"Taylor" singularities in the phonon spectrum of metals

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The existence of lines of parabolic points on the Fermi surface of metals leads to the appearance of singularities in the phonon spectrum $\Delta\omega$ and in the value of the inverse lifetime Γ of the phonons; we have called these "Taylor" singularities [P. L. Taylor, Phys. Rev. **131**, 1995 (1963)]. Because of the presence of antipode points on the Fermi surface, Taylor singularities show up most clearly in Γ. The loci of singular points in $\Delta\omega$ and Γ in the momentum space of the phonons are considered, and the relation between the local geometry of the Fermi surface and the form of these loci is investigated, together with the nature of the Γ singularity. It is shown that the presence of a plane of symmetry in the Fermi surface leads to the appearance of an enhanced singularity in $\Delta\omega$ and in Γ.

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Singularities in the dispersion law $\omega=\omega(\mathbf{q})$ of phonons, produced by their interaction with the conduction electrons (see Migdal[1] and Kohn[2]), are observed at $q=2p_F$, if the Fermi surface (FS) is a sphere of radius p_F. The nature of the singularity is $\Delta\omega\sim x\ln|x|$, $x=q-2p_F$. At the same value of the phonon quasimomentum, the derivative with respect to q of the quantity Γ (where $\Gamma=1/\tau_{\mathbf{q}}$, and $\tau_{\mathbf{q}}$ is the lifetime of a phonon) experiences a discontinuity. Afanas'ev and Kagan[3] showed that the singularity is enhanced if the FS contains finite cylindrical or plane sections, and Kaganov and Semenenko[4] showed that the nature of the singularity is influenced by the local properties of the FS. In all the cited papers, the phonon momenta $\mathbf{q}$ considered were close to the value of the diameter of the FS. The existence of dents and bridges on the FS leads to singularities in the phonon spectrum at $q\to 0$ in those cases in which sound is propagated in the dierction of a tangent at a parabolic point.[5,6] According to Ref. 5, there are parabolic points of two types, the O and the X types. At an O-type point there is a discontinuity, and at an X-type point a logarithmic singularity, in the absorption coefficient of sound.

In the present paper, we investigate singularities in the phonon spectrum with $q\neq 0$; these are possible only in metals whose Fermi surfaces contain lines of parabolic points. The singularities considered in Refs. 5 and 6 are the limiting case of these singularities for $q\to 0$.

To determine the singularities of the quantity Γ and of the frequency shift $\Delta\omega$, we shall use the expressions obtained in the first order of perturbation theory:

$$\Gamma=\int |M|^2[n(\varepsilon_{\mathbf{p}})-n(\varepsilon_{\mathbf{p+q}})]\delta(\varepsilon_{\mathbf{p}}+\hbar\omega_{\mathbf{q}}-\varepsilon_{\mathbf{p+q}})\,d^3p, \tag{1}$$

$$\Delta\omega=\fint\frac{|M|^2[n(\varepsilon_{\mathbf{p}})-n(\varepsilon_{\mathbf{p+q}})]}{\varepsilon_{\mathbf{p}}+\hbar\omega_{\mathbf{q}}-\varepsilon_{\mathbf{p+q}}}\,d^3p. \tag{2}$$

Here $\varepsilon_{\mathbf{p}}$ is the energy of the electrons, $n=n(\varepsilon)$ is the Fermi function, and M is the matrix element of the electron-phonon interaction [all factors of the type $1/(2\pi\hbar)^3$ and the like are included in it]. The expressions (1) and (2) are correct under the condition $ql/\hbar\to 0$, where l is the free path length of the electrons.

For a comparatively crude estimate of the singularities, we may neglect the phonon energy, since $\hbar\omega_{\mathbf{q}}\ll\varepsilon_F$ (ε_F is the Fermi energy). Then at the absolute zero of temperature, the expression (1) can be put into the following form:

$$\Gamma\approx\hbar\omega_{\mathbf{q}}\int|M|^2\delta(\varepsilon_{\mathbf{p}}-\varepsilon_F)\delta(\varepsilon_{\mathbf{p+q}}-\varepsilon_F)\,d^3p. \tag{3}$$

It is evident that singularities of Γ, and hence of $\Delta\omega$, occur in those and only in those cases in which there is a change of topology of the line of intersection of the surfaces $\varepsilon_{\mathbf{p}}=\varepsilon_F$ and $\varepsilon_{\mathbf{p+q}}=\varepsilon_F$. Consequently the locus of singular points (LSP) in the phonon spectrum is determined as the set of those values of the vector $\mathbf{q}$ for which the surfaces $\varepsilon_{\mathbf{p}}=\varepsilon_F$ and $\varepsilon_{\mathbf{p+q}}=\varepsilon_F$ are tangent. We shall call these values of the vector $\mathbf{q}$ critical values and shall designate them by $\mathbf{q}_c$.

The phonon momentum values $\mathbf{q}=\mathbf{q}_c$ corresponding to Kohn singularities connect points on the FS at which the electron velocities $\mathbf{v}_{\mathbf{p}}$ and $\mathbf{v}_{\mathbf{p+q}}$ are *antiparallel*. If there are parabolic points on the FS, then there are singularities of another type: the surfaces $\varepsilon_{\mathbf{p}}=\varepsilon_F$ and $\varepsilon_{\mathbf{p+q}}=\varepsilon_F$ may touch at points at which the velocities $\mathbf{v}_{\mathbf{p}}$ and $\mathbf{v}_{\mathbf{p+q}}$ are *parallel*; we shall designate the corresponding phonon momentum values also by $\mathbf{q}_c$. The existence of such singularities was first pointed out by Taylor.[7] We therefore call them Taylor singularities.

