Criteria for superconductivity and the macroscopic stability of electron-phonon systems

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The problem of the conditions for the onset of the Cooper instability and for the occurrence of the structural transitions involving a doubling of the lattice constant is investigated in the framework of the electron-phonon model of superconductivity. It is shown that in the strong-screening approximation for the degenerate Fermi system the conditions for the existence of both types of instabilities reduce to the inequality $\rho s^2 < N^2 \rho_F^{-1}$ (for an isotropic phonon spectrum), where ρ is the density, s is the (renormalized) velocity of sound, N is the electron concentration, ρ_F is the number of states per unit energy interval at the Fermi level, and the relation between the quantities T_c and T_p (the Cooper-pairing and Peierls-doubling temperatures) is determined by the degree of three-dimensionality (the magnitude of the overlap integral U for neighboring conducting chains), i.e., by the deviation from flatness of the Fermi surface. This criterion can be refined by allowing for logarithmic corrections due to the effects of tight binding, phonon-frequency softening near the structural instability point, and three-dimensional interactions. The transition temperatures T_c and T_p are estimated in an electron-phonon interaction model in which the deformation and Coulomb effects are taken into account in a self-consistent manner (a generalized "jellium" model or a "two-boson" scheme).

1. INTRODUCTION

The purpose of the present paper is to analyze the conditions for the existence of superconductivity and structural transitions due to electron-phonon interactions in conducting solids. In our view, this problem has not been satisfactorily solved even for the simple metals, and is a particularly pressing problem in the case of the intermetallic compounds with the β-tungsten structure[1,2], laminar structures intergrafted with certain organic materials[3], and TCNQ-based quasi-one-dimensional compounds[4]. Interest in the last class of substances, which possess practically one-dimensional metallic conductivities, is due at present to the prospects of obtaining high-temperature superconductors[5]. A distinctive feature of the (quasi-one-dimensional) compounds[1,4,5] is the strong temperature dependence of the lattice characteristics, a dependence which is closely connected with the order-disorder phenomena in the electron system.

In 1964 the present author[6] proposed a model for describing the electron-phonon interaction in metals which practically unites the elements of the so-called "jellium" model[7] and the ordinary (Fröhlich) electron-phonon scheme[8]. A distinguishing feature of the proposed approach is, in the language of the theory of elastic waves in metals[9], the allowance for the long-range Coulomb fields connected with the lattice deformations and not consistently describable in the framework of the purely phonon scheme. In fact, we have to introduce two Bose fields[10] that describe the metal-lattice vibrations: the field of the phonons and that of the "photons" (i.e., the longitudinal electric oscillations) interacting with each other and with the electrons. In such a scheme we can describe in a self-consistent manner the effects of the phonon-induced attraction between the electrons and the Coulomb repulsion due to the exchange of the quanta of the boson fields. In contrast to the simple jellium model[7], the present scheme leads to the conclusion that there exists at the frequency $\omega = 0$ a nonvanishing electron-electron interaction whose sign is determined by the relation between the experimentally determinable parameters (i.e., by the renormalized elastic constants of the lattice and the density of electron states at the Fermi surface)[1)]. On the basis of this, a "criterion" for superconductivity was proposed in the papers[6] which, as was demonstrated in[6,12], reproduces quite well the experimental situation for many metals.

The aim of the present paper is to extend a similar approach to substances possessing substantial anisotropy—in particular, substances possessing two- or one-dimensional conductivity. In the latter case, besides undergoing a superconducting transition, the electron-phonon system turns out under certain conditions to be unstable against a doubling of the lattice constant (the Peierls-Fröhlich instability[13,14]). This instability is connected with the appearance of a "soft" phonon mode, i.e., with the softening of the lattice, which, on account of the results of[6], facilitates an increase in the interelectron attraction. Thus, both phenomena should be considered in a consistent fashion.

It should be noted that in the strictly one-dimensional model[15] the phenomena of lattice-constant doubling also manifest themselves in the appearance of logarithmically diverging diagrams at the vertex part of the electron-electron scattering. At the same time, according to Dzyaloshinskiĭ and Kats[16], the existence of correlation between the one-dimensional chains is necessary for the appearance of long-range superconducting order. The model considered by us is not a strictly one-dimensional model, but includes (although weak) three-dimensional interactions between the conducting chains in the crystal. As to the phonon spectrum, it is fully three dimensional. The conditions under which the present model satisfies the adiabaticity criterion are discussed. In spite of the presence of the chain-chain interaction, the structural transition (i.e., the Peierls instability) can occur. In this respect, our treatment differs from Bychkov, Gor'kov, and Dzyaloshinskiĭ's work[15], in which a scheme with a direct (and not an electron-phonon) interaction is studied.

The contents of the present paper are as follows. In Sec. 2 we construct an electron-phonon interaction scheme, which we call the "two-boson" model and

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which takes the deformation and Coulomb effects into account in a self-consistent manner. In the long-wave ($k \to 0$) limit, it reproduces the results of the classical calculation based on the ideas used in[6] (with the exception of the generalization to the anisotropic case). Thus, for $k \to 0$ the results of the classical and quantum treatments coincide, but at large momenta there appear new distinctive features—the Migdal-Kohn anomalies in the phonon dispersion[17-19] and the corresponding (to these anomalies) change in the interaction between the charges. In Sec. 3 we study the distinctive features of the electron-electron vertex part (K) of the two-body interaction. We determine the poles of K on the temperature axis that are connected with the Cooper ($T = T_c$) and Peierls ($T = T_p$) instabilities. The higher of these temperatures determines the nature of the phase transition that occurs in the system. We find the conditions for the existence of the points T_c and T_p (the conditions for the occurrence of superconductivity and lattice instability) and the relation between these quantities. The latter problem is analyzed in greater detail in Sec. 4, where the logarithmic corrections to the above-indicated criteria are due to the effects of tight binding and phonon-frequency softening near the structural transition point and to the role of three dimensionality (the deviation from flatness of the Fermi surface) are considered.

