

SINGULARITIES OF THE PHONON ABSORPTION COEFFICIENT AND THE GEOMETRY OF THE FERMI SURFACE

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Singularities of the phonon spectrum and the phonon damping coefficient in metals due to phonon-electron interaction are considered. A relation is established between the singularities and the local properties of the Fermi surface. It is shown that the difference in the singularities is due not so much to differences of the local properties on the Fermi surface as to differences in the nature of the contact with the surface and its shifted analog. The relation between the attenuation coefficient and the singularities in the spectrum is established by means of dispersion relations which are similar to the Kramers-Kronig relations.

IN considering sound propagation in metals, the usual approximation (used by others in specific studies of the problem) is the neglect of the phonon momentum \mathbf{q} in comparison with the Fermi momentum of the electrons \mathbf{p}_F . In most cases, such an approximation is entirely valid. When the interaction of Debye (thermal) phonons with electrons is considered, e.g., for large phonon momenta, more interesting phenomena can be observed, which are due to the interaction of the phonons with the electrons. Thus, for $q = 2p_F$ (we are dealing with free electrons) a singularity exists in the phonon spectrum. For the same value of the momentum, the absorption coefficient falls discontinuously to zero.^[1, 2] On the other hand, the expression for the change in the phonon energy $\Delta\omega$ and for the absorption coefficient Γ (due to phonon-electron interaction) can be written in a form which is valid over a wide range of phonon momenta:

$$\Gamma = \int |M|^2 (n_p - n_{p+q}) \delta(\epsilon_p + \hbar\omega_q - \epsilon_{p+q}) d\tau, \quad (1)$$

$$\Delta\omega = \oint \frac{|M|^2 (n_p - n_{p+q}) d\tau}{\epsilon_p + \hbar\omega_q - \epsilon_{p+q}}, \quad d\tau = dp_x dp_y dp_z. \quad (2)$$

Here ϵ_p is the energy of electrons with momentum \mathbf{p} , and $n_p \equiv n(\epsilon_p)$ is the Fermi distribution function. The symbol \oint denotes the principal value of the integral. All the factors (of the type $2\pi/\hbar$ etc.) are taken into the square of the matrix element $|M|^2$.

The dependence of $|M|^2$ on the momenta (of the electron and the phonon) cannot be obtained in the general case. For small phonon momenta \mathbf{q} , starting with a macroscopic approach, one can establish the fact that $|M|^2 \sim q^2/\omega(\mathbf{q})$.

Use of perturbation theory, with the help of which Eqs. (1)-(2) were obtained, is justified by the condition^[3]

$$\omega\tau \gg u/v_F, \quad (3)$$

where τ is the electronic relaxation time, u the sound velocity, and v_F the speed of electrons with energy equal to the Fermi energy ϵ_F .

If, as a result of the absorption of a phonon, the electron undergoes a transition to another band (interband transition), then the absorption coefficient (we shall denote it by Γ') is written in the following fashion:

$$\Gamma' = \int |M'|^2 (n_p - n'_{p+q}) \delta(\epsilon_p + \hbar\omega_q - \epsilon'_{p+q}) d\tau, \quad (4)$$

where the prime on the energy means that $\epsilon'(\mathbf{p}) \neq \epsilon(\mathbf{p})$; $n'_{p+q} \equiv n(\epsilon'_{p+q})$. It is natural that the interband absorption of phonons is possible only in very special cases, in which the energy bands overlap,¹⁾ since, in the opposite case, the energy of the phonon is generally smaller than the band separation.

The problem of the present research is the establishment of the connection between the singularities of the absorption coefficient of the phonons Γ and the properties of the Fermi surface $\epsilon_p = \epsilon_F$. It is natural that the existence of singularities in the absorption coefficient corresponds to singularities in the phonon energy spectrum (for example, the finite jump in Γ for $q = 2p_F$ corresponds to a

¹⁾Overlap of the energy bands (zones) does not mean degeneracy, at which $\epsilon(\mathbf{p}) = \epsilon'(\mathbf{p})$ in some points of \mathbf{p} space. The case of degeneracy will be considered separately with graphite as an example.

logarithmic singularity in the dependence of $d\omega/dq$ on q in this same region.²⁾ This can be established directly (see [1, 4]); one can use dispersion relations similar to the well-known Kramers-Kronig relations (see, for example, [5] and also [6]). The second course is more convenient for us, since Eqs. (1) and (2) are analyzed comparatively simply (because of the δ function which describes the law of energy conservation).

Afnas'ev and Kagan^[4] have shown that the character of the Kohn singularity^[1] depends on the shape of the Fermi surface, while, in a number of cases, the singularity can be significantly strengthened. Taylor^[7] has shown how the shape of the Fermi surface determines those values of the quasimomentum of the Fermi phonons for which singularities are observed. However, in the work cited, the possible variation of the local properties of the Fermi surface was not taken into account. As will be shown in this work, a change in the local properties can lead to a significant sharpening of the singularity in the phonon spectrum.

The entire analysis has been carried out for a temperature of absolute zero (however, see Appendix II). A finite temperature, as well as various scattering mechanisms of the electrons, leads to a smoothing out of the singularities, in which the temperature plays the principal role for $T \gg \hbar/\tau$ while the scattering mechanisms play this role for $T \ll \hbar/\tau$. For a mean free path of the electron of the order of 10^{-3} cm, we have $\hbar/\tau \approx 1^\circ$ K.