All types of Taylor singularities can be investigated on FS of two types: "dumbbells" (Fig. 1) and "tops" (Fig. 2). In the case of a "dumbbell", a Taylor singu-

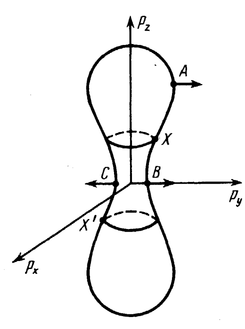

FIG. 1. Fermi surface of "dumbbell" type. Points X and X' lie on collars of parabolic points of X type. The arrows indicate the directions of the velocities at the corresponding points of the Fermi surface.

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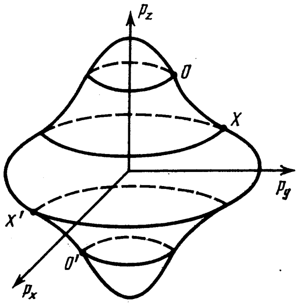


FIG. 2. Fermi surface of "top" type. Collars of parabolic points of O and of X type are marked on the surface.

larity occurs when the surfaces $\varepsilon_p=\varepsilon_F$ and $\varepsilon_{p+q_c}=\varepsilon_F$ are tangent, for example at points A and B; a Kohn singularity, for tangency at points A and C (see Fig. 1). Since a singularity is determined by the local properties of the FS, the treatment given here is of general character. The "dumbbell" and the "top" are chosen only for illustration (on a "dumbbell" there are parabolic points only of X type; on a "top", both of X and of O types).

We note an important difference of Taylor singularities from Kohn. In consequence of the central symmetry of the dispersion law of electrons, each of two chosen points on the FS with parallel velocities (they are connected by the vector $\mathbf{q}_c$) has a point with antiparallel velocity (the antipode point). We shall designate by $\mathbf{q}_c^{(a)}$ the critical momentum connecting the antipode points corresponding to the two chosen points. If we neglect the phonon energy $\hbar\omega_q$ in the expressions (1) and (2), then the singularities corresponding to these two pairs of points occur at a single point of q space ($\mathbf{q}_c=\mathbf{q}_c^{(a)}$); the singularities in Γ add, while those in $\Delta\omega$ cancel. When the value of $\hbar\omega$ is taken into account, first, the momenta $\mathbf{q}_c$ and $\mathbf{q}_c^{(a)}$ differ somewhat in value and in direction: $|\mathbf{q}_c-\mathbf{q}_c^{(a)}|\sim\hbar\omega_{q_c}/v_F$, and the angle between them is of order $\hbar\omega_{q_c}/(q_c v_F)$ (v_F is the Fermi velocity); second, each of the two singularities is split and weakened. The structure of singularities, for example of O and X type (see below), is shown in Ref. 5. Fig. 7 (for visualizability, we neglect the splitting of the singularities). In our case, the width of the step on this figure for angular singularities $\sim\hbar\omega_{q_c}/(q_c v_F)$; and for singularities due to change of the phonon momentum in magnitude, $\sim\hbar\omega_{q_c}/v_F$. Hence it follows that Taylor singularities show up most clearly in Γ. Therefore we shall hereafter be interested chiefly in singularities in the value of the inverse lifetime of the phonons.

We shall consider the LSP of Taylor singularities. For this purpose, by use of the equations of the surfaces $\varepsilon_p=\varepsilon_F$ and $\varepsilon_{p+q}=\varepsilon_F$ in the vicinity of an arbitrarily chosen point of tangency ($\mathbf{p}=\mathbf{p}_c$ when $\mathbf{q}=\mathbf{q}_{c0}$), we shall determine the equation of the LSP in q space in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$. We shall designate by the letter A the point of tangency on the surface $\varepsilon_p=\varepsilon_F$, with coordinates $p_x=p_{cx}$, $p_y=p_{cy}$, $p_z=p_{cz}$, and by the letter B the point of tangency on the surface $\varepsilon_{p+q}=\varepsilon_F$ ($\mathbf{p}=\mathbf{p}_c+\mathbf{q}_{c0}$). We shall attach to the point A an orthogonal system of coordinates, whose p_z axis is directed along the normal to the FS at this point, while the p_x and p_y axes are located in principal sections of the surface. If we assume for simplicity that the points A and B are located in planes of local symmetry of thecorresponding surfaces (with respect to p_x), the equation of the surface $\varepsilon_p=\varepsilon_F$ in the vicinity of the point A can be written in the following form:

$$p_z^A(p_x,\ p_y)={}^1/_2 f_{xx}p_x^2+{}^1/_2 f_{yy}p_y^2+{}^1/_2 f_{xxy}p_x^2p_y+{}^1/_6 f_{yyy}p_y^3+{}^1/_{24}f_{xxxx}p_x^4+\ldots; \tag{4}$$

and for the equation of the surface $\varepsilon_{p+q}=\varepsilon_F$ in the vicinity of the point B we have

$$\begin{aligned}p_z^B(p_x,\ p_y,\ \delta_x,\ \delta_y,\ \delta_z)&={}^1/_2\varphi_{xx}(p_x+\delta_x)^2\\&+{}^1/_2\varphi_{yy}(p_y+\delta_y)^2+{}^1/_2\varphi_{xxy}(p_x+\delta_x)^2(p_y+\delta_y)\\&+{}^1/_6\varphi_{yyy}(p_y+\delta_y)^3+{}^1/_{24}\varphi_{xxxx}(p_x+\delta_x)^4-\delta_z+\ldots,\end{aligned} \tag{5}$$

where $\delta_x=q_x-q_{c0x}$, $\delta_y=q_y-q_{c0y}$, $\delta_z=q_z-q_{c0z}$; $|\boldsymbol{\delta}|\ll|\mathbf{q}_{c0}|$. In the expressions (4) and (5), the coefficients f_{ij}, φ_{ij}, and so on are determined by the partial derivatives of the quantities ε_p and ε_{p+q} with respect to the components of the momentum p at the respective points A and B; for example,

$$f_{xx}=-\frac{1}{v_A}\frac{\partial^2\varepsilon(A)}{\partial p_x^2},\quad \varphi_{xx}=-\frac{1}{v_B}\frac{\partial^2\varepsilon(B)}{\partial p_x^2}.$$