2. THE THEORY OF THE ELECTRON-PHONON INTERACTION (THE TWO-BOSON MODEL)

There exist at present several approaches to the determination of the electron-electron interaction strength in solids. In the simplest variant, which was proposed about the time the first papers based on the BCS model appeared, the interaction is assumed to be additively made up of two uncoupled parts: attraction due to purely deformation effects in the Fröhlich model and (screened) Coulomb repulsion. Since the two terms are computed in the framework of different model approximations, the resulting interaction turns out to be largely ambiguous, and does not allow the establishment of a reliable criterion for superconductivity. Moreover, the two terms are actually not independent, since the "deformation" interaction is also partly electromagnetic in nature. This is especially apparent in the so-called "jellium" model, in which the two terms cancel each other out—at least for low frequencies[7]. In the jelly model the attraction is purely electromagnetic, and it does not take into account the residual interactions between the core electrons of the deformed ions—interactions which are of nonelectrostatic (exchange) origin.

Following the arguments employed in the analysis of elastic-wave propagation in metals[9], we can construct a self-consistent phenomenological scheme that takes into account electromagnetic interactions, as well as other types of interaction (called, for brevity, deformation interactions) and that is valid in the limit of long (compared to the lattice constant) wavelengths. We shall then assume that the scheme under consideration can be extended to the case of large k. The basis for this is the fact that the interaction does not have a singularity as $k \to 0$ and can, upon the introduction of a reasonably defined cutoff at large momenta, describe the real situation. It would not have been difficult to introduce phenomenological form factors $\Lambda(k)$ that decrease with increasing k, but such an approach is not constructive

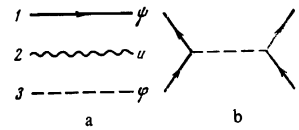

FIG. 1

and does not, in the framework of the phenomenological scheme, give significantly new results.

The determination of the electron-electron interaction strength in the quantum scheme amounts to the computation of the Green functions for the Bose particles that carry out the transfer of energy and momentum between the electrons. In accordance with the foregoing, we shall consider a system that is a combination of three fields: the fields of 1) the electrons, 2) the elastic lattice vibrations (phonons) with a bare $\omega^0_{k\alpha}$-dispersion law (α is the polarization index), and 3) the "photons"—the oscillations of the electromagnetic field. We shall represent the Green functions of the corresponding fields as shown in Fig. 1a.

We represent the interaction between the systems 1)—3) in the form

$$H_{int}=H_{12}+H_{13}+H_{23}, \tag{2.1}$$

where H_{ij} is the Hamiltonian coupling the subsystems i and j to each other. Without specifying—for the moment—the form of the terms H_{ij}, let us note that a methodological difficulty encountered in such a scheme is that it is impossible to introduce (bare) longitudinal field oscillations in the absence of interactions. Nevertheless, all that we shall need is the noninteracting-photon Green function, whose form is known from quantum electrodynamics. Considering the simplest two-particle scattering diagram shown in Fig. 1b, which corresponds to the Coulomb interaction, we find that this function has the form $4\pi e^2/k^2$.

Let us represent the interaction Hamiltonian H_{12} in the form

$$H_{12}=\sum_\sigma \int d^3r\, \psi_\sigma^+(\mathbf{r})\Lambda_{ik}\frac{\partial u_i}{\partial x_k}\psi_\sigma(\mathbf{r}), \tag{2.2}$$

where $\psi^+_\sigma(\mathbf{r})$ is the operator that creates an electron at the point r (σ is a spin component):

$$\psi_\sigma^+(\mathbf{r})=\frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}\sigma}^+\psi_{\mathbf{p}}(\mathbf{r}),$$

u is the quantized phonon field:

$$\mathbf{u}(\mathbf{r})=-\frac{i}{\sqrt{V}}\sum_{k\alpha}\frac{1}{\sqrt{2\rho\omega_{k\alpha}^0}}(\mathbf{e}_{k\alpha}b_{k\alpha}e^{i\mathbf{kr}}-\mathbf{e}_{k\alpha}^*b_{k\alpha}^+e^{-i\mathbf{kr}});$$

a^+ and b^+ are electron and photon creation operators, and the $e_{k\alpha}$'s are unit polarization vectors. $\Lambda_{ik}\partial u_i/\partial x_k$ is the change in the energy of the electron in the elastic-deformation field (Λ_{ik} is the strain tensor in the laboratory frame of reference[9]). Below we shall set $\Lambda_{ik} = \Lambda\delta_{ik}$ and assume that the phonon spectrum is an isotropic line spectrum. In such a model the electrons interact only with the longitudinal vibrations. The changes due to the role of the anisotropy effects will be discussed below.

Similarly, the terms H_{13} and H_{23} in the formula (2.1) can be written as

$$H_{13}=\sum_\sigma\int d^3r\,\psi_\sigma^+(\mathbf{r})e\varphi\psi_\sigma(\mathbf{r}),$$
$$H_{23}=Ne\int d^3r\,\varphi\,\mathrm{div}\,\mathbf{u}. \tag{2.3}$$

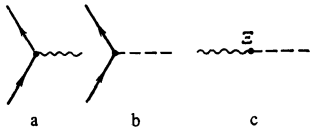

FIG. 2

Here φ is the scalar potential of the electromagnetic field. As can be shown, owing to the condition $s \ll v_F$ (s is the velocity of sound), the electric field in the metal can be assumed to be irrotational (curl **E** = 0), while the magnetic field **H** = 0 (we are dealing here with variable fields accompanying the elastic deformation). The form of the first term in (2.3) is obvious; as to the second term, it is simply the energy of the excess charge arising in the medium upon the deformation of a positive ion core ($\rho' = Ne \operatorname{div} \mathbf{u}$) in the field of the potential φ; N is the equilibrium electron concentration.

