

ON THE PROBLEM OF THE RENORMALIZATION OF THE ENERGY SPECTRUM OF  
ELECTRONS IN METALS AS A CONSEQUENCE OF THE ELECTRON-PHONON  
INTERACTION

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Submitted October 7, 1970

Zh. Eksp. Teor. Fiz. 60, 1141–1149 (March, 1971)

An attempt is made to generalize, analyze, and present in the most clear form the results of theoretical work devoted to the investigation of the influence of the electron-phonon interaction on the energy spectrum of electrons in metals in the normal and superconducting states. An anomalously strong reduction of the cyclotron mass of electrons in non-transition metals subjected to pressure is predicted on the basis of the analysis which is carried out.

1. It is known that during the motion of electrons in a lattice, the ions are displaced (one can treat this process as the successive emission and absorption of phonons by the electrons). The displacement of the ions leads, on the one hand, to the appearance of an attraction between the electrons and to superconductivity at low temperatures, and on the other hand it leads to a renormalization of the energy spectrum for electrons in metals in the normal state.

In spite of the fact that a considerable number of articles have been devoted to the study of the electron-phonon interaction, at the present time a number of questions are not sufficiently clearly understood. First of all, this touches upon the connection between the interactions that lead to superconductivity and the nature of the change in the spectrum of the electrons in metals in the normal state. In this connection it is important to represent more or less intuitively the nature of the changes in the spectrum of the electrons which appear as the result of renormalization and the physical consequences of renormalization: these consequences develop in what kind of phenomena, under what kind of conditions (for example, in what frequency interval), and in what temperature interval.

The method of the pseudopotential<sup>[1]</sup> has been widely used in recent years in order to construct the energy spectrum of electrons in metals. In the zero-order approximation of this method, the electrons are regarded as free, which enables one to obtain an extremely intuitive and physically clear picture of the spectrum. Taking account of the first-order corrections due to the nonlocality of the pseudopotential and the corrections of second order associated with the transition to the many-wave approximation (taking account of the influence of the Bragg planes of reflection) leads, without taking the electron-phonon interaction into account, as a rule to a small change of the initial electron parameters. The basic parameters of the resulting model—that is, the dimensions and shape of the equal-energy surfaces in the bands, and also the quantities characterizing the

energy gaps between the bands—are in good agreement with the experimental data in the overwhelming majority of cases.

It is of interest to determine what kind of changes the electron-phonon interaction introduces into the classical spectrum of the free electrons. The analysis of the known experimental data shows that the electron-phonon interaction leads to an increase of the electron's mass  $m_{bs}$  at the Fermi surface. The values of the effective mass of the electrons and their density of states  $N_{bs}$  for  $E = E_F$ , calculated by the pseudopotential method, turn out to be appreciably smaller (by 20 to 100%) than the experimental values (the subscript bs denotes the calculated values of the band structure parameters).

2. The influence of the electron-phonon interaction on the spectrum of free electrons was first considered by Buckingham and Schaffroth.<sup>[2]</sup> Using the Brillouin-Wigner form of perturbation theory, the authors found that the mass  $m_0$  of the free electrons near the Fermi surface undergoes the following renormalization:  $m^* = m_0(1 - \lambda)^{-1}$ . The more exact calculations by Migdal,<sup>[3]</sup> carried out according to perturbation theory for a many-particle system (using a diagram technique), showed that  $m^* = m_0(1 + \lambda)$ . In both cases the parameter  $\lambda$  is determined by the following integral:<sup>[4]</sup>

$$\lambda = 2 \int_0^{\infty} d\omega \frac{\alpha^2(\omega)g(\omega)}{\omega}, \quad (1)$$

where  $\alpha(\omega)$  denotes the electron-phonon coupling constant, and  $g(\omega)$  and  $\omega$  denote the density of states of the phonons and their frequency, respectively. For example, for Na, Al, and Pb the calculated values of  $\lambda$  are equal, respectively, to 0.19, 0.50, and 1.6 (see below).