We first consider intraband absorption. Since $\epsilon_{p+q} = \epsilon_p + \hbar\omega_q$ and the Fermi function at $T = 0$ differs from zero only for an argument smaller than the Fermi energy ϵ_F , the difference $n_p - n_{p+q}$ differs from zero only in a narrow range in p space, where

$$\epsilon_F - \hbar\omega_q \leq \epsilon_p \leq \epsilon_F, \quad (5)$$

while the δ function differs from zero only if

$$\epsilon_{p+q} - \epsilon_p = \hbar\omega_q. \quad (6)$$

Equation (6) is the equation of a surface in p space. Thus the absorption coefficient differs from zero only for those values of the Fermi momentum q for which the surface (6) intersects the region (5). Singularities in the dependence of $\Gamma(q)$ ought to be observed in those cases in which the topology of the cross section changes, in particular, when $\Gamma(q)$ vanishes (Fig. 1).

Since the Fermi energy ϵ_F for most metals is much larger than the limiting frequencies of the

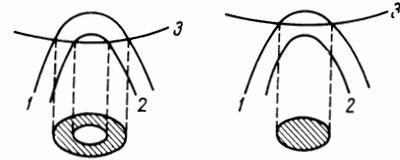


FIG. 1. 1—surface $\epsilon_p = \epsilon_F$; 2—surface $\epsilon_p = \epsilon_F - \hbar\omega_q$; 3—surface $\epsilon_p + \hbar\omega_q - \epsilon_{p+q} = 0$.

phonon spectrum, then the energy of the phonons can be neglected everywhere in a comparatively rough estimate of the character of the discontinuity. In this case the absorption coefficient takes the form

$$\Gamma = -\hbar\omega \int |M|^2 \frac{\partial n_F}{\partial \epsilon} \delta(\epsilon_p - \epsilon_{p+q}) d\tau$$

or, since

$$-\partial n_F / \partial \epsilon = \delta(\epsilon_p - \epsilon_F),$$

we get

$$\Gamma = \hbar\omega \int |M|^2 \delta(\epsilon_p - \epsilon_F) \delta(\epsilon_{p+q} - \epsilon_F) d\tau. \quad (7)$$

It is clear from the last equation that Γ differs from zero only for those values of q for which the Fermi surface $\epsilon_p = \epsilon_F$ and the Fermi surface $\epsilon_{p+q} = \epsilon_F$, shifted by an amount $-q$, intersect. Neglect of the quantity $\hbar\omega_q$ in comparison with the Fermi energy leads to the result that the two nearby singularities in the dependence on $\Gamma(q)$ merge, and the resultant singularity is sharper. Below, we shall trace the splitting of the singularity, but meanwhile (neglecting the splitting, that is, by using Eq. (7) and not (1)), we shall first determine the geometric locus of the singular points and then (in the same approximation) determine the character of the singularity as a function of the geometry of the Fermi surface.

Before undertaking an exposition of the new results, we note the following two circumstances:

1) For free electrons, as is well known,^[1, 2] the geometric locus of the singularities of $\Gamma(q)$ is a sphere of radius $2p_F$, while the character of the singularity is a finite jump. The reason for the fact that $\Gamma(q)$ vanishes jumpwise (while the line of intersection of the surfaces $\epsilon_p = \epsilon_F$ and $\epsilon_{p+q} = \epsilon_F$ reduces to a point) is clear from the following manner of expressing the absorption coefficient:

$$\Gamma(q) = \hbar\omega_q \oint \frac{|M|^2}{v_p v_{p+q}} \frac{dl_q}{\sin \theta_q} \quad q \leq 2p_F;$$

$$\Gamma(q) = 0, \quad q > 2p_F. \quad (8)$$

Here the integration is carried out along the inter-

²⁾This singularity is often called Kohn a singularity.

section line of the surfaces $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{F}}$ and $\epsilon_{\mathbf{p}+\mathbf{q}} = \epsilon_{\mathbf{F}}$; the quantity $dl_{\mathbf{q}}$ is an element of arc on this line, while $\theta_{\mathbf{q}}$ is the angle between the vector velocities $\mathbf{v}_{\mathbf{p}} = \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}$ and $\mathbf{v}_{\mathbf{p}+\mathbf{q}} = \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}+\mathbf{q}}$. When \mathbf{q} approaches $2\mathbf{p}_{\mathbf{F}}$, the circle which is the intersection line reduces to a point, but the angle $\theta_{\mathbf{p}}$ simultaneously goes to zero.

2) Under those conditions for which the Fermi surface is very close to a sphere (Na, K, etc.), because of the periodicity in \mathbf{p} space, the geometric locus of the singularities of $\Gamma(\mathbf{q})$ can differ appreciably from a sphere. Let us consider a simple cubic periodic structure (the edge of the cube is equal to b). If $2p_{\mathbf{F}} < b/2$, then the geometric locus of the singular points is a sphere, just as for free electrons, but if the radius of the spherical Fermi surface satisfies the condition

$$b/2 < 2p_{\mathbf{F}} < b,$$

then the geometric locus of the singular points of $\Gamma(\mathbf{q})$ is much more complicated. The plane case is shown in Fig. 2 for illustrative purposes. In the transition to the doubly-hatched region, the absorption coefficient is doubled jumpwise, while the absorption coefficient is equal to zero in the singly shaded region.