Decomposing φ in terms of plane waves in exactly the same way as was done for the phonons, and introducing the new operators

$$\varphi_k^{\,t} = \frac{\Lambda_0 k}{\sqrt{2\rho\omega_k^{\,0}}}(b_k + b_{-k}^{+}), \quad \varphi_k^{\,2} = c_k + c_{-k}^{+},$$

we represent H_{int} in the form

$$H_{int} = \frac{1}{\sqrt{V}} \sum_{p\sigma k} a_{p+k,\sigma}^{+} a_{p\sigma} (\varphi_k^{\,t} + \varphi_k^{\,2}) + \Xi \sum_k \varphi_k^{\,t} \varphi_{-k}^{\,2}, \tag{2.4}$$

where Ξ is a constant:

$$\Xi = N/\Lambda_0. \tag{2.5}$$

The interaction (2.4), which is depicted by the diagrams shown in Fig. 2, is the basis of our subsequent investigation. In accordance with the formula (2.4) the vertices of the diagrams of Figs. 2a and 2b are each equal to unity, while the vertex of the diagram of Fig. 2c is equal to the quantity Ξ, (2.5). Further, introducing in the usual fashion the Green functions for the Fermi (G) and Bose (D_{ij}) fields (i, j = 1, 2), and denoting the polarization operator by Π, we construct the Dyson equations shown in Fig. 3. In these diagrams, the functions D_{11}, D_{22}, D_{12}, and D_{21} are respectively represented by wavy, wavy-dashed (a wavy line that changes into a dashed line), and dashed-wave lines. For example, the first equation in Fig. 3 has the analytic form

$$D_{11}(k, \omega) = D_{11}^{\,0} + D_{11}^{\,0} \Pi D_{11} + D_{11}^{\,0} (\Pi + \Xi) D_{21}.$$

Writing out the remaining equations, and solving the corresponding system, we obtain

$$D_{11} = \frac{D_{11}^{\,0}(1 - \Pi D_{22}^{\,0})}{[\ldots]}, \quad D_{22} = \frac{D_{22}^{\,0}(1 - \Pi D_{11}^{\,0})}{[\ldots]},$$
$$D_{12} = D_{21} = \frac{D_{11}^{\,0} D_{22}^{\,0} (\Pi + \Xi)}{[\ldots]}, \tag{2.6}$$

where

$$[\ldots] = (1 - \Pi D_{11}^{\,0})(1 - \Pi D_{22}^{\,0}) - (\Pi + \Xi)^2 D_{11}^{\,0} D_{22}^{\,0}. \tag{2.7}$$

Using the techniques of thermodynamics[8], we obtain

$$D_{11}^{\,0} = -\frac{\Lambda_0^2 \mathbf{k}^2}{\rho\omega^2 + \lambda_0 \mathbf{k}^2}, \quad D_{22}^{\,0} = \frac{4\pi e^2}{k^2}, \quad G = \frac{1}{i\omega - \xi_p}, \tag{2.8}$$

$$\Pi(k) = 2 \int d^4p \, G(p) G(p+k), \tag{2.9}$$

where ω denotes discrete frequencies, which are even for the Bose field and odd for the Fermi field, k is the four-dimensional momentum ($\mathbf{k}$, ω), and we have introduced the symbolic notation

$$T \sum_{\omega} \int \frac{d^3p}{(2\pi)^3} \to \int d^4p.$$

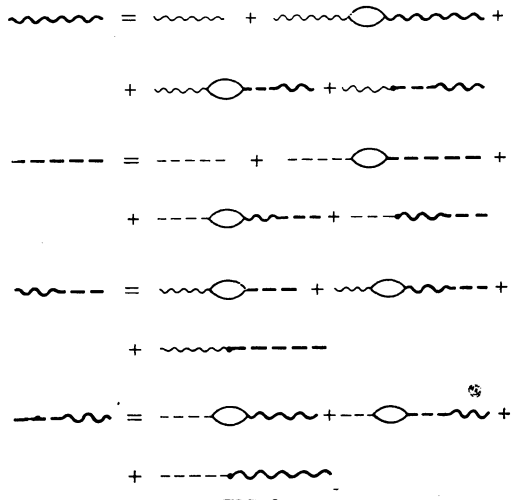

FIG. 3

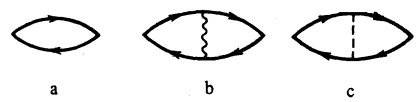

FIG. 4

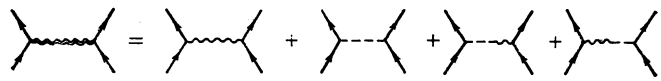

FIG. 5

The expression (2.9) corresponds to the simple electron loop (Fig. 4a). The question of the allowance for higher-order diagrams like those shown in Figs. 4b and 4c will be discussed in the following section.

The total interaction between the electrons is given by the sum of the diagrams shown in Fig. 5. Using (2.6) and (2.7), we obtain

$$D = \left(\frac{1}{D_{11}^{\,0}} + \frac{1}{D_{22}^{\,0}} + 2\Xi\right) \times \left[\frac{1}{D_{11}^{\,0} D_{22}^{\,0}} - \Pi\left(\frac{1}{D_{11}^{\,0}} + \frac{1}{D_{22}^{\,0}} + 2\Xi\right) - \Xi^2\right]^{-1}. \tag{2.10}$$

Further, we must perform an analytic continuation to real frequencies. Since we are interested in the transferred-energy region $\omega \sim sk \ll v_F k$, we can set $\omega = 0$ in the expression for $\Pi(\mathbf{k}, \omega)$.