The equation of the line of intersection of the surfaces $\varepsilon_p=\varepsilon_F$ and $\varepsilon_{p+q}=\varepsilon_F$—the equation of a "collar" on the FS—is found from the relation

$$p_z^A(p_x,\ p_y)-p_z^B(p_x,\ p_y,\ \delta_x,\ \delta_y,\ \delta_z)=0. \tag{6}$$

The collar formed when the surfaces $\varepsilon_p=\varepsilon_F$ and $\varepsilon_{p+q_c}=\varepsilon_F$ are tangent we shall call a critical collar. Thus the expression (6) with $\delta=0$ determines a critical collar. The equation of the LSP of Taylor singularities in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$, i.e., the relation $\delta_z=\delta_z(\delta_x,\ \delta_y)$, is determined by the requirement that equation (6) with $\delta\neq0$ shall give a new critical collar (a critical point on this collar of course does not coincide with the points A and B; therefore in writing of the equation of the collar in standard form, a shift is required—a translation of the coordinate system).

We shall investigate the various cases that are encountered oftenest. The structure of the LSP is determined by the relations between the coefficients f_{ij}, φ_{ij}, and so on in the expansions (4) and (5).

I. Suppose that $f_{xx}\neq\varphi_{xx}$, $f_{yy}\neq\varphi_{yy}$, and any one of these coefficients is nonzero. For the equation of the LSP we get from (6), with the necessary accuracy,

$$\delta_z=\frac{1}{2}\frac{\varphi_{xx}f_{xx}}{f_{xx}-\varphi_{xx}}\delta_x^2+\frac{1}{2}\frac{\varphi_{yy}f_{yy}}{f_{yy}-\varphi_{yy}}\delta_y^2. \tag{7}$$

If

$$\varphi_{xx}f_{xx}\varphi_{yy}f_{yy}(f_{xx}-\varphi_{xx})(f_{yy}-\varphi_{yy})>0,$$

then the surface (7) represents an elliptic paraboloid; if the sign of this product is the opposite, then (7) determines a hyperbolic paraboloid. The coordinate axes in q space are parallel to the corresponding axes in p space. The topology of the critical collar does not change along the LSP in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$:

$${}^1/_2(\varphi_{xx}-f_{xx})p_x^2+{}^1/_2(\varphi_{yy}-f_{yy})p_y^2=0. \tag{8}$$

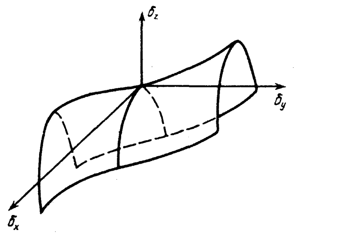


FIG. 3. Locus of singular points in the vicinity of a chosen point $\mathbf{q}=\mathbf{q}_{c0}$ in case II.

If $(\varphi_{xx}-f_{xx})(\varphi_{yy}-f_{yy})>0$, then the critical collar is a point, and the value of Γ experiences a discontinuity; but if $(\varphi_{xx}-f_{xx})(\varphi_{yy}-f_{yy})<0$, then the critical collar near the critical point is two intersecting straight lines, and Γ has a logarithmic singularity. Hereafter we shall classify and name these Taylor singularities as in Ref. 5: O type (discontinuity of Γ) and X type (logarithmic singularity of Γ).

II. Suppose that $f_{xx}\neq\varphi_{xx}$, $f_{xx}\neq 0$, $\varphi_{xx}\neq 0$, and $f_{yy}\neq\varphi_{yy}=0$; that is, the point B is a parabolic point. The equation of the LSP is written as follows:

$$\delta_z=\frac{1}{2}\frac{\varphi_{xx}f_{xx}}{f_{xx}-\varphi_{xx}}\delta_x^2+\frac{1}{6}\varphi_{yyy}\delta_y^3. \qquad (9)$$

The form of the surface (9) is shown in Fig. 3 ($\mathbf{q}\approx\mathbf{q}_{c0}$). The topology of the critical collar does not change with change of the vector $\boldsymbol{\delta}_c=\mathbf{q}_c-\mathbf{q}_{c0}$ ($|\boldsymbol{\delta}_c|\ll|\mathbf{q}_{c0}|$):

$$^1/_2(\varphi_{xx}-f_{xx})p_x^2-{}^1/_2 f_{yy}p_y^2=0. \qquad (10)$$

The structure of the critical collar and the nature of the singularity are similar to those of case I.

