T)$. Solution of this equation leads to the expression

$$\Delta(T) = d_k\left[2\left(\mathrm{th}^2\frac{d}{2T} - \frac{d}{d_k}\right)\right]^{1/2}. \qquad (19')$$

We find from this, in particular, that the transition temperature tends to zero as $d \to d_k$ like

$$T_c = d/\ln\frac{4d_k}{d_k - d}.$$

The quantity d, which characterizes the relative position of the bands of the non-realigned spectrum, depends on the pressure, and generally speaking decreases with increasing pressure. Therefore, if d is positive at normal pressure, that is, the crystal is a dielectric, then at large pressures d can become negative, and for a specified temperature T the transition to the metallic state occurs at a pressure p which satisfies the equation $T = T_c(d_c(p))$.

The spectrum of elementary excitations for $d < d_k$ and $T < T_c$ belongs to the superconducting type, but no superconductivity arises, inasmuch as the electron-hole pairs are neutral. Nonetheless, the phenomenon of superfluidity can take place, since, unlike an ordinary dielectric, in this model the entire system of electrons can move as a unit in the absence of elementary excitations. Superfluidity can become manifest in the existence of super-thermal-conductivity, or more accurately energy flow is possible in the absence of a temperature gradient and a chemical-potential gradient.

In conclusion let us note the causes which may make pairing of electrons with holes impossible. Such a factor may be the electron-phonon interaction, which leads to a mutual repulsion of the electrons and holes in a layer of thickness $2\omega_D$ at the Fermi surface. In view of this, the possibility of pairing is determined by the sign of the effective interaction, which is a sum of the Coulomb attraction and phonon repulsion of the electrons and holes. Thus, the pairing criterion is roughly speaking the inverse of the superconductivity criterion. A factor hindering pairing is also the deviation of the dispersion law from spherical symmetry, which occurs at large overlaps.

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