Let us set $\Pi(\mathbf{k}, 0) = \Pi(\mathbf{k})$ and first consider the long-wave region. For $ka \ll 1$, we have

$$\Pi(0) = 2 \int \frac{d^3p}{(2\pi)^3} \frac{\partial n_p}{\partial \varepsilon} = -\rho_F, \tag{2.11}$$

where the quantity ρ_F is the density of electron states at the Fermi surface. Substituting (2.11) into (2.10), we find

$$D(k, \omega) = \frac{1}{\rho_F}\left[(\lambda_0 - 2N\Lambda_0)k^2 - \rho\omega^2 - \frac{\Lambda_0^2 k^4}{4\pi e^2}\right]\left[(\lambda_0 k^2 - \rho\omega^2)\left(1 + \frac{k^2}{4\pi e^2 \rho_F}\right) - 2N\Lambda_0 k^2 + \frac{N^2 k^2}{\rho_F} - \frac{\Lambda_0^2 k^4}{4\pi e^2}\right]^{-1}, \tag{2.12}$$

where $\lambda_0 = \rho s_0^2$ is the "bare" elastic modulus of the medium (ρ is the lattice density). The formula (2.12)

was obtained earlier[6] by another method. From it we can find the expressions corresponding to the jellium and Fröhlich models.

Setting $\lambda_0 = \Lambda_0 = 0$ in (2.12), we obtain in the case of a quadratic dispersion law for the electrons the expression

$$D_1(k,\omega)=\frac{mv_F^2}{3N}\frac{\rho\omega^2}{\rho\omega^2(1+k^2v_F^2/3\omega_0^2)-Nmv_F^2k^2/3}, \qquad (2.13)$$

where v_F is the Fermi velocity and $\omega_0 = (4\pi Ne^2/m)^{1/2}$ is the plasma frequency. This expression coincides exactly with the two-charge interaction potential in the jellium model[7]. The pole of (2.13) gives the dispersion law for the elastic waves: $\omega_k = sk$ for $k \to 0$ and $\omega_k \to (4\pi Ne^2/M)^{1/2} = \text{const}$ for $k \to \infty$ (M is the mass of the unit cell). For $\omega \to \infty$ the formula (2.13) describes the screened Coulomb potential:

$$D_c(k)=\lim_{\omega\to\infty}D_1(k,\omega)=\frac{4\pi e^2}{k^2+k_s^2}, \quad k_s^2=4\pi e^2\rho_F. \qquad (2.14)$$

If, on the other hand, we set the electron charge $e = 0$ in (2.12), then we shall have the phonon Green function in the Fröhlich model[8]:

$$D_2(k,\omega)=\frac{\Lambda_0^2k^2}{\rho\omega^2-(\lambda_0-\Lambda_0^2\rho_F)k^2}. \qquad (2.15)$$

The quantity $\lambda = \lambda_0 - \Lambda_0^2\rho F$ is the renormalized elastic constant of the lattice in the approximation under consideration.

Returning to the general case, we note that in the long-wave limit the expression (2.12) gets simplified and assumes the form

$$D(k,\omega)=\frac{1}{\rho_F}\frac{(\lambda_0-2N\Lambda_0)k^2-\rho\omega^2}{(\lambda_0-2N\Lambda_0+N^2\rho_F^{-1})k^2-\rho\omega^2}. \qquad (2.16)$$

The formula (2.16) can be obtained by formally setting the electron charge $e = \infty$ in (2.12). The expression (2.16) is valid provided $k \ll k_S$, where k_S is the inverse Debye (Thomas-Fermi) screening radius given in (2.14). Although in the approximation under consideration the magnitude of the charge does not enter into the formula (2.16), we see, nonetheless, that this expression differs significantly from the phonon Green function (2.15) in the Fröhlich model. The formula (2.16), in contrast to (2.15), describes both the phonon (attraction-related) and Coulomb (repulsion-related) effects in the long-wave approximation (just adding the Coulomb potential (2.14) to (2.15) would not have been the correct procedure). The fact that the Coulomb effects are taken into account in (2.16) can also be seen from the fact that for $\omega \to \infty$ (2.16) coincides with the limiting form $4\pi e^2/k_S^2$, (2.14), of the Coulomb potential. Analysis of the expression (2.16) led in[6] to the establishment as a consequence of the condition for superconductivity in metals the condition for the function $D(k, \omega)$ to be negative at $\omega = 0$:

$$\rho s^2 < N^2/\rho_F, \qquad (2.17)$$

where s is the renormalized sound velocity, which, according to (2.16), is determined by the relation

$$\rho s^2 = \lambda_0 - 2N\Lambda_0 + N^2\rho_F^{-1}. \qquad (2.18)$$

The latter quantity should clearly be positive. Notice, however, that this cannot, generally speaking, be said of the bare constants λ_0 and Λ_0. Although methodologically this requires an explanation, we can assert that λ_0 and Λ_0 can be consistently assumed to be both positive and negative.

In the anisotropic case the form of the function $D(k, 0)$ can also be easily found (in the long-wave limit). This is most easily done by resorting to the "classical" method expounded in[6]. The result has the form

$$D(k,0)=(1-\mathbf{ng})/\rho_F, \quad \mathbf{n}=\mathbf{k}/k,$$

where $g(n)$ is a vector determinable from the matrix equation

$$\lambda_{ikjl}n_kn_lg_j=N^2\rho_F^{-1}n_i;$$

λ_{ikjl} is the renormalized elastic-modulus tensor:

$$\lambda_{ikjl}=\lambda^0_{ikjl}-N\Lambda_{ik}\delta_{jl}-N\Lambda_{jl}\delta_{ik}+N^2\rho_F^{-1}\delta_{ik}\delta_{jl}. \qquad (2.19)$$

The condition for the function $D(k, 0)$ to be negative has the form (cf. (2.17))

$$\sum_\alpha (\mathbf{ne}_\alpha)^2/\rho s_\alpha^2 > \rho_F/N^2, \qquad (2.20)$$

where $s_\alpha(n)$ are the (renormalized) velocities of the elastic waves.