Migdal's results have been confirmed by more recent articles.<sup>[5-7]</sup> The additional consideration of the Coulomb repulsion of the electrons and of the band structure<sup>[4,8-10]</sup> leads to the following expression for the cyclotron mass in non-superconducting metals:

$$m^* = m_{bs}(1 + \lambda + \mu). \quad (2)$$

Here  $m_{bs}$  denotes the band mass, and  $\lambda$  and  $\mu$  take into consideration, respectively, the interaction of the elec-

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trons with the phonons and the Coulomb interaction of the electrons. At the present time the value of  $\mu$  is not exactly known; however, one can believe that it is small (according to the data given in article<sup>[11]</sup>  $\mu \approx 0.01$  for Al; for certain other metals values of  $\mu$  are given in<sup>[8-10]</sup>).

In accordance with Migdal's results,<sup>[3]</sup> the specific heat  $C_V^*$  of an electron gas and the density of states  $N^*$  at the Fermi surface for real metals are changed with respect to the same quantities ( $C_V$ ,  $N$ ) for free electrons:

$$\frac{C_V^*}{C_V} = \frac{N^*}{N} = \frac{\langle m^* \rangle}{m_0} = \frac{\langle m_{bs} \rangle}{m_0} (1 + \lambda + \mu), \quad (3)$$

where the angular brackets denote averaging over the Fermi surface. This must lead to a change of the cyclotron resonance frequency and a change in the nature of the temperature dependence of the amplitude for all oscillating effects (the Shubnikov-de Haas effect, the de Haas-van Alphen effect, and others). The resistance to a constant current and the anomalous skin effect,<sup>[6]</sup> the tunneling current, the spin-lattice relaxation time, the thermal conductivity, and the Pauli paramagnetic susceptibility do not change in this connection.<sup>[11]</sup>

The very same quantity  $\lambda$  given by Eq. (1), which determines the renormalization of the spectrum of the electrons for normal metals (and for superconductors when  $T > T_C$  where  $T_C$  denotes the temperature of the transition into the superconducting state), appears in the equation of the BCS theory for the energy gap in superconductors,  $\Delta = 2\omega_D \exp(-1/ND)$  ( $\omega_D$  denotes the characteristic frequency of the phonon spectrum, and  $V$  is the parameter characterizing the electron-phonon interaction). The result obtained from the Gor'kov-Eliashberg equation<sup>[12,13]</sup> for the Einstein model of the phonon spectrum ( $\omega(\mathbf{k}) = \omega_E = \text{const}$ ) is that  $NV$  is simply equal to  $\lambda$ . More exact calculations,<sup>[14,15]</sup> taking the Coulomb repulsion of the electrons and the band structure of the metal into consideration, give

$$NV = \left( \ln \frac{2\omega_D}{\Delta} \right)^{-1} = \frac{\lambda}{N^*/N - \gamma} - \mu', \quad (4)$$

$$\gamma = 2 \int_0^{\omega_D} d\omega \frac{\alpha^2(\omega)g(\omega)}{\omega} \ln \frac{\omega}{\omega_D}, \quad (5)$$

where  $\lambda$  and  $N^*/N$  are determined by expressions (1) and (3), the quantity  $\mu'$  takes the Coulomb repulsion of the electrons into account ( $\mu'$  is not equal to  $\mu$  in expression (2)). For Al the calculated value  $\mu' = 0.1$ ,  $\gamma = 0.05$ ,  $N^*/N = 1.6$ , and  $\lambda = 0.5$ ,<sup>[14,15]</sup> which gives  $NV = 0.2$ . The resulting value of  $NV$  is appreciably smaller than  $NV = \lambda = 0.5$  in the simple BCS theory.