III. Suppose that $f_{xx}\neq\varphi_{xx}$, $f_{xx}\neq 0$, $\varphi_{xx}\neq 0$, $\varphi_{yy}=f_{yy}\neq 0$, $\varphi_{yyy}\neq f_{yyy}$. In this case, we get two "sheets" of the LSP, $\delta_z=\delta_z^{(1)}(\delta_x,\delta_y)$ and $\delta_z=\delta_z^{(2)}(\delta_x,\delta_y)$, when $\delta_y>0$:

$$\begin{aligned}\delta_z^{(1)}&=\frac{1}{2}\frac{\varphi_{xx}f_{xx}}{f_{xx}-\varphi_{xx}}\delta_x^2+\frac{2}{3}\varphi_{yy}\left(\frac{2\varphi_{yy}}{f_{yyy}-\varphi_{yyy}}\right)^{1/2}\delta_y^{3/2},\\ \delta_z^{(2)}&=\frac{1}{2}\frac{\varphi_{xx}f_{xx}}{f_{xx}-\varphi_{xx}}\delta_x^2-\frac{2}{3}\varphi_{yy}\left(\frac{2\varphi_{yy}}{f_{yyy}-\varphi_{yyy}}\right)^{1/2}\delta_y^{3/2},\end{aligned} \qquad (11)$$

[for definiteness we suppose that $\varphi_{yy}(f_{yyy}-\varphi_{yyy})>0$]. The surface (11) is shown in Fig. 4. The LSP contains a line of reentry points on the plane $\delta_y=0$:

$$\delta_z={}^1/_2\varphi_{xx}f_{xx}\delta_x^2/(f_{xx}-\varphi_{xx}).$$

The evolution of the critical collar with change of the vector δ_c along the first "sheet" of the LSP is determined by the equation

$$\begin{aligned}&{}^1/_2(\varphi_{xx}-f_{xx})p_x^2-{}^1/_2[2\varphi_{yy}(f_{yyy}-\varphi_{yyy})]^{1/2}\delta_{cy}^{1/2}p_y^2\\ &\quad+{}^1/_6(\varphi_{yyy}-f_{yyy})p_y^3=0,\quad \delta_{cy}>0;\end{aligned} \qquad (12)$$

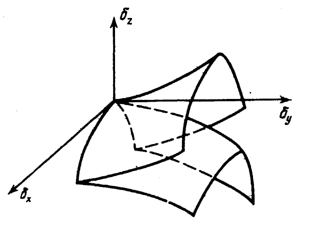


FIG. 4. Locus of singular points in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$ in case III.

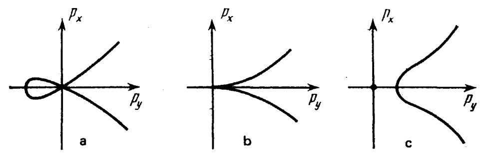


FIG. 5. Change of topology of the critical collar (12) on transition from one "sheet" of the locus of singular points to another [for definiteness, we suppose that $(\varphi_{xx}-f_{xx})>0$, $(\varphi_{yyy}-f_{yyy})<0$]: a) structure of the critical collar along the first "sheet" of the locus; b) structure of the critical collar at the transition points; c) structure of the critical collar along the second "sheet" of the locus.

along the second "sheet", by

$$\begin{aligned}&{}^1/_2(\varphi_{xx}-f_{xx})p_x^2+{}^1/_2[2\varphi_{yy}(f_{yyy}-\varphi_{yyy})]^{1/2}\delta_{cy}^{1/2}p_y^2\\ &\quad+{}^1/_6(\varphi_{yyy}-f_{yyy})p_y^3=0,\quad \delta_{cy}>0.\end{aligned} \qquad (12')$$

It is clear from (12) and (12′) that on passage from one "sheet" of the LSP to the other, the topology of the critical collar changes (Fig. 5). Consequently, the type of singularity also changes: a singularity of O type is transformed to a singularity of X type (and conversely). We emphasize that the points of transition from O- to X- singularities (and conversely) on the LSP are not directly related to the local structure of the FS but are determined by the relation of the corresponding derivatives at various points on it (of course with paralel velocities $\mathbf{v}_{\mathbf{p}_c}$ and $\mathbf{v}_{\mathbf{p}_c+\mathbf{q}_{c0}}$).

At the transition points ($\delta_{cy}=0$), the singularity is enhanced:

$$\Delta\Gamma\sim|\delta_z|^{-1/6}. \qquad (13)$$

In the expression (13), we have for singularities due to change of magnitude of the phonon momentum: $\delta_z=\delta_q\cos\theta$, where $\delta_q=q-q_{c0}$ and where θ is the angle between the vectors $\mathbf{q}_{c0}$ and $\mathbf{v}_{\mathbf{p}_c}$, and the vector $\mathbf{q}$ is directed along the vector $\mathbf{q}_{c0}$. For angular singularities $\delta_z\approx -q_{c0}\sin\theta\cdot\delta\theta$, where $\delta\theta$ is the deviation of the vector $\mathbf{q}$ from the critical momentum $\mathbf{q}_{c0}$. We shall not consider here the singularities in those cases in which the approach to the critical value of the momentum occurs in the plane $\delta_z=0$. The singularity can be easily calculated in each concrete case.

IV. Suppose that $f_{xx}=\varphi_{xx}\neq 0$, $f_{yy}\neq\varphi_{yy}$, $f_{yy}\neq 0$, $\varphi_{yy}\neq 0$, and $\beta\neq 0$. To avoid unnecessary complexity, in this case we restrict ourselves to the equation of the section of the LSP by the plane $\delta_x=0$. The section has two branches $\delta_z=\delta_z^{(1)}(\delta_y)$ and $\delta_z=\delta_z^{(2)}(\delta_y)$:

$$\begin{aligned}\delta_z^{(1)}&=\frac{1}{2}\frac{f_{yy}\varphi_{yy}}{f_{yy}-\varphi_{yy}}\delta_y^2,\\ \delta_z^{(2)}&=\frac{1}{2}\left(\frac{f_{yy}\varphi_{yy}}{f_{yy}-\varphi_{yy}}+\frac{3\alpha^2}{\beta(f_{yy}-\varphi_{yy})}\right)\delta_y^2,\end{aligned} \qquad (14)$$

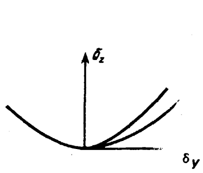


FIG. 6. Line of intersection of the locus of singular points by the plane $\delta_x=0$ in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$ (case IV).