In the general case, the geometric locus of singular points of the coefficient $\Gamma(\mathbf{q})$ is found to be the set of values of the vector \mathbf{q} for which the surfaces $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{F}}$ and $\epsilon_{\mathbf{p}+\mathbf{q}} = \epsilon_{\mathbf{F}}$ make contact. We shall denote these values of the phonon momenta by $\mathbf{q}_0 = q_0\boldsymbol{\kappa}$ and shall be interested in the dependence of the absorption coefficient on the quantity $\Delta = \mathbf{q}_0 - \mathbf{q}$, assuming that $|\Delta| \ll q_0$. Furthermore, we shall assume that the approach to the critical value takes place along the direction of $\boldsymbol{\kappa}$, that is, $\mathbf{q} = q\boldsymbol{\kappa}$. (Naturally, other variants can also be considered.) If we exclude special cases (where the Fermi surface is a cylinder or a plane), then it is natural that the contact takes place at a single point. For $|\Delta| \ll q_0$, this allows us, in the calculation of the absorption coefficient, to use the expansion of the functions $\epsilon(\mathbf{p})$ and $\epsilon(\mathbf{p} + \mathbf{q})$ in powers of the vectors $\mathbf{p} - \mathbf{p}_0$ and $\mathbf{q} - \mathbf{q}_0$, where \mathbf{p}_0 is the contact point corresponding to the value of the phonon momentum \mathbf{q}_0 . Depending on the properties of the surfaces $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{F}}$ and $\epsilon_{\mathbf{p}+\mathbf{q}} = \epsilon_{\mathbf{F}}$ in the vicinity of the contact point \mathbf{p}_0 , different cases are possible, to the study of which we now turn. For the calculations, we shall make use of Eq. (8). We introduce the notation

$$\Delta\mathbf{p} = \mathbf{p} - \mathbf{p}_0, \quad \Delta p_x \equiv x, \quad \Delta p_y \equiv y, \quad \Delta p_z \equiv z \quad (9)$$

(the z axis is directed along the common normal

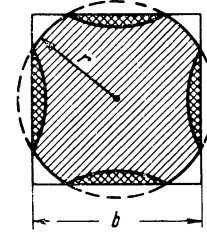


FIG. 2. $r = 2p_{\mathbf{F}}$.

to the surfaces). Integration in Eq. (8) is carried out over the curve of intersection of the surfaces $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{F}}$ and $\epsilon_{\mathbf{p}+\mathbf{q}} = \epsilon_{\mathbf{F}}$. Expanding $\epsilon(\mathbf{p})$ and $\epsilon(\mathbf{p} + \mathbf{q})$ in powers of the components of the vectors $\mathbf{p} - \mathbf{p}_0$ and $\mathbf{q} - \mathbf{q}_0$, we find the equation of these surfaces in the vicinity of the contact point ($x = y = z = 0$) with accuracy up to terms of fourth order of smallness: the surface $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{F}}$,

$$z_1(x, y) = -[A_{xx}x^2 + 2A_{xy}xy + A_{yy}y^2 + a_1x^3 + \dots + a_4y^3 + a_5x^4 + \dots + a_9y^4]; \quad (10)$$

the surface $\epsilon_{\mathbf{p}+\mathbf{q}} = \epsilon_{\mathbf{F}}$,

$$z_2(x, y) = B_{xx}x^2 + 2B_{xy}xy + B_{yy}y^2 + b_1x^3 + \dots + b_4y^3 + b_5x^4 + \dots + b_9y^4 - \nu\Delta. \quad (11)$$

In Eq. (11) there are other terms of the form $\Delta(\Delta + x + y + x^2 + \dots)$, but they can be neglected in comparison with $(-\nu\Delta)$ (in view of the smallness of Δ, x, y).

Here, $\nu = -(\mathbf{n} \cdot \boldsymbol{\kappa})$, where \mathbf{n} and $\boldsymbol{\kappa}$ are unit vectors in the directions of $\mathbf{v}_{\mathbf{p}_0}$ and \mathbf{q} , $\Delta = \mathbf{q} - \mathbf{q}_0$,

$$A_{\alpha\beta} = \frac{1}{2} \frac{1}{v_{\mathbf{p}_0}} \frac{\partial^2 \epsilon(\mathbf{p}_0)}{\partial p_\alpha \partial p_\beta},$$

$$B_{\alpha\beta} = \frac{1}{2} \frac{1}{v_{\mathbf{p}_0+\mathbf{q}_0}} [-(\mathbf{n}, \mathbf{n}_0)] \frac{\partial^2 \epsilon(\mathbf{p}_0 + \mathbf{q}_0)}{\partial p_\alpha \partial p_\beta},$$

$$\mathbf{n}_0 = \frac{\mathbf{v}_{\mathbf{p}_0+\mathbf{q}_0}}{v_{\mathbf{p}_0+\mathbf{q}_0}}.$$

The coefficients a_1, \dots, a_4 and b_1, \dots, b_4 contain derivatives of third order and products of derivatives of second order; the coefficients $a_5, \dots, a_9, b_5, \dots, b_9$ contain derivatives of fourth order and products of derivatives of third and second orders. All these products are divided by the corresponding velocity.

The equation of the intersection curve $y(x)$ can be found from the condition

$$z_2(x, y) - z_1(x, y) = 0. \quad (12)$$

Using (10) and (11), we find the equation for the determination of the function $y(x)$:

$$C_{xx}x^2 + 2C_{xy}xy + C_{yy}y^2 + c_1x^3 + \dots + c_4y^3 + c_5x^4 + \dots + c_6y^4 - v\Delta = 0, \tag{13}$$

where $C_{\alpha\beta} = A_{\alpha\beta} + B_{\alpha\beta}$ and $c_i = a_i + b_i$.