In article<sup>[10]</sup> the quantity  $\lambda$  is calculated by integration over the Fermi surface  $S(\mathbf{k})$  ( $\mathbf{k}$  is the wave vector):

$$\lambda = \frac{1}{4\pi^2} \int \frac{dS_k}{|V_k E|} \int \frac{dS_{k'}}{|V_{k'} E|} \sum_{\xi} \frac{|M_{kk', \xi}|^2}{\omega_{q, \xi}} / \int \frac{dS_k}{|V_k E|}, \quad (6)$$

where  $M_{kk', \xi}$  is the matrix element of the electron-phonon interaction,  $E$  denotes the electron energy,  $\omega_{q, \xi}$  denotes the phonon frequency, and  $\xi$  is the subscript indicating the polarization. The phonon spectrum obtained from neutron scattering experiments<sup>[10]</sup> was used in articles<sup>[8-10]</sup> in order to calculate  $\lambda$ , and the Born-von Karman model for the lattice dynamics was used in<sup>[4]</sup>.

The matrix element  $M_{kk', \xi}$  is calculated with the aid of the method of orthogonalized plane waves in the theory of the pseudopotential. The numerical values of  $\lambda$  and  $NV$  which are thus obtained are in good agreement with the experimental data.<sup>[10]</sup> Theoretical and experimental values of  $\lambda$  and  $NV$  for certain alloys of the Pb-Tl-Bi group ( $\lambda = 1.5$  to  $0.7$ ) are presented in<sup>[4, 2)</sup>

Umklapp processes, and also the transverse branches of the phonon spectrum, were taken into consideration in all of the articles. Their contribution to  $\lambda$  reaches 50%.<sup>[16]</sup> The additional calculation of the not exactly transverse and not exactly longitudinal nature of the phonons leads to an anisotropy of the effective mass. For Na Grimval<sup>[16]</sup> found that the associated anisotropy of  $\lambda$  does not exceed 2% whereas the anisotropy of the inverse relaxation time  $\Gamma$ , which is equal to the uncertainty  $\Delta\epsilon$  in the energy of the elementary excitations near the Fermi surface, in order of magnitude amounts to 45%. For Na, Grimval<sup>[16,17]</sup> also calculated the temperature dependence of  $\lambda$  and  $\Delta\epsilon$ .  $\lambda(T) = 1.2\lambda(0)$  reaches its maximum value for  $T \approx 0.4 T_D$  ( $T_D$  denotes the Debye temperature). For  $T \ll T_D$  we have  $\lambda \propto T^2 \ln T$ , and at the Fermi surface the damping is given by  $\Gamma = \Delta\epsilon = T^3$ . For  $T \gg T_D$  the parameter  $\lambda$  falls off in proportion to  $T^{-2}$ .

One can also take account of the electron-phonon interaction on the basis of the theory of strongly compressed matter developed by Abrikosov.<sup>[15]</sup> The assumption that for the majority of metals the kinetic energy of the electrons substantially exceeds the energy of interaction with the lattice makes it possible to apply perturbation theory and to thus calculate the basic parameters associated with renormalization.

3. Let us attempt to intuitively interpret the results of the known theoretical investigations of the electron-phonon interaction in metals. We start from the fact that the spectrum of elementary excitations is determined by the poles of the single-particle Green's function:

$$G^{-1}(\mathbf{p}, \epsilon) \equiv \epsilon - \epsilon_0(\mathbf{p}) - \Sigma(\mathbf{p}, \epsilon) = 0; \quad (7)$$

here  $\epsilon_0(\mathbf{p}) = E(\mathbf{p}) - E_F$  denotes the energy of the electrons in the absence of any electron-phonon interaction. For  $|\epsilon_0| \ll E_F$  one has

$$\epsilon_0(\mathbf{p}) \approx p_F(p - p_F)/m$$

( $p = |\mathbf{p}|$ ,  $E_F$  and  $p_F$  are the Fermi energy and momentum, and  $\epsilon$  and  $\mathbf{p}$  are the variables appearing in the Green's function).