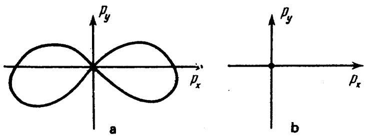


FIG. 7. Structure of the critical collar (15) as it depends on the value of δ_{cy} when $\beta > 0$: a) $\alpha\delta_{cy} < 0$; b) $\alpha\delta_{cy} \geq 0$. For definiteness, we suppose that $(\varphi_{xxy} - f_{xxy})(\varphi_{yy} - f_{yy}) > 0$.

where

$$\alpha = \varphi_{yy} f_{xxy} - f_{yy}\varphi_{xxy}, \quad \beta = (f_{xxxx} - \varphi_{xxxx})(f_{yy} - \varphi_{yy}) - 3(\varphi_{xxy} - f_{xxy})^2;$$

the second branch of the LSP exists for those δ_y for which $\alpha\delta_y/\beta \leq 0$.

The line (14) of intersection of the LSP by the plane $\delta_x = 0$ is shown in Fig. 6. The evolution of the critical collar with change of the vector $\boldsymbol{\delta}_c$ along the first branch of the LSP is determined by the equation

$$\frac{1}{2}(\varphi_{yy} - f_{yy}) p_y^2 + \frac{1}{2}\frac{\varphi_{xxy} f_{yy} - f_{xxy}\varphi_{yy}}{f_{yy} - \varphi_{yy}} \delta_{cy} p_x^2 + \frac{1}{2}(\varphi_{xxy} - f_{xxy}) p_x^2 p_y + \frac{1}{24}(\varphi_{xxxx} - f_{xxxx}) p_x^4 = 0. \quad (15)$$

As is evident, the type of singularity changes: a singularity of O type is transformed to a singularity of X type (and conversely). We shall consider the various cases as they depend on the relation of the coefficients of equation (15).

1) $\beta > 0$: that is, the quadratic form in p_x^2 and p_y is of one sign. Then the critical collar for $\delta_{cy} = 0$ degenerates to a point (Fig. 7), and we have for the singular part of Γ at the transition point

$$\Delta\Gamma \sim |\delta_z|^{-1/4} \text{ when } \delta_z \operatorname{sign}(\varphi_{yy} - f_{yy}) > 0, \quad \Delta\Gamma = 0 \text{ when } \delta_z \operatorname{sign}(\varphi_{yy} - f_{yy}) < 0. \quad (16)$$

2) $\beta < 0$: that is, the quadratic form in p_x^2 and p_y is hyperbolic. When $\delta_{cy} = 0$, the critical collar has a point of self-tangency (Figs. 8 and 9), and the singular part of the quantity Γ is

$$\Delta\Gamma \sim |\delta_z|^{-1/4}. \quad (17)$$

On the second branch of the LSP, the singularity may be a singularity of O or of X type; it is transformed to the enhanced singularity (16) or (17) for $\delta_{cy} = 0$.

V. Suppose that $\varphi_{yy} \neq f_{yy}$, $\varphi_{yy} \neq 0$, $f_{yy} \neq 0$, $f_{xxy} = \varphi_{xxy} \neq 0$, $f_{xx} = \varphi_{xx} \neq 0$, $f_{xxxx} = \varphi_{xxxx}$, and all the subsequent coefficients of terms p_x^6, p_x^8, etc. in the expansions (4) and (5) are equal to each other. We have for the equation of the LSP

$$-\delta_y\delta_z + \frac{1}{2}\frac{f_{yy}\varphi_{yy}}{f_{yy} - \varphi_{yy}}\delta_y^3 = \frac{1}{2}\frac{f_{xx}^2}{f_{xxy}}\delta_x^2; \quad (18)$$

in the plane $\delta_x = 0$, the LSP line is determined by the equation

$$\delta_z = {}^1/_2 f_{yy}\varphi_{yy}\delta_y^2/(f_{yy} - \varphi_{yy}),$$

but the solution $\delta_y = 0$ for arbitrary δ_z must be rejected. The surface (18) is shown in Fig. 10.

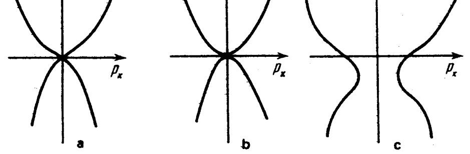


FIG. 8. Structure of the critical collar (15) as it depends on the value of δ_{cy} when $\beta < 0$ and $(f_{xxxx} - \varphi_{xxxx})(f_{yy} - \varphi_{yy}) < 0$: a) $\alpha\delta_{cy} < 0$; b) $\delta_{cy} = 0$; c) $\alpha\delta_{cy} > 0$. For definiteness, we suppose that $(\varphi_{xxy} - f_{xxy})(\varphi_{yy} - f_{yy}) > 0$.

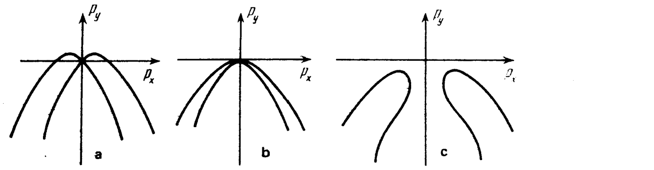


FIG. 9. Structure of the critical collar (15) as it depends on the value of δ_{cy} when $\beta < 0$ and $(f_{xxxx} - \varphi_{xxxx})(f_{yy} - \varphi_{yy}) > 0$: a) $\alpha\delta_{cy} < 0$; b) $\delta_{cy} = 0$; c) $\alpha\delta_{cy} > 0$. For definiteness, we suppose that $(\varphi_{xxy} - f_{xxy})(\varphi_{yy} - f_{yy}) > 0$.