As can be seen from (2.17) and (2.20), in order for the electrons to attract each other, the density of states of the single-particle excitations should be sufficiently low and the electron concentration N should be high. This is possible in the case of sufficiently broad bands with small effective masses. In[6] it was shown that the condition (2.20) is, as a rule, satisfied if the metal is a superconductor, and not satisfied for metals that do not go over into the superconducting state. The above-employed approximation, according to which the deformation-interaction constants Λ_{ik} are assumed to be independent of the electron momentum p, can be justified if we neglect the variation of the electron dispersion in the band and consider only the displacement of its edge at the given point of the crystal as a result of the local deformation of the medium.

As essential difference between the above-considered scheme and the ordinary electron-phonon interaction model consists in the necessity for the consideration of two boson fields—one elastic and the other electromagnetic. The topological structure of the diagrams in Figs. 2 and 3 is such that they cannot be reduced to a single boson field (save, perhaps, as a purely effective field). The "two-boson scheme considered in the present paper is a synthesis of the traditional Fröhlich model and the jellium model.

Let us proceed to consider the effects that obtain when the momentum transfers are not small (i.e., when $k \sim p_F$). As shown in[17,18], the polarization operator (2.9) has a singularity at the point $k = 2p_F$, where p_F is the Fermi momentum. This singularity is strongest in the one-dimensional case, i.e., for the plane electron Fermi surface[19]. For the strictly one-dimensional case at low temperatures

$$\Pi(2p_F)=-\rho_F\ln(\varepsilon_F/T), \qquad (2.21)$$

i.e., $\Pi(2p_F)$ tends logarithmically to infinity as $T \to 0$. The expression (2.10) for the interaction between two charges assumes the form

$$D(k,\omega)=\frac{(\lambda_0-2N\Lambda_0)k^2-\rho\omega^2}{\rho_F[(\lambda_0-2N\Lambda_0)k^2-\rho\omega^2]L(k_z)+N^2k^2}, \qquad (2.22)$$

where the function $L(k)$ is the ratio $\Pi(k)/\Pi(0)$. Like (2.16), this formula is valid when the screening is strong (i.e., for $k \ll k_S$). As can be seen from (2.22), in the long-wave ($k \to 0$) limit the elastic properties of the metal do not depend on the direction of the vector k,

since $L(0) = 1$[2]. As k increases, there arises an anisotropy due to the presence of atomic chains (parallel to the z axis) effecting a one-dimensional conductivity.

The phonon-dispersion law is, according to (2.22), given by the expression

$$\rho\omega_k^2=(\lambda_0-2N\Lambda_0)k_\perp^2+\rho_F^{-1}N^2k_z^2L^{-1}(k_z) \qquad (2.23)$$

and has a singularity at $k_z = 2p_F$[3]. In this connection it is significant that in the one-atom-per-unit-cell case under consideration the point $2p_F$ coincides with the boundary π/a (where a is the lattice constant in the z direction) of the one-dimensional Brillouin zone.

The important question of the corrections to the polarization operator due to the higher-order diagrams will be discussed in the following section, since it is closely connected with the general problem of the stability of the electron-phonon system.

3. THE STABILITY OF THE ELECTRON-PHONON SYSTEM AND THE CONDITION FOR SUPERCONDUCTIVITY

We shall analyze here the behavior of the electron-phonon system at low temperatures. It is known that a system of interacting Fermi particles becomes at sufficiently low T unstable against pairing, which can be described as the appearance of a pole in the vertex part of the electron-electron interaction in the case when the sum of the 4-momenta of the impinging particles vanishes, i.e., when $p_1 + p_2 = 0$[8].

Let us consider the two-particle Green function

$$\mathcal{G}(1, 2; 3, 4)=\langle T\psi(1)\psi(2)\bar\psi(3)\bar\psi(4)\rangle, \qquad (3.1)$$

where the numerals number the interacting particles. The perturbation-theory series for $\mathcal{G}$ contains the diagrams shown in Fig. 6, in which the wavy line corresponds to the total electron-electron interaction (2.10). Beside the number of each diagram is indicated the sign with which the corresponding expression obtained with the aid of the rules of the diagrammatic technique enters into $\mathcal{G}$.

The diagrams 1—3 (and those similar to them) correspond to the Cooper effect, i.e., to the pairing of states with momenta p and −p. The vertex part of such diagrams satisfies the equation depicted by Fig. 7; whence

$$K_1(p, k)=D(k)-\int d^4q\, D(q)G(p+q)G(-p-q)K_1(p+q, k-q). \qquad (3.2)$$

Here we have used the four-dimensional notation used in (2.9). $K_1(p, k)$ is the vertex function $K(p_1, p_2; p_1 + k, p_2 - k)$ for $p_1 = -p_2 = p$. Noting that the momentum sum $p + k$ for the quantity K_1 has the same value on both sides of Eq. (3.2), we obtain an equation for the pole ($T = T_c$) as the eigenvalue of the homogeneous equation

$$\varphi(p)+\int d^4p'D(p-p')G(p')G(-p')\varphi(p')=0. \qquad (3.3)$$

This is none other than the gap equation in the electron-

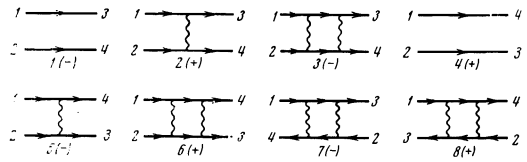

FIG. 6

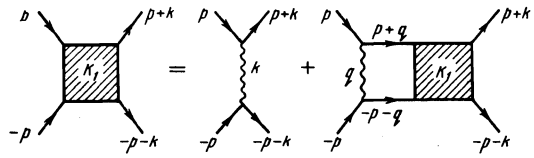

FIG. 7

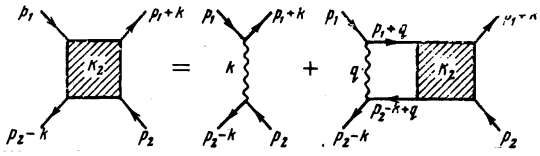

FIG. 8

phonon model of the theory of superconductivity[20]. The product $G(p)G(-p)$ guarantees a logarithmic singularity of the kernel of (3.3).