Equation (7) determines the complex function  $\epsilon(\mathbf{p})$ . In what follows we shall only consider those cases where  $|\text{Im } \epsilon| \ll \text{Re } \epsilon$ . Then one can interpret the quantity  $|\epsilon| \approx |\text{Re } \epsilon|$  as the energy of the quasiparticles. As is well-known the self-energy part  $\Sigma$  of the Green's function for electrons interacting with phonons does not depend on  $\mathbf{p}$ .<sup>[3]</sup> Its real and imaginary parts (see Fig. 1) in the limits of small and large energies have the following form: for  $|\epsilon| \ll \omega_D$

<sup>2)</sup>We note that the larger values of  $\lambda$  for a number of metals and alloys do not contradict the criterion for the stability of the lattice since the corresponding values of the parameter  $NV$  in the BCS formula do not exceed 0.5.

$$\text{Re } \Sigma = -\lambda \epsilon, \quad \text{Im } \Sigma \approx -\lambda \epsilon^2 / \omega_D^2, \quad (8a)$$

and for  $|\epsilon| \gg \omega_D$

$$\text{Re } \Sigma' = -\lambda \omega_D^2 / \epsilon, \quad \text{Im } \Sigma \approx -\lambda \omega_D. \quad (8b)$$

In these two limiting cases the spectrum of the electrons can be obtained from relations (7) and (8): for  $|\epsilon| \ll \omega_D$

$$\epsilon_1(p) = \frac{\epsilon_0(p)}{1 + \lambda} = \frac{p_F(p - p_F)}{m(1 + \lambda)} \quad (9a)$$

and for  $|\epsilon| \gg \omega_D$

$$\epsilon_{II}(p) = \epsilon_0(p). \quad (9b)$$

Under these conditions  $|\epsilon_I| \gg \text{Im } \Sigma(\epsilon_I)$  and  $|\epsilon_{II}| \gg \text{Im } \Sigma(\epsilon_{II})$ , which permits us to consider the electrons as quasiparticles (elementary excitations with energies  $|\epsilon(p)|$ ) with a rather large relaxation time (weak damping). In the region where the energy  $|\epsilon|$  is comparable with  $\omega_D$ , the damping becomes appreciable ( $|\text{Im } \Sigma(\epsilon)| \approx |\lambda \epsilon|$ ) and such a consideration becomes invalid. From expressions (9) it follows that the renormalization effects should appear only in the frequency range  $\omega \ll \omega_D \approx 10^{13} \text{ sec}^{-1}$ .

The picture of the energy spectrum of the electrons associated with the interaction with the phonons is also complicated by the appearance of new branches of the spectrum near the Fermi energy. It is already clear from simple considerations that different branches of quasiparticles (the so-called electron-like and phonon-like elementary excitations) must appear in the region where the electron curve  $\epsilon(p)$  and the phonon curve  $\omega(k)$  intersect.

Figure 2 illustrates the emergence of renormalization of the electron branch near  $\epsilon = 0$  and the appearance of new branches of the spectrum. In order to explain this question in more detail, let us consider the spectral function of the electrons

$$A(\mathbf{p}, \epsilon) = \pi^{-1} |\text{Im } G(\mathbf{p}, \epsilon)|. \quad (10)$$

It satisfies the sum rule

$$\int_{-\infty}^{\infty} A(\mathbf{p}, \epsilon) d\epsilon = 1. \quad (11)$$

With the aid of the spectral function one can express the Green's function of the perturbed system in the form

$$G(\mathbf{p}, \epsilon) = \int_{-\infty}^{\infty} G_0(\mathbf{p}, \epsilon - \epsilon') A(\mathbf{p}, \epsilon') d\epsilon', \quad (12)$$

where  $G_0(\mathbf{p}, \epsilon)$  is the Green's function for free electrons.