The evolution of the critical collar with change of the vector $\boldsymbol{\delta}_c$ along the LSP in the plane $\delta_x = 0$ is determined by the equation

$$^1/_2(\varphi_{yy} - f_{yy}) p_y^2 + {}^1/_2 f_{xxy}\delta_{cy} p_x^2 = 0. \quad (19)$$

It is evident from the expression (19) that along the LSP there occurs a transition of a singularity of O type to a singularity of X type; when $\delta_c = 0$, tangency of the surfaces $\varepsilon_{\mathbf{p}} = \varepsilon_F$ and $\varepsilon_{\mathbf{p}+\mathbf{q}_{c0}} = \varepsilon_F$ occurs along the line $p_y = 0$.

On calculating the singularity due to a change in magnitude of the phonon momentum, we have for the singular part of Γ at the transition point, depending on the form of the FS ($\delta_q = q - q_{c0}$),

$$\Delta\Gamma \sim \delta_q^{-1/2} \text{ when } \delta_q > 0, \quad \Delta\Gamma = 0 \text{ when } \delta_q < 0, \quad (20)$$

or

$$\Delta\Gamma = 0 \text{ when } \delta_q > 0, \quad \Delta\Gamma \sim \delta_q^{-1/2} \text{ when } \delta_q < 0. \quad (20')$$

VI. We consider the singularity of Γ due to a plane of symmetry σ on the FS [for example, on a "dumbbell" (Fig. 11)]. We introduce an orthogonal system of coordinates such that the p_z axis is directed perpendicular to the plane of symmetry σ, while the p_y axis is directed along the normal to the FS, parallel to the plane σ. The critical vector $\mathbf{q}_{c0}$ is parallel to the p_z axis and

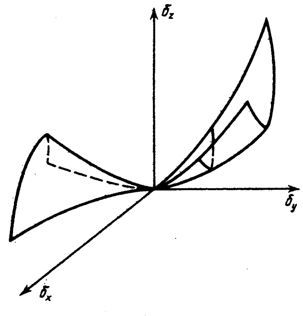


FIG. 10. Locus of singular points in the vicinity of the point $\mathbf{q} = \mathbf{q}_{c0}$ in case V.

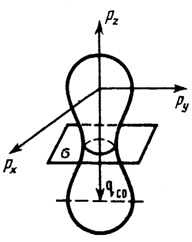


FIG. 11.

is equal in magnitude to the distance between the planes that contain the normals to the FS parallel to the plane σ. For small values of the quantity p_z ($p_z \ll p_F$, where p_F is the Fermi momentum), we may write

$$\begin{aligned} \varepsilon_p &= \frac{1}{2m}\left[(p_x^2+p_y^2)(1+cp_z^2+dp_z^3)+ap_z^2+bp_z^3\right], \\ \varepsilon_{p+q} &= \frac{1}{2m}\left[(p_x^2+p_y^2)(1+c(p_z+\delta_z)^2-d(p_z+\delta_z)^3)\right. \\ &\quad \left.+a(p_z+\delta_z)^2-b(p_z+\delta_z)^3\right]; \end{aligned} \tag{21}$$

here $a+2m\varepsilon_F c>0$ and $\delta_z=-\delta_q$. In order of magnitude the coefficients in the expressions (21) are estimated thus: $a\sim 1$, $b\sim 1/p_F$, $c\sim 1/p_F^2$, $d\sim 1/p_F^3$.

For a comparatively rough estimate of the singularity due to change in magnitude of the phonon momentum, we have, using (3),

$$\Delta\Gamma \approx \frac{4\pi m^2\hbar\omega_q|M_0|^2}{\xi}\cdot\begin{cases} |\delta_z|^{-1}, & \eta\delta_z>0 \\ {}^1/_2|\delta_z|^{-1}, & \eta\delta_z<0 \end{cases}, \tag{22}$$

where

$$|M_0|^2 \equiv |M(\mathbf{p}_c,\mathbf{q})|^2,\quad \xi\equiv a+2m\varepsilon_F c,\quad \eta\equiv b+2m\varepsilon_F d.$$

The equation of the line of intersection of the LSP with the plane $\delta_x=0$ in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$ has the following form:

$$\delta_z=\frac{3}{\xi}\left(\frac{\eta m\varepsilon_F}{2}\right)^{1/3}\delta_y^{2/3}, \tag{23}$$

and the surface is obtained by rotation of the line (23) about the δ_z axis (Fig. 12). On passage through the point $\mathbf{q}=\mathbf{q}_{c0}$ along the LSP, the type of singularity of Γ does not change. When $\mathbf{q}_c\neq\mathbf{q}_{c0}$, Γ has a logarithmic singularity (this applies specifically to the "dumbbell").

The treatment given enables us to construct the form of the LSP of Taylor singularities for FS of the "dumbbell" (Fig. 1) and "top" (Fig. 2) types. For simplicity we are supposing that the FS is a solid of revolution. From the continuity of the LSP for arbitrarily chosen small sections of the FS, it follows that for closed-cavity FS the LSP is continuous and closed. In the case

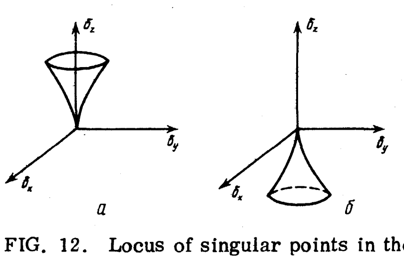


FIG. 12. Locus of singular points in the vicinity of the point $\mathbf{q}=\mathbf{q}_{c0}$ in case VI: a) $\eta>0$; b) $\eta<0$.

