

OSCILLATIONS OF THE ELECTRONIC THERMODYNAMIC CHARACTERISTICS OF A METAL FILM AT HIGH PRESSURES

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It is demonstrated that quantization of the energy of a conduction electron in a film may lead to the appearance of logarithmic singularities in the state density. The singularities are responsible for the peculiar oscillations of the electronic thermodynamic characteristics of metallic films at low temperatures and high pressures.

1. INTRODUCTION

THE singularities of the energy spectrum of conduction electrons in metals can give rise, as shown by I. M. Lifshitz^[1], to a unique electronic transition, due to the change in the topology of the Fermi surface as the latter is continuously deformed at high pressures. In the vicinity of the transition point, anomalies of the surface quantities become significant^[2], besides the anomalies in the volumetric thermodynamic characteristics of the metal. A study of similar effects in the thermodynamic properties of metal films shows that under certain conditions the character of the transition is greatly altered by the quantization of the conduction-electron conductivity in the film.

For certain equal-energy surfaces, the quantization of the energy spectrum leads to logarithmic singularities in the density of the states. A characteristic feature of a surface of this kind are saddle points. This circumstance is clearly manifest in the giant oscillations of the thermodynamic quantities, resulting from the shift of the chemical potential ζ upon deformation of the film. The amplitude of the oscillations is quite large, and at sufficiently low temperatures it is of the order of or even larger than the smooth part of the corresponding quantities. In this respect, the oscillations under consideration differ greatly from the oscillations investigated by I. M. Lifshitz and A. M. Kosevich^[3]

To observe the oscillations, low temperatures $T \lesssim 10^3/L_0$ [deg] are required (L_0 is the number of atomic layers in the film), according to estimates of Itskovich^[4], and also a film deformation such that the chemical potential $\delta\zeta$ is at least of the order of the distance between the energy levels near the limiting Fermi energy, i.e., $\delta\zeta \sim \zeta/L_0$. Accord-

ing to Kosevich^[5], the deformation necessary for this purpose is $u_{ik} \sim 1/L_0$. The observed displacements of the chemical potential^[6] upon deformation of the metal are sufficient, for example, for films of thickness $L \sim 10^{-6}$ cm.

2. DENSITY