From (11) and (12) it is seen that  $A(\mathbf{p}, \epsilon)$  can be inter-

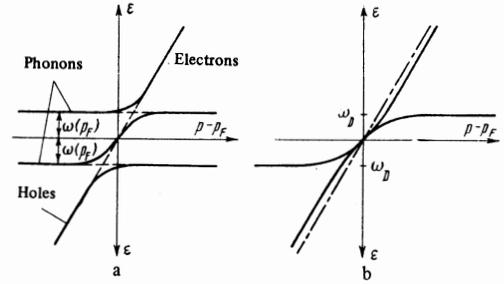


FIG. 2. Illustrations of the change in the spectra of electrons and phonons upon taking account of the interaction between them: a—the one-dimensional case, b—the poles of the Green's function for electrons in the three-dimensional case according to the data given in article [17] are represented by the solid curves, and by the dot-dash line for the case of free electrons. For clearness the energies of electrons and holes are measured from the Fermi energy toward different sides.

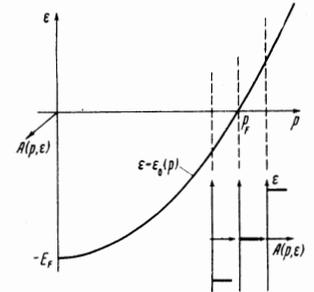


FIG. 3. The spectral function  $A(\mathbf{p}, \epsilon)$  for free electrons. For arbitrary values of the energy  $\epsilon_0(\mathbf{p})$  the function  $A(\mathbf{p}, \epsilon)$  is expressed by a  $\delta$ -function whose coordinate axis is directed perpendicular to the plane of the figure. The cross sections of the planes perpendicular to  $\mathbf{p}$  are depicted in the lower right-hand corner.

preted as the probability of finding "bare" electrons with momentum  $\mathbf{p}$  and energy  $\epsilon$  in the system. For electrons which are only interacting with phonons, this function was calculated in article<sup>[18]</sup> (in<sup>[16]</sup> the function  $A(\mathbf{p}, \epsilon)$  is obtained for  $N\alpha$ ). For free electrons the function  $A(\mathbf{p}, \epsilon) = \delta(\epsilon - \epsilon_0(\mathbf{p}))$  is shown in Fig. 3. On Fig. 4 we have tried to graphically illustrate the results of article<sup>[18]</sup> for the spectral function of electrons interacting with phonons.

The general nature of the function  $A(\mathbf{p}, \epsilon)$  for electrons interacting with phonons does not depend on the quantity  $\lambda$ :<sup>3)</sup> in the immediate vicinity of the Fermi surface ( $|\epsilon(p)| \ll \omega_D$ ) the spectral function has several branches ( $A = A_I + A_{II}$ ).

The branch  $A_I$  is a narrow Lorentzian function with its maximum at  $\epsilon_I = \epsilon_0 / (1 + \lambda)$  and with the half-width  $\Gamma = \Delta \epsilon_I = |\text{Im } \epsilon_I| \approx |\lambda \epsilon_I \omega_D| \ll |\epsilon_I|$ . It is approximately described by

$$A_I \approx \frac{1}{1 + \lambda} \delta\left(\epsilon - \frac{\epsilon_0}{1 + \lambda}\right).$$

This branch describes the electrons (or holes) surrounded by a cloud of virtual phonons.

The branch  $A_{II}$  describes electrons (or holes) which absorb or emit real phonons. In the region  $|\epsilon(p)| \lesssim \omega_D$  it is impossible to interpret this branch as describing a quasiparticle since in this case it is impossible to express the corresponding part of the spectral function in terms of one or several Lorentzian functions. At larger energies  $|\epsilon(p)| \gg \omega_D$  the sum rule (11) almost com-

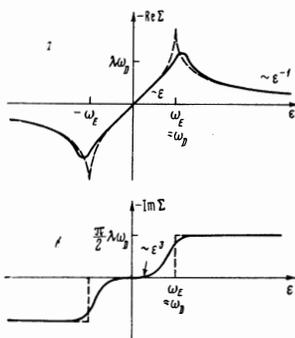


FIG. 1. Self-energy part  $\Sigma$  of the Green's function for electrons interacting with phonons, calculated for the exact phonon spectrum (the solid curve) and for the approximate spectrum in the Einstein model (the dashed curve); a—the real part, b—the imaginary part.