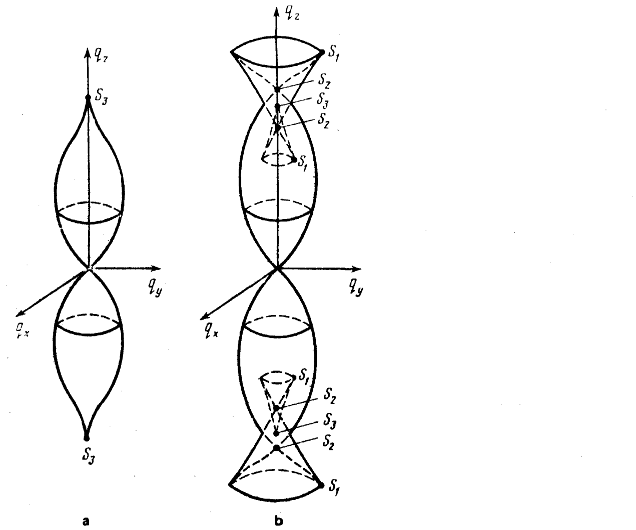


FIG. 13. Locus of singular points of Taylor singularities for a surface of the "dumbbell" type, in the case $\eta>0$.

of the "dumbbell", which is symmetric with respect to the plane $p_z=0$, we obtain different forms of LSP (Figs. 13 and 14), depending on the sign of the quantity η [see (22)]; when $\eta>0$, depending on the specific structure of the FS, two types of LSP are possible (Fig. 13a and b). The LSP of Taylor singularities in the case of the "top" is shown in Fig. 15. The q_z axis in these figures is chosen parallel to the axes of symmetry of the FS considered. We note that in the case of the "top", depending on the specific structure of the FS, three different forms of LSP are possible, whose surfaces differ from each other in the vicinity of the points S_1 (Fig. 15).

We shall identify the points on the LSP in accordance with the type of singularity in Γ. At points S_1 in Figs. 13–15 there are singularities of the type (13); at points S_2, singularities of the types (20) and (20′); at points S_3, singularities of the type (22). At other points of the LSP, $\Gamma=\Gamma(\mathbf{q})$ has a standard singularity: either of O type or of X type. The critical directions $\mathbf{n}_c$ (see Ref. 5) for singularities at $q\to 0$ lie along the generatrices

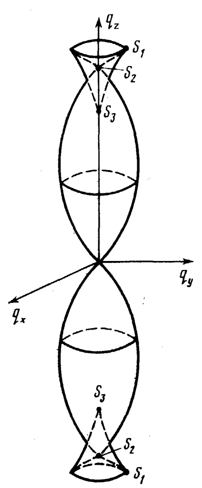


FIG. 14. Locus of singular points of Taylor singularities for a surface of the "dumbbell" type, in the case $\eta<0$.

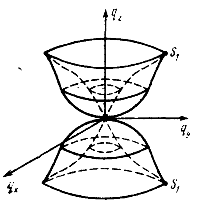


FIG. 15. Locus of singular points of Taylor singularities for a surface of the "top" type.

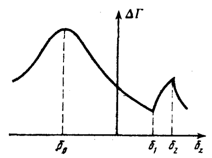


FIG. 17. The function $\Delta\Gamma(\delta_z)$. For definiteness, we suppose that $\eta > 0$ and $\xi d - 3\eta c > 0$.

of the cones, tangent at the point $\mathbf{q} = \mathbf{q}_c = 0$.

Openness of the FS is reflected in the properties of the LSP of Taylor singularities. As an example, we consider a FS of the "corrugated cylinder" type (Fig. 16a). The LSP in this case, in a system of recurrent zones, is shown in Fig. 16b. The first Brillouin zone in the planes $p_x = 0$ and $q_x = 0$ is distinguished by dotted lines in Fig. 16.

Earlier, in the calculation of the singularities and the construction of the LSP, we neglected the quantity $\hbar\omega_{\mathbf{q}}$ in comparison with ε_F. As was mentioned above, allowance for the values of $\hbar\omega_{\mathbf{q}}$ leads to the result that the singularities described split and weaken; correspondingly, the LSP splits into two surfaces (allowance for antipode points leads to the result that the LSP splits into four surfaces). As a rule, the velocities $\mathbf{v}_{\mathbf{p}_c}$ and $\mathbf{v}_{\mathbf{p}_c+\mathbf{q}_c}$ are not equal to each other; therefore the amount of the splitting is of order $\hbar\omega_{\mathbf{q}_c}/v_F$, and the derivative with respect to q of the quantity Γ has the singularities described in sections I–IV. If the velocities are equal then the amount of the splitting Δq_c is usually of order $(\hbar\omega_{\mathbf{q}_c})^2/(\varepsilon_F v_F)$. The case of equal velocities is realized in sections V–VI. In V, the singular part of Γ has a root-type singularity.

We shall determine the fine structure of the singularity in case VI. Using (1), we have for $\Delta\Gamma$ (for definiteness, we suppose that $\eta > 0$)