If, on the other hand, we sum the diagrams 1, 2, etc., in Fig. 6 in which the upper and lower lines are directed in opposite directions, then we obtain for the value of the vertex part K_2 corresponding to these diagrams the equation depicted by Fig. 8, or, analytically,

$$K_2(p_1, p_2; k)=D(k)-\int d^4q\, D(q)G(p_1+q)G(p_2-k+q)K_2(p_1+q, p_2; k-q). \qquad (3.4)$$

Under the condition when $p_1 - p_2 + k = K = (2p_F, 0)$ (i.e., at zero frequency and for the wave number $k_z = 2p_F$) in the one-dimensional case this equation also has a logarithmic singularity, whose position is determined by the equation

$$\psi(p)+\int d^4p'D(p-p')G(p')G(p'+K)\psi(p')=0. \qquad (3.5)$$

On account of (2.8), we have

$$G(p)G(-p)=\frac{1}{\omega^2+\xi_p^2}, \quad G(p)G(p+K)=-\frac{1}{\omega^2+\xi_p^2} \qquad (3.6)$$

provided the spectrum ξ_p has the property

$$\xi_{p+K}=-\xi_p. \qquad (3.7)$$

In the one-dimensional case, the last equality is always fulfilled in the vicinity of the point $\xi_p = 0$, i.e., near $p = \pm p_F$, which leads to a logarithmic singularity of the kernel of Eq. (3.5) similar to the Cooper instability. Notice that the kernels of Eqs. (3.3) and (3.5) have different signs; therefore, if the interaction D should be negative (attractive interaction) in order for the Cooper effect to appear, then "pairing" in the channel (3.5) appears when the interaction between the electrons is repulsive (and the electron-hole interaction is attractive). The phenomenon[15] under consideration is reminiscent of the Keldysh-Kopaev effect[21]—the exciton pairing of carriers from different bands—and, like the latter effect, is extremely sensitive to small deviations from the ideal form (3.7) of the spectrum. For example, when the Fermi surface differs slightly from the ideal shape—the plane—in the strong-binding approximation, instead of a logarithmic singularity of the integral (3.5) of the form $\ln(\tilde\omega/T)$ ($\tilde\omega$ is the characteristic cutoff energy), we obtain (at temperatures $T \ll U$) an expression $\sim\ln(\tilde\omega/U)$, where U is the wave-function overlap integral for neighboring chains. The interpolation expression for the singular part of (3.5) that is valid for any arbitrary relation between U and T will be (see the Appendix):

$$\int d^4p\, G(p)G(p+K)\approx-\frac{1}{2}\rho_F\ln\frac{\tilde\omega}{T+U}. \qquad (3.8)$$

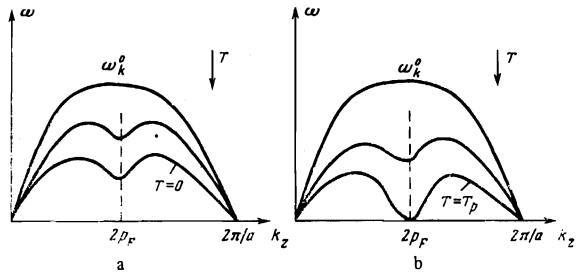

FIG. 9

Thus, we see that in a quasi-one-dimensional system ($U \ll \tilde{\omega}$), only the Cooper singularity of the vertex part remains when $T \ll U$, which allows us to not consider the specific problem of the summation of the "parquet" diagrams[15][4)]. Besides this problem, however, there arises in the electron-phonon model the possibility of the appearance of a second pole, since the function $D(k)$ itself becomes infinite at some value of T. The symbolic solution to Eq. (3.2)

$$K_1=D/(1+\langle DGG\rangle) \tag{3.9}$$

has a pole at the point at which the denominator vanishes ($T = T_c$) and at the pole of the quantity $D(T = T_p)$. Of course, only the higher of the two temperatures T_c and T_p, which determines the point of reconstruction of the state of the electron-phonon system, has a direct meaning. Below we shall estimate the temperatures T_c and T_p and find the conditions for the existence of the points $T_c > 0$, $T_p > 0$, and $T_c > T_p$.

1. The computation of T_p is simpler. The pole of the function (2.22) at $\omega = 0$ and $k_z = 2p_F$ is determined, according to (3.8), by the equation

$$\rho_F \ln\frac{\varepsilon_F}{T+U}(\rho s_0^2-2N\Lambda_0)+N^2=0, \tag{3.10}$$

where $s_0 = \sqrt{\lambda_0/\rho}$ is the renormalized velocity of sound. Introducing the renormalized velocity s according to Eq. (2.18), we obtain $\rho s_0^2 - 2N\Lambda_0 = \rho s^2 - N^2\rho_F^{-1}$, from which it is evident on the basis of (3.10) that the pole of D on the temperature axis exists only when the following conditions are satisfied: 1) $\rho s^2 < N^2\rho_F^{-1}$ (cf. (2.17)) and 2) the overlap integral U ($U = |U|$) is sufficiently small.