<sup>3)</sup>The distribution of the intensities between branches I and II depends on the quantity  $\lambda$  (see Fig. 4).

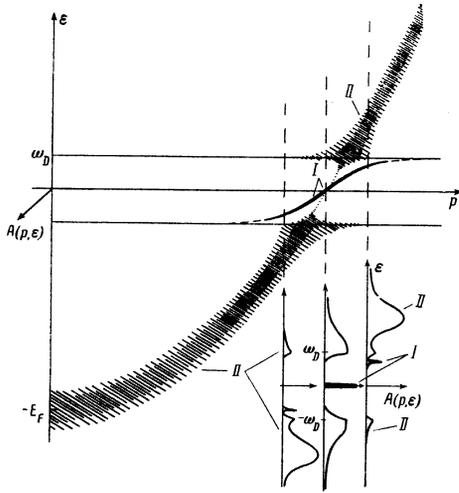


FIG. 4. The spectral function  $A(p, \epsilon)$  for the case of electrons interacting with phonons. The width of the crosshatching on the branches II and the thickness of the line representing branch I correspond to the height of the function  $A(p, \epsilon)$  above the  $(p, \epsilon)$  plane. The distribution of the intensities in the function  $A(p, \epsilon)$  for three fixed values of  $p(p > p_F, p = p_F, \text{ and } p < p_F)$  is given in the lower right-hand corner of the figure.

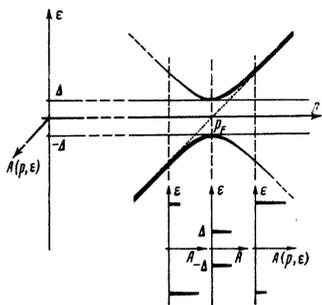


FIG. 5

FIG. 5. The spectral function  $A(p, \epsilon)$  for the case of superconducting electrons. The dotted line depicts the dependence of  $\epsilon$  on  $p$  for electrons in the normal state ( $\Delta = 0$ ).

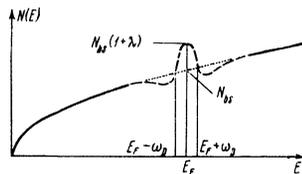


FIG. 6

FIG. 6. The change in the density of the electron states near the Fermi surface for metals in the normal state. The segments of the curve which pertain to the region in which it is impossible to regard the electrons as quasiparticles are indicated by the dashed line.

pletely exhausts the branch  $A_{II}$ , which is now described by a Lorentzian function having its maximum at  $\epsilon_{II} = \epsilon_0$  and with a half-width  $\Gamma = \lambda \omega_D$  (the weight of branch I in this region decreases exponentially:  $A_I \sim \exp(-2\lambda \epsilon / \omega_D)$ ).

Upon the transition of the metal into the superconducting state, an energy gap  $\Delta \ll \omega_D$  appears in the immediate vicinity of the Fermi energy. It is natural to assume that this gap appears on branch I of the electron spectrum, which is shown in Fig. 4. The spectral function for superconducting electrons,  $A(p, \epsilon) = u_p^2 \delta(\epsilon - \epsilon_p) + v_p^2 \delta(\epsilon + \epsilon_p)$  where

$$\begin{aligned} \epsilon_p &= [\epsilon_1^2(p) + \Delta^2]^{1/2}, \\ u_p^2 &= \frac{1}{2} \left( 1 + \frac{\epsilon_1(p)}{\epsilon_p} \right), \\ v_p^2 &= \frac{1}{2} \left( 1 - \frac{\epsilon_1(p)}{\epsilon_p} \right), \end{aligned}$$

is depicted in Fig. 5.