Knowing $z_1(x, y)$ and $z_2(x, y)$, it is easy to find $\sin \theta_q$:

$$\sin \theta_q = \left(\frac{(z_{2x}' - z_{1x}')^2 + (z_{2y}' - z_{1y}')^2 + (z_{1x}'z_{2y}' - z_{1y}'z_{2x}')^2}{(1 + z_{1x}'^2 + z_{1y}'^2)(1 + z_{2x}'^2 + z_{2y}'^2)} \right)^{1/2}. \tag{14}$$

The primes denote derivatives with respect to the corresponding coordinate: $z'_{1x} = \partial z_1 / \partial x$ and so forth. In Eq. (14), one must substitute $y(x)$.

Let us consider various cases:

1) The quadratic form $C_{\alpha\beta}x_\alpha x_\beta$ is positive definite, that is $C_{yy} > 0$ and $C_{xx}C_{yy} - C_{xy}^2 > 0$. It suffices to limit ourselves to terms of second order of smallness in Eq. (13). For $\Delta = 0$, the equation has only the trivial solution $x = y = 0$, that is, the only common point (for $\Delta = 0$) in the vicinity of the contact point will be this very point. For $\Delta > 0$, the lines of intersection will be curves of second order; for $\Delta < 0$, there is no intersection line, and the absorption drops jumpwise to zero (Fig. 3a). A simple calculation leads to the following expression for the quantity $\Gamma(\Delta > 0)$:

$$\Gamma(\Delta > 0) = \frac{\pi \hbar \omega_q |M(\mathbf{p}_0, \mathbf{q})|^2}{v_{\mathbf{p}_0} v_{\mathbf{p}_0 + \mathbf{q}} (C_{xx}C_{yy} - C_{xy}^2)^{1/2}}. \tag{15}$$

The form $C_{\alpha\beta}x_\alpha x_\beta$ can be negative definite. In this case, absorption is absent for $\Delta > 0$.

2) The quadratic form $C_{\alpha\beta}x_\alpha x_\beta$ is hyperbolic, that is, $C_{xx}C_{yy} - C_{xy}^2 < 0$. Then it also suffices to limit ourselves to terms of second order in Eq. (13). The surfaces intersect along the curves 1 ($\Delta = 0$), 2 ($\Delta > 0$), 3 ($\Delta < 0$) (see Fig. 5 below). This intersection, which recalls the intersection of the saddle surface by a plane, shows that the topology of the intersection line can be changed in the contact. The absorption coefficient differs from zero also for $\Delta > 0$ and for $\Delta < 0$. A sharp change in the absorption coefficient takes place at low values of the quantity Δ , while after this, a sharp change corresponds to that part of the absorption

coefficient which is connected with the integration near the point \mathbf{p}_0 . Therefore, one must use the expansion of the functions $\epsilon(\mathbf{p})$ and $\epsilon(\mathbf{p} + \mathbf{q})$ in the calculation. The calculation shows that

$$\Gamma(\Delta) \sim - \frac{\hbar \omega_q |M|^2}{v_{\mathbf{p}_0} v_{\mathbf{p}_0 + \mathbf{q}} (C_{xy}^2 - C_{xx}C_{yy})^{1/2}} \ln \left| \Delta \frac{v}{C_{xx}^{-1}} \right|, \tag{16}$$

The dependence of $\Gamma(\Delta)$ is shown schematically in Fig. 3b.

We still have to consider the case in which $C_{\alpha\beta}x_\alpha x_\beta$ is of parabolic form. By rotation of the x and y axes, this expression can be put in the form $C_{yy}y^2 \neq 0$. Use of the second approximation in this case is not sufficient. In order to determine the point of contact, it is necessary to consider the subsequent terms of the expansion in Eq. (13). We note that if the coefficients of x^3, y^3, \dots were identically equal to zero, then the contact would be made along a line. Naturally, such a situation is possible only as an exceptional case.

First, let us consider the case in which the coefficient of x^3 in Eq. (13) is equal to zero. This is always the case for limit singularities, for which the total coefficient is equal to zero for $q > q_0$, but there can also be intermediate singularities. It is then necessary to investigate the quadratic form in x^2, y :

$$C_{yy}y^2 + 2c_2x^2y + c_5x^4. \tag{17}$$

3) If the form (17) is positive definite, that is, $C_{yy} > 0$ and $C_{yy}c_5 - c_2^2 > 0$, then it suffices in Eq. (13) to confine ourselves only to this form. It isolates the contact point (for $\Delta = 0$) as the only common point of the surfaces, to which the curve of intersection of the surfaces contracts as $\Delta \rightarrow 0$. Calculation shows that

$$\Gamma(\Delta) \sim \frac{\pi \hbar \omega_q |M|^2 C_{yy}^{-1/4}}{v_{\mathbf{p}_0} v_{\mathbf{p}_0 + \mathbf{q}} v^{1/4} (C_{yy}c_5 - c_2^2)^{1/4}} \Delta^{-1/4}, \quad \Delta > 0, \tag{18}$$

$$\Gamma(\Delta) = 0, \quad \Delta < 0.$$

Such a dependence is shown in Fig. 3c.

If the form (17) is negative definite, then

$$\Gamma(\Delta > 0) = 0, \quad \Gamma(\Delta < 0) \sim |\Delta|^{-1/4}.$$

4) If the form (17) is hyperbolic, that is, $C_{yy}c_5 - c_2^2 < 0$, then it suffices to consider only this form in Eq. (13). The situation here is the same as in case 2), but it is necessary to assume that the "saddle" in the given case is not a surface of second order. Calculation leads to the result

$$\Gamma \sim \frac{\hbar \omega_q |M|^2 C_{yy}^{-1/4}}{v_{\mathbf{p}_0} v_{\mathbf{p}_0 + \mathbf{q}} v^{1/4} (c_2^2 - c_5 C_{yy})^{1/4}} |\Delta|^{-1/4} \tag{19}$$

(see Fig. 3b).