A schematic form of the phonon dispersion law for the case when the wave vector is directed along the z axis is shown in Fig. 9 for the cases when: a) $\rho s^2 > N^2\rho_F^{-1}$ and b) $\rho s^2 < N^2\rho_F^{-1}$. If the above-formulated conditions are satisfied, then $\omega(2p_F)$ vanishes at $T = T_p$. Upon further lowering of the temperature the frequency becomes purely imaginary, which implies a lattice instability. The temperature of this instability is determined by the equation

$$T_p=\varepsilon_F e^{-1/\lambda_p}-U, \quad \lambda_p=\frac{N^2\rho_F^{-1}-\rho s^2}{N^2\rho_F^{-1}}. \tag{3.11}$$

It can be seen from (3.11) that U has the meaning of a "depairing" factor (in analogy to superconductivity[23]) that lowers the critical temperature of the transition.

2. Let us now proceed to estimate T_c. The expression (2.22) can be represented in the form $D_{ph} + D_C$, where

$$D_c(\mathbf{k})=D(\mathbf{k},\infty), \quad D_{ph}=D-D_c. \tag{3.12}$$

The "Coulomb" potential D_C is positive and decreases as we approach the point $k_z = 2p_F$; D_{ph} describes the interelectron attraction. In the loose-binding limit the gap equation (3.3)

$$\varphi(\mathbf{p},\omega)=-T\sum_{\omega'}\int\frac{d^3p'}{(2\pi)^3}D(\mathbf{p}-\mathbf{p}',\omega-\omega')\frac{\varphi(\mathbf{p}',\omega')}{\omega'^2+\xi_{\mathbf{p}'}^2} \tag{3.13}$$

is determined by the value of D at the point $\omega = \omega' = 0$[5)]. Allowing for the fact that the characteristic phonon frequency ω_D is low compared to the Fermi energy ϵ_F, we obtain

$$T_c=\omega_D e^{-1/\lambda_c}, \quad \lambda_c=-\frac{1}{2}\rho_F\langle D(\mathbf{k},0)\rangle, \tag{3.14}$$

where the angle brackets denote averaging over the Fermi surface. The quantity $D(\mathbf{k}, 0)$ is, according to (2.22), equal to

$$D(\mathbf{k},0)=\frac{\rho s^2-N^2\rho_F^{-1}}{N^2+\rho_F(\rho s^2-N^2\rho_F^{-1})L(k_z)}, \tag{3.15}$$

where for $|k_z - 2p_F| \ll p_F$, we can, in analogy to (3.8), approximate $L(k_z)$ by

$$L(k_z)\approx\ln\frac{p_F v_F}{T+|(k_z-2p_F)|v_F+U}. \tag{3.16}$$

It can be seen that in the case when $U \to 0$ the quantity $D(\mathbf{k}, 0)$ is negative when the inequality $\rho s^2 < N^2\rho_F^{-1}$, which is the condition for superconductivity in the framework of the model under consideration[6], is satisfied. Neglecting, further, the dependence of D on k_z, we obtain for the Cooper interaction constant defined in (3.14) the expression

$$\lambda_c\approx(N^2\rho_F^{-1}-\rho s^2)/2\rho s^2. \tag{3.17}$$

This expression can be refined by allowing for a temperature dependence in the formula (3.15). It should, however, be noted that since the "softening" of the phonon spectrum occurs in a narrow range of wave-vector values ($|k_z - 2p_F| \sim T/v_F$), these corrections are, generally speaking, not very large.

It can be seen from (3.17) that the loose-binding case is realized when the quantities ρs^2 and $N^2\rho_F^{-1}$ (the elastic constants of the lattice and the electron gas) are close in value. In the jellium model these quantities coincide[7], but this is not so in the general case, in which, moreover, there does not exist any a priori prescribed relation between ρs^2 and $N^2\rho_F^{-1}$.

4. CONCLUSIONS

The main result of the investigation carried out above amounts to the assertion that the criteria for superconducting and structural transitions require, as a necessary condition, the fulfilment of the close inequality (2.17) (or, in the more general case, (2.20)):

$$\rho s^2<N^2\rho_F^{-1}, \tag{4.1}$$

where ρ is the lattice density, s the velocity of sound, N the conduction-electron density, and ρ_F the number of states per unit energy interval at the Fermi level, and that comparison of the expressions (3.11), (3.14), and (3.17) enables us to determine the regions of the values of the parameters s, ρ_F, N, and the overlap integral U (the ratio U/ϵ_F determines the extent to which the Fermi surface deviates from the plane surface) where the superconducting transition precedes the structural instability. Notice that the inequality (4.1) can also be rewritten in another form:

$$\overline{M}\overline{\omega^2}<N\hbar v_F\eta, \tag{4.2}$$

where $\overline{\omega^2}$ is the mean square of the phonon frequency, while the numerical coefficient $\eta \sim 10$ corresponds to

the Debye model of the phonon spectrum. In a more realistic picture of the solid body, this coefficient can be different, but we hope that the relation (4.2) (like (4.1)) reflects the general tendency toward the appearance of low-temperature transitions: the decrease of the vibrational frequency of the lattice, the increase of the electron density, the decrease of the effective electron mass (the growth of the Fermi velocity).