Fortunately, one can calculate physical quantities with the aid of the Green's function even in those cases when the simple picture of quasiparticles turns out to be inapplicable, and in individual cases one can physically interpret the obtained results by isolating the contributions of various branches to a given phenomenon. Thus, for example, one can show that only the electrons of branch I give a contribution to the heat capacity.<sup>4)</sup> This same electron branch determines the phenomenon of cyclotron resonance.

Thus, at the present time one can apparently assume that the electron-phonon interaction leads to the appearance of a layer of "heavy" electrons near the Fermi surface, the thickness of this layer amounting to several tens of  $\omega_D$ . To a rather high degree of accuracy one can regard the electrons in this layer as quasiparticles. The change in the effective mass of the electrons in this layer leads to an increase in the density of electron states at the Fermi surface for normal metals:  $N^* = N_{BS}(1 + \lambda)$  (see Fig. 6).

The picture of the renormalization of the electron spectrum in metals considered above is apparently qualitatively preserved over a rather broad range of temperatures, substantially below the Debye temperature.<sup>[16,17]</sup> As to the Pauli paramagnetic susceptibility  $\chi_p$ , in this case the energies of the subsystems of electrons with spins directed up and down are changed independently of whether the electrons interact with the phonons or not. Therefore  $\chi_p$  does not depend on the magnitude of the electron-phonon interaction.

At the present time the question as to how the diamagnetism of the electrons is changed by the phonon interactions remains unclear. One can calculate the diamagnetic susceptibility with the aid of the two-particle Green's function. This was done in article<sup>[19]</sup> for the case of a free electron gas without taking the electron-phonon interaction into account.

Apparently there is still another question which is not clear: what kind of role do the different branches of the electron spectrum play, for example, in transport phenomena? In article<sup>[20]</sup> where this question was investigated, the spectral function was replaced by a single Lorentzian function of unit weight. But since the weight of the side branches of the spectrum  $\lambda/(1 + \lambda)$  is of the order of the renormalization effects themselves, then perhaps such an investigation is incorrect.

In conclusion we wish to point out that the renormalization of the electron spectrum as a result of the electron-phonon interaction should lead to an anomalously strong dependence of the effective cyclotron mass of the electrons on the pressure. From experiments on the effect of pressure on superconductivity<sup>[21]</sup> it follows that the density of states of normal electrons at the Fermi surface is markedly reduced under hydrostatic pressure for practically all non-transition metals. Since the band density  $N_{BS}$  should change very slightly

<sup>4)</sup>In the formula given in [5] (Russian page 231) from the heat capacity of the electrons in a metal at  $T = 0^\circ\text{K}$ , the product  $(\partial \ln G(\epsilon)/\partial \epsilon) (\partial f(\epsilon)/\partial \epsilon)$  appears inside the integral sign, where  $f(\epsilon)$  is the Fermi distribution function. Since  $\partial f(\epsilon)/\partial \epsilon$  is a  $\delta$ -function, the heat capacity is determined only by the behavior of the Green's function for  $\epsilon = 0$ . At this point  $G(\epsilon)$  is uniquely given by branch I of the electron spectrum (see Fig. 4).

under pressure, it is natural to assume that the observed strong reduction of  $N^*(E_F)$  is a consequence of the decrease of the parameter  $\lambda$  under compression. On this basis one can anticipate that the effective cyclotron mass of the electrons at the Fermi surface will also decrease under pressure. A similar effect should be observed in connection with the investigation of the effect of pressure on the electronic specific heat.

We take this opportunity to express our sincere gratitude to A. A. Abrikosov for a detailed discussion of this work and for valuable advice.

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Translated by H. H. Nickle  
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