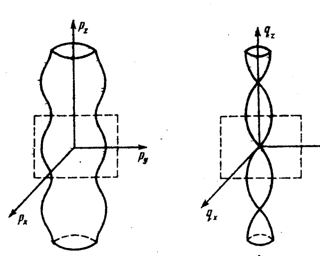
$$\Delta\Gamma \approx \frac{4\pi |M_0|^2 \xi (\eta\xi)^{1/2}}{3^{1/2}\hbar\omega_{\mathbf{q}_c}(\xi d - 3\eta c)} \cdot \begin{cases} (\delta_z - \delta_1)^{1/2}, & |\delta_z - \delta_1| \ll \delta_1 \\ -(\delta_z - \delta_2)^{1/2}, & |\delta_z - \delta_2'| \ll \delta_2, \end{cases} \tag{24}$$

$$\Delta\Gamma \approx \frac{2^{4/3}\pi m (m\hbar\omega_{\mathbf{q}_c})^{1/3} |M_0|^2}{3\eta^{1/3}} \left(1 - \frac{\xi^2(\delta_z - \delta_0)^2}{9 \cdot 2^{1/3}(m\hbar\omega_{\mathbf{q}_c})^{4/3}\eta^{2/3}}\right)$$

when $|\delta_z - \delta_0| \ll |\delta_0|$, where

$$\delta_0 = -\frac{3\eta^{2/3}(m\hbar\omega_{\mathbf{q}_c})^{2/3}}{2^{4/3}\xi}, \quad \delta_1 = \frac{3\eta^{1/3}(m\hbar\omega_{\mathbf{q}_c})^{2/3}}{2^{2/3}\xi} - \frac{2^{1/3}(\xi d - 3\eta c)(m\hbar\omega_{\mathbf{q}_c})^{5/3}}{\eta^{2/3}\xi^2},$$

$$\delta_2 = \frac{3\eta^{1/3}(m\hbar\omega_{\mathbf{q}_c})^{2/3}}{2^{2/3}\xi}.$$



a b

FIG. 16. a) Fermi surface of the "corrugated cylinder" type. b) Locus of singular points of Taylor singularities for a "corrugated cylinder."

Here in the expressions for δ_1 and δ_2, only the shift of these quantities with respect to each other is calculated with accuracy $(\hbar\omega_{\mathbf{q}_c})^{5/3}/(v_F\varepsilon_F^{2/3})$. The function $\Delta\Gamma(\delta_z)$ is shown in Fig. 17. It is clear from (24) that the amount of the splitting in this case is of order $(\hbar\omega_{\mathbf{q}_c})^{5/3}/(v_F\varepsilon_F^{2/3})$. In this case, because of the presence of a plane of symmetry σ in the FS, the singularity in $\Delta\omega$ with allowance for antipode points does not cancel out. From the expression (2) we have for $\Delta\omega$ ($\eta > 0$): if $|\delta_z - \delta_1| \ll |\delta_2 - \delta_1|$, then

$$\Delta\omega \sim -\frac{\xi |M_0|^2}{\hbar\omega_{\mathbf{q}_c}(\xi d - 3\eta c)} \begin{cases} \xi(\eta/m\hbar\omega_{\mathbf{q}_c})^{1/3}(\delta_z - \delta_1), & \delta_z > \delta_1, \\ (\xi\eta)^{1/2}(\delta_1 - \delta_z)^{1/2}, & \delta_z < \delta_1; \end{cases} \tag{25}$$

if $|\delta_z - \delta_2| \ll |\delta_2 - \delta_1|$, then

$$\Delta\omega \sim \frac{\xi |M_0|^2}{\hbar\omega_{\mathbf{q}_c}(\xi d - 3\eta c)} \begin{cases} \xi(\eta/m\hbar\omega_{\mathbf{q}_c})^{1/3}(\delta_z - \delta_2), & \delta_z > \delta_2, \\ (\xi\eta)^{1/2}(\delta_2 - \delta_z)^{1/2}, & \delta_z < \delta_2. \end{cases} \tag{25'}$$

In (25) and (25′), the notation is the same as in (24).

It must be noted that a finite temperature T and various scattering mechanisms lead to a smoothing out of the singularities; the fine structure of the singularities can be observed when the very strict conditions $T \ll \hbar\omega_{\mathbf{q}_c}$ and $ql \gg \varepsilon_F/\omega_{\mathbf{q}_c}$ are satisfied.

Use of formulas (1) and (2) for analysis of singularities of the phonon spectrum means, in particular, neglect of the electromagnetic fields that accompany the propagation of sound waves in a metal.[8] The following can be said in favor of the model adopted: when $q/\hbar k_{em} \gg 1$ (where k_{em} is the value of the wave vector of the electromagnetic field at frequency $\omega_{\mathbf{q}}$), the electromagnetic field is insignificant (the amplitude of the accompanying field approaches zero when $q/\hbar k_{em} \to \infty$). It is this fact that enables us to "separate" phonons with finite momentum from other elementary excitations (photons in the medium, plasmons, weakly attenuating waves, and so on). For $q \to 0$ (the region at the origin of coordinates in Figs. 13–16), the situation is more complicated. Formally (for $\hbar\omega_{\mathbf{q}} \to 0$ and $l \to \infty$), allowance for the longitudinal electric field that accompanies the sound wave eliminates the singularity.[9,10] But the conditions for elimination are so strict (for example, $ql/\hbar \gg \exp(v_F/s)$, where s is the velocity of sound) that in real metals, the singularities investigated here should undoubtedly show up.

Experimental observation of singularities of the phonon spectrum is related to investigation of inelastic scattering of thermal neutrons (see Refs. 11 and 12 and references in Ref. 11). Model calculations[11] show that the intensity of Taylor singularities is less than that of Kohn singularities, and perhaps also than that of the three-particle singularities predicted by Brovman and Kagan.[13] Therefore for experimental detection of Taylor singularities, it is apparently necessary to apply methods different from inelastic scattering of neutrons. For example, it is possible to use the fact that according to the results of the present treatment, the values of the critical momenta q_c in certain directions approach zero. This enables us to seek singularities on the basis of angular anomalies in the absorption of ultrasound (cf. Refs. 5 and 6 and also Refs. 14 and 15); for detection of singularities at finite values of q_c, it is necessary to use hypersound (the maximum frequency of hypersound so far attained is $\omega_{max} = 2\pi \cdot 2 \cdot 10^{12}$ sec^{-1} Ref. 16).

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