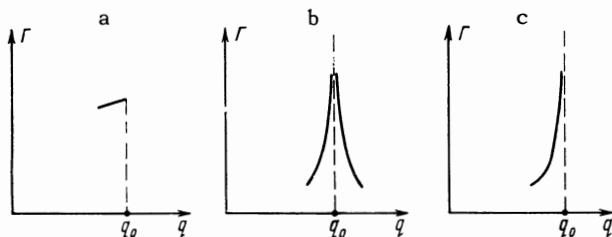


FIG. 3

5) We now consider the case in which $c_1x^3 \neq 0$. Equation (13) can be put in the form

$$C_{yy}y^2 + 2c_2x^2y + c_1x^3 - v\Delta = 0, \quad (20)$$

since the role of the remaining terms is insignificant. Solution of Eq. (20) gives the curve of intersection of the surfaces. The situation here is the same as in case 4). Simple calculation leads to the result:

$$\Gamma \sim \frac{\hbar\omega_{\mathbf{q}} |M|^2 C_{yy}^{-1/2}}{v_{p_0} v_{p_0+\mathbf{q}} c_1^{1/2} v^{1/6}} |\Delta|^{-1/6} \quad (21)$$

(see Fig. 3b).

6) Finally, let $C_{\alpha\beta}x_{\alpha}x_{\beta} \equiv 0$, that is, if we limit ourselves to the second approximation, then the contact is effected over part of the surface. Therefore, for the determination of the contact point, it is necessary to take the next terms of the expansion into account in (13). Here we consider the case in which the coefficients for terms of third order are equal to zero, which is always the case for limit singularities.

Terms of fourth order remain in Eq. (13). These form a positive definite expression, isolating (for $\Delta = 0$) the contact point as the only common point of the surfaces. The line of intersection is closed and contracts to the contact point as $\Delta \rightarrow 0$. Simple calculation leads to the result:

$$\Gamma \approx \frac{\pi\hbar\omega_{\mathbf{q}} |M|^2}{v_{p_0} v_{p_0+\mathbf{q}} \sqrt[3]{vc_7}} \times \begin{cases} \Delta^{-1/2}, & \Delta > 0 \\ 0, & \Delta < 0, \quad c_7 > 0, \quad c_6 = c_8 = 0 \end{cases} \quad (22)$$

(see Fig. 3c). The same singularity in the given approximation is observed in the case of a cylindrical Fermi surface.

We note that the singularities of $\Gamma(\mathbf{q})$ should be observed not only on the main diameters of the Fermi surface, but also on the "outside" diameters which characterize the location of different cavities of the Fermi surface in \mathbf{p} space. Naturally, it is a matter of indifference here as to whether these cavities formally belong to one band or to different bands, or are a periodic replica of the Fermi surface in the fundamental cell. The latter circumstance makes it unnecessary for us to consider the interband transitions as a special case.

Furthermore, we emphasize that the difference in the singularities of the coefficient $\Gamma(\mathbf{q})$ is associated not only with the difference in the local properties of the points on the Fermi surface, but also with the difference in the contact of the Fermi surface and its displaced analog.

Up to this point, we have neglected the quantity $\hbar\omega_{\mathbf{q}}$ in comparison with $\epsilon_{\mathbf{F}}$, which allows us to reduce the region $\epsilon_{\mathbf{F}} - \hbar\omega \leq \epsilon_{\mathbf{p}} \leq \epsilon_{\mathbf{F}}$ to the surface $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{F}}$. Account of the value of $\hbar\omega_{\mathbf{q}}$ (which can be especially important for metals with a comparatively small number of electrons—Bi, As, Sb, C (graphite)) leads to the result that the singularities described above split up, while at the points \mathbf{q}_1 and \mathbf{q}_2 ,

$$(\mathbf{q}_1 \approx \kappa(q_0 - \hbar\omega_0 / v v_{p_0}), \quad \mathbf{q}_2 \approx \kappa(q_0 + \hbar\omega_0 / v v_{p_0+q_0}))$$

the coefficient $\Gamma(\mathbf{q})$ has much weaker singularities than those described above (see Appendix I). As a rule, $d\Gamma(\mathbf{q})/d\mathbf{q}$ has the singularities described above in items 1)–6) (for fixed κ).

We emphasize two more circumstances. First, as we have already said, a finite temperature and different scattering mechanisms break up the singularities. Temperature diffusion will be considered in the simplest example in Appendix II, while the role of scattering leads to the result that the minimum value which the parameter Δ can take on is \hbar/l where l is the smallest of the mean free path lengths—of an electron with momentum \mathbf{p}_0 or a phonon with momentum \mathbf{q}_0 .

The anomalies of the absorption coefficient described above can be directly observed in the width of the line of inelastic neutron scattering, and also in the anomalies in the phonon spectrum. The character of the anomalies can be obtained directly (by using Eq. (2)), and is also clear on the basis of the dispersion relations.^[5, 6]

However, we must consider the following circumstance: too sharp a singularity in expressions $\Gamma(\mathbf{q})$ and $\Delta\omega(\mathbf{q})$ is evidently not possible because of the renormalization of the electron-phonon interaction, thanks to the account of the electron-electron interactions.³⁾ This means that the formulas given above are valid for not too small values of the parameter Δ .

Moreover, the transition to the exact (split) singularities (see Appendix I) leads to the result that all the values of the frequency $\omega(\mathbf{q})$ are shown to be not only finite but also not too strongly different from the unperturbed value.

The complicated surface of graphite^[8, 9] allows in principle the possibility of observing all the anomalies described above. The interaction of the electrons of graphite with sound will be the subject of a separate paper.