The relation (4.1) can be refined by taking into account the role of the three-dimensional interactions and the logarithmic corrections due to the fact that the Coulomb part of the potential (2.22) (see (3.12)) falls off more slowly than the phonon part. This leads to the condition for superconductivity

$$\rho s^2 < N^2 \rho_F^{-1} \left(1 + \frac{1}{2} \ln \frac{\varepsilon_F}{\omega_D}\right) \tag{4.3}$$

and the condition for a structural transition

$$\rho s^2 < N^2 \rho_F^{-1} \left(1 - \frac{1}{\ln(\varepsilon_F/U)}\right). \tag{4.4}$$

Comparison of these formulas with the formula (4.1) shows that (4.3) is a weaker, and (4.4) a stronger, condition than (4.1). It follows from this that a superconducting transition can, in principle, occur in the absence of a doubling of the lattice constant. A more typical situation is the one (in particular, for the A-15 group of compounds[2]) in which both transitions exist; in this case the scale of the quantity T_P is, generally speaking, greater than that of T_C (cf. (3.11) for U = 0 with (3.14)), although this is not a hard and fast rule. The relation between the quantities T_C and T_P depends essentially on the degree of three dimensionality of the system, i.e., on the relative role of the interaction between the one-dimensional chains.

A detailed experimental investigation of the above-introduced quantities s^2 (or $\overline{\omega^2}$), ρ_F, and U as functions of the parameters of the quasi-one-dimensional (e.g., organic) crystals[5] is desirable, for this will enable us to tackle the problem of the purposeful alteration of the properties of a substance with a view to increasing the critical temperature of the transition to the superconducting state.

In conclusion, I express my deep gratitude to L. P. Gor'kov for a useful discussion of the paper and for critical comments. I am also grateful to V. M. Kontorovich for a joint discussion of the problems of lattice dynamics and to Yu. V. Kopaev for his comments and for pointing out to me a number of papers on the subject touched upon here.

APPENDIX

Let us compute the phonon polarization operator, taking into account the interaction between the chains. In the tight-binding approximation, we choose the dispersion law in the form

$$\xi_p = -\varepsilon_0 \cos a p_z + U(p_\perp^2 b^2 - \langle p_\perp^2 b^2 \rangle), \tag{A.1}$$

where a is the lattice constant in the direction of the z axis, $v_F = a\epsilon_0$ is the Fermi velocity, and U is a quantity of the order of the integral of the transition of an electron between neighboring conducting chains (b is the characteristic lattice constant in the direction of the transition). Substituting (A.1) into the formula (2.9) and integrating over the unit cell of the reciprocal lattice, we represent Π in the form

$$\Pi = -\rho_F L(T, q, U), \quad \rho_F = 2/\pi S_\perp v_F, \tag{A.2}$$

$$L \cong T \sum_{\omega} \int_{-\epsilon_0}^{\epsilon_0} d\xi \int_0^1 dx \frac{1}{\xi^2 - (i\omega + q v_F + \tilde{U} x)^2}, \tag{A.3}$$

where $q = |p_F - k_z/2| \ll p_F$, $p_F = \pi/2a$ is the Fermi momentum, and $\tilde{U} = 4\pi U$. For q = U = 0 the integral (A.3) is equal to $\ln(\epsilon_0/T)$, for T = 0 and U = 0 to the quantity $\sim \ln(\epsilon_0/q v_F)$. If we assume for the moment that U = 0, then we find

$$L = \ln \frac{\varepsilon_0}{\gamma \overline{T^2 + (q v_F)^2}} - \varphi(\lambda), \quad \lambda = \frac{T^2}{T^2 + (q v_F)^2}, \tag{A.4}$$

where

$$\varphi(\lambda) = \int_0^\infty \frac{\ln|[1 - \lambda(1 + x^2)]|}{(e^x + 1)(e^{-x} + 1)} dx. \tag{A.5}$$

The parameter λ varies from zero to unity, and the quantity $\varphi(\lambda)$, which is of the order of unity, is then small compared to the large logarithmic quantity in (A.4). To the same degree of accuracy (neglecting terms $\sim$1), we can replace the logarithm in (A.4) by $\ln(\epsilon_0/(T + q v_F))$. A similar estimate can be made in the general case, i.e., when $U \neq 0$. Neglecting terms of the order of unity (which affect only the value of the preexponential factor in the determination of T_P), we obtain for T, $q v_F$, $U \ll \epsilon_0$ the expression

$$L(T, q, U) \approx \ln \frac{\varepsilon_0}{T + |\tilde{U}| + q v_F}.$$

[1)] Notice that in the framework of the jellium model the inequality $D(k, 0) < 0$ violates the stability condition $1/\epsilon(k, 0) \leqslant 0$ [11] ($\epsilon(k, \omega)$ is the permittivity) for the system. In the present case, however, it is necessary to introduce a few response functions—both electromagnetic (of the ϵ) and deformation types of response functions—as a result of which the stability condition assumes a more complicated form. The negativeness of the electron-electron interaction function for $\omega = 0$ is not, as can be verified, inconsistent with the requirement that the energy be a minimum.

[2)] This is due to the model chosen by us, in which the phonon spectrum is isotropic. The quasi-one-dimensional properties manifest themselves only in the characteristics of the electron dispersion, i.e., in the shape of the Fermi surface.

[3)] Upon allowance for the three-dimensional interactions this singularity is smoothed out (see Sec. 3).

[4)] A similar result was also obtained in [22]. There arises in the computation of the corrections to a polarization operator of the type of the diagram in Fig. 4b an additional small quantity of the form $\ln(\omega_D/U)/\ln(\epsilon_F/U)$, since the characteristic "cutoff" energies for the diagrams in Figs. 4a and 4b are different—in the first case it is the Fermi energy ϵ_F, while in the second case it is the maximum phonon energy $\sim\omega_D$. Thus, we see that there appears in the problem an adiabatic small parameter $\omega_D/\epsilon_F \sim (m/M)^{1/2}$, which is analogous to the Migdal theorem [17] for three-dimensional systems. An important difference is that in the one-dimensional case this smallness is only logarithmic.

[5)] In this approximation, we can neglect the logarithmic renormalization of the Coulomb potential $\mu \to \mu/[1 + \mu \ln(\epsilon_F/\omega_D)]$ (see, for example [11]). The refinement connected with the allowance for such a renormalization (the tight-binding effects) is discussed in Sec. 4.

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