In conclusion, we note that for metals which possess magnetic structure (ferro- or antiferro-

³⁾We are grateful to E. Brovman for this remark (see also [7]).

magnetic), all the singularities noted above should be observed not only in the phonon spectrum, but also in the spin-wave spectrum.

APPENDIX I

We shall make clear the character of the split singularities. Inasmuch as we are interested in the region $\mathbf{p} \approx \mathbf{p}_0$ and $\mathbf{q} \approx \mathbf{q}_0$, Eq. (1) for the quantity $\Gamma(\mathbf{q})$ must lead to the form

$$\Gamma \approx \frac{|M(p_0, q)|^2}{|v_{p_0} - v_{p_0+q}|} \int_{(\epsilon_F - \hbar\omega \leq \epsilon_p \leq \epsilon_F)} dS_{(\epsilon_p + \hbar\omega - \epsilon_{p+q} = 0)} \quad (\text{I.1})$$

The notation used in items 1)–6) is kept here. New symbols are $\Delta_2 = q_2 - q_1$ and $\Delta_1 = q_1 - q$ (see above).

The functions $\epsilon(\mathbf{p})$ and $\epsilon(\mathbf{p} + \mathbf{q})$ are expanded in powers of $(\mathbf{p} - \mathbf{p}_0)_\alpha$ and $(\mathbf{q} - \mathbf{q}_0)_\alpha$, where, as before, \mathbf{p}_0 is the contact point of the surfaces $\epsilon_p = \epsilon_F$ and $\epsilon_{p+q} = \epsilon_F$ for $\mathbf{q} = \mathbf{q}_0$. In accord with (I.1), we find the area enclosed between the intersection curve of the surfaces $\epsilon_p = \epsilon_F$ and $\epsilon_{p+q} = \epsilon_F + \hbar\omega$ and the intersection curve of the surfaces $\epsilon_p = \epsilon_F - \hbar\omega$ and $\epsilon_{p+q} = \epsilon_F$. The intersection curve of the surfaces $\epsilon_p = \epsilon_F$ and $\epsilon_{p+q} = \epsilon_F + \hbar\omega$ is determined from the equation

$$C_{xx}x^2 + 2C_{xy}xy + C_{yy}y^2 + c_1x^3 + \dots + c_4y^3 + c_5x^4 + \dots + c_9y^4 - \nu_2\Delta_2 = 0, \quad (\text{I.2})$$

where ν_2 is determined from the condition

$$-\nu_2\Delta_2 + \hbar\Delta\omega_2 / v_{p_0+q_0} = -\nu_2\Delta_2, \quad \Delta\omega_2 = \omega_2 - \omega.$$

The intersection curve of the surfaces $\epsilon_p = \epsilon_F - \hbar\omega$, $\epsilon_{p+q} = \epsilon_F$ is determined from the equation

$$C_{xx}x^2 + 2C_{xy}xy + C_{yy}y^2 + c_1x^3 + \dots + c_4y^3 + c_5x^4 + \dots + c_9y^4 - \nu_2\Delta_2 + \hbar\omega(1/v_{p_0} + 1/v_{p_0+q_0}) = 0. \quad (\text{I.3})$$

The possible cases here are the same as were encountered in the study of Eq. (13); therefore we only list the results.

1) The quadratic form $C_{\alpha\beta}x_\alpha x_\beta$ is positive definite. Simple calculation leads to the result (see Fig. 4a)

$$\Gamma \approx \frac{\pi|M|^2}{|v_{p_0} - v_{p_0+q}| (C_{xx}C_{yy} - C_{xy}^2)^{1/2}} \times \begin{cases} \nu_2\Delta_2, & q_1 < q < q_2 \\ (1/v_{p_0} + 1/v_{p_0+q_0})\hbar\omega_q, & q < q_1. \end{cases} \quad (\text{I.4})$$

2) The quadratic form $C_{\alpha\beta}x_\alpha x_\beta$ is hyperbolic. In Fig. 5, $y_2(x)$ is a curve which is determined by Eq. (1.3) for $|\Delta_2| \ll |\Delta_1|$ while curves 1 ($\Delta_2 = 0$),

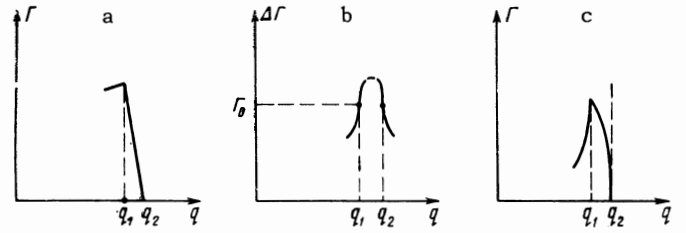


FIG. 4

2 ($\Delta_2 > 0$), and 3 ($\Delta_2 < 0$) are determined by Eq. (I.2) for the same conditions. Change in the area at the expense of a shift of the curve $y_2(x)$ is unimportant and can be neglected. The basic change in the area takes place between curves 1 and 2 (positive increment) for $\Delta_2 > 0$, and between curves 1 and 3 (negative increment) for $\Delta_2 < 0$. The basic contribution to the value of $\Delta\Gamma$ ($\Gamma = \Gamma_0 + \Delta\Gamma$, where Γ_0 is the smooth part and $\Delta\Gamma$ is determined by the area between curves 1 and 2 for $\Delta_2 > 0$, and 1 and 3 for $\Delta_2 < 0$) is made by the vicinity of the zero point, which is small enough to make the expansion of the functions $\epsilon(\mathbf{p})$ and $\epsilon(\mathbf{p} + \mathbf{q})$ correct.

If $|\Delta_1| \ll \Delta_2$, then the curve $y_2(x)$ occupies the position of curves 1, 2, and 3, depending on the sign of Δ_1 , while the curve (I.2) takes the position indicated by the dashed line in Fig. 5. Increase in the area here changes the sign opposite to the corresponding sign of Δ_1 (in comparison with the case described).

For this case, the quantity $\Delta\Gamma$ has the form (see Fig. 4b)

$$\Delta\Gamma \sim \frac{|M|^2}{|v_{p_0} - v_{p_0+q}| (C_{xx}C_{yy} - C_{xy}^2)^{1/2}} \times \begin{cases} -\nu_2\Delta_2 \ln \left| \Delta_2 \frac{\nu_2}{C_{xx}^{-1}} \right|, & |\Delta_2| \ll |\Delta_1| \\ \nu_1\Delta_1 \ln \left| \Delta_1 \frac{\nu_1}{C_{xx}^{-1}} \right|, & |\Delta_1| \ll \Delta_2. \end{cases} \quad (\text{I.5})$$

3) Form (17) is positive definite. Simple calculation for this case leads to the result (see Fig. 4c)

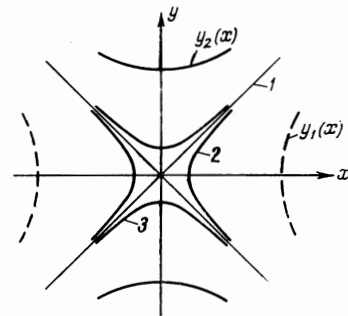


FIG. 5

$$\Gamma \approx \frac{4|M|^2 v_2^{3/4} \alpha_1}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| C_{yy}^{1/4} (c_5 C_{yy} - c_2^2)^{1/4}} [\Delta_2^{3/4} - \alpha_2 \Delta_1^{3/4}];$$

$$\alpha_1 = \frac{1}{6\sqrt{2}\pi} \left[\Gamma \left(\frac{1}{4} \right) \right]^2, \quad \alpha_2 = \left(\frac{v_1}{v_2} \right)^{3/4}, \quad (\text{I.6})$$

ν_1 is determined from the condition

$$-v\Delta_1 - \mathfrak{H}\Delta\omega_1 / v_{p_0} = -v_1\Delta_1, \quad \Delta\omega_1 = \omega_1 - \omega.$$

4) Form (17) is hyperbolic. The calculation, carried out on the same principle as in case 2) leads to the result (see Fig. 4b): for $|\Delta_2| \ll |\Delta_1|$

$$\Delta\Gamma \sim \frac{|M|^2 v_2^{3/4}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| C_{yy}^{1/4} (c_2^2 - c_5 C_{yy})^{1/4}} \begin{cases} \Delta_2^{3/4}, & \Delta_2 > 0 \\ -|\Delta_2|^{3/4}, & \Delta_2 < 0 \end{cases}; \quad (\text{I.7})$$

for $|\Delta_1| \ll \Delta_2$

$$\Delta\Gamma \sim \frac{|M|^2 v_1^{3/4}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| C_{yy}^{1/4} (c_2^2 - c_5 C_{yy})^{1/4}} \begin{cases} -\Delta_1^{3/4}, & \Delta_1 > 0 \\ |\Delta_1|^{3/4}, & \Delta_1 < 0 \end{cases}$$

5) $C_{\alpha\beta x_\alpha x_\beta} = C_{yy} y^2 \neq 0$, $c_1 x^3 \neq 0$. Calculation is performed according to the same principle as in cases 2) and 4). The result is the following (see Fig. 4b): for $|\Delta_2| \ll |\Delta_1|$

$$\Delta\Gamma \sim \frac{|M|^2 v_2^{5/6}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| C_{yy}^{1/2} c_1^{1/3}} \begin{cases} \Delta_2^{5/6}, & \Delta_2 > 0 \\ -|\Delta_2|^{5/6}, & \Delta_2 < 0 \end{cases}; \quad (\text{I.8})$$

for $|\Delta_1| \ll \Delta_2$,

$$\Delta\Gamma \sim \frac{|M|^2 v_1^{5/6}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| C_{yy}^{1/2} c_1^{1/3}} \begin{cases} -\Delta_1^{5/6}, & \Delta_1 > 0 \\ |\Delta_1|^{5/6}, & \Delta_1 < 0 \end{cases}$$

6) $C_{\alpha\beta x_\alpha x_\beta} \equiv 0$, the coefficients for the terms of third order are equal to zero, while the remaining expression is positive definite. The result is given by the expression (see Fig. 4c)

$$\Gamma \approx \frac{2|M|^2 v_2^{1/2}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| c_7^{1/2}} [\Delta_2^{1/2} - \beta \Delta_1^{1/2}];$$

$$\beta = (v_1/v_2)^{1/2}, \quad c_7 > 0, \quad c_6 = c_8 = 0. \quad (\text{I.9})$$

Below, we shall present formulas for the singularities in the phonon spectrum corresponding to different types of contact of the surfaces $\epsilon_p = \epsilon_F$ and $\epsilon_{p+q} = \epsilon_F$. The numbering is the same as in the consideration of the singularities of $\Gamma(\mathbf{q})$.

A detailed derivation of these formulas, and also the proof of the dispersion relations will be the subject of a separate publication of one of the authors (A. I. Semenenko).

The expressions for the split singularities of $\Delta\omega$ in cases 1)–6) have the following form:

$$1) \Delta\omega = \frac{\pi|M|^2}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| (C_{xx} C_{yy} - C_{xy}^2)^{1/2}} \times \begin{cases} v_2 \Delta_2 \ln \left| \frac{v_2}{C_{xx}^{-1}} \Delta_2 \right|, & |\Delta_2| \ll |\Delta_1| \\ v_1 \Delta_1 \ln \left| \frac{v_1}{C_{xx}^{-1}} \Delta_1 \right|, & |\Delta_1| \ll \Delta_2 \end{cases} \quad (\text{I.10})$$

2) The same expression, but $C_{xx} C_{yy} - C_{xy}^2$ is taken in terms of the modulus.

3) For $|\Delta_2| \ll |\Delta_1|$

$$\Delta\omega = \frac{\pi|M|^2 F_1 v_2^{3/4}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}|} \begin{cases} -\Delta_2^{3/4}, & \Delta_2 > 0 \\ \sqrt{2} |\Delta_2|^{3/4}, & \Delta_2 < 0 \end{cases}. \quad (\text{I.11})$$

Here $F_1 = 4C_{yy}^{-1/4} (C_{yy} c_5 - c_2^2)^{-1/4}$. For $|\Delta_1| \ll \Delta_2$, the expression for $\Delta\omega$ is obtained from (I.11) by the replacement of ν_2 and Δ_2 by ν_1 and Δ_1 , respectively.

4) For $|\Delta_2| \ll |\Delta_1|$

$$\Delta\omega \sim \frac{|M|^2 F_2 v_2^{3/4}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}|} \begin{cases} \left(\frac{v_{p_0+q_0}}{\hbar\omega_0} \right)^{1/4} \Delta_2, & \Delta_2 > 0 \\ |\Delta_2|^{3/4}, & \Delta_2 < 0 \end{cases}. \quad (\text{I.12})$$

Here $F_2 = C_{yy}^{-1/4} (c_2^2 - C_{yy} c_5)^{-1/4}$. For $|\Delta_1| \ll \Delta_2$ in Eq. (I.12) the quantities ν_2 , Δ_1 , and $v_{p_0+q_0}$ must be replaced by ν_1 , Δ_1 , and v_{p_0} , respectively.

5) For $|\Delta_2| \ll |\Delta_1|$,

$$\Delta\omega \sim \frac{|M|^2 F_3 v_2^{5/6}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}|} \begin{cases} -\Delta_2^{5/6}, & \Delta_2 > 0 \\ |\Delta_2|^{5/6}, & \Delta_2 < 0 \end{cases}. \quad (\text{I.13})$$

Here $F_3 = C_{yy}^{-1/2} c_1^{-1/3}$. For $|\Delta_1| \ll \Delta_2$, the quantities ν_2 , Δ_2 in Eq. (I.13) must be replaced by ν_1 , Δ_1 , respectively.

6) For $|\Delta_2| \ll |\Delta_1|$

$$\Delta\omega \sim \frac{2\pi|M|^2 \sqrt{v_2}}{|\mathbf{v}_{p_0} - \mathbf{v}_{p_0+q}| c_7^{1/2}} \begin{cases} \left(\frac{v_{p_0+q}}{\hbar\omega_0} \right)^{1/2} \Delta_2, & \Delta_2 > 0 \\ |\Delta_2|^{1/2}, & \Delta_2 < 0 \end{cases}. \quad (\text{I.14})$$

For $|\Delta_1| \ll \Delta_2$, the quantities ν_2 , Δ_2 , $v_{p_0+q_0}$ in Eq. (I.14) must be replaced by ν_1 , Δ_1 , v_{p_0} , respectively.

The singularities 1), 2), 3), and 5) are shown schematically in Fig. 6a, and the singularities 4)–6) in Fig. 6b.

APPENDIX II

We consider the temperature diffusion in the simplest case in which $\epsilon_p = p^2/2m$. For the absorption coefficient, we use Eq. (1), in which

$$n_p - n_{p+q} \approx -\hbar\omega \frac{\partial n}{\partial \epsilon} = \frac{\hbar\omega}{kT} \frac{e^{(\epsilon_p - \epsilon_F)/kT}}{(e^{(\epsilon_p - \epsilon_F)/kT} + 1)^2},$$

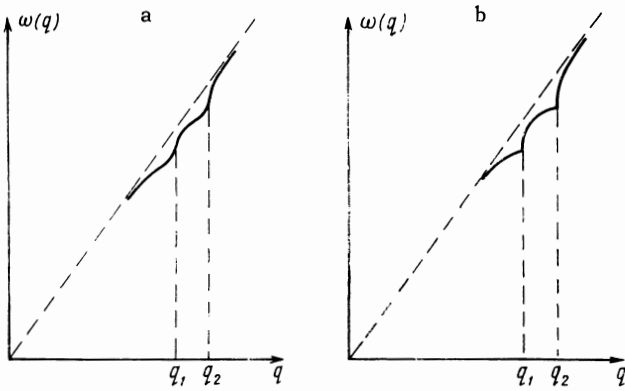


FIG. 6

while the quantity $\hbar\omega_0$ is neglected in the δ function. The temperature is sufficiently low. Simple calculation then leads to the result

$$\Gamma \approx \frac{\hbar\omega_q}{q} \frac{2\pi m^2 |M(\mathbf{p}_F, \mathbf{q})|^2}{\exp(p_F \Delta / 2mkT) + 1}, \quad \Delta = q - 2p_F. \quad (\text{II.1})$$

It is seen from (II.1) that the temperature diffusion takes place in the interval

$$-2mkT / p_F < \Delta < 2mkT / p_F.$$

The width of the interval is much less than $2p_F$. Outside of this interval, the quantity Γ remains basically the same as for $T = 0$ (see (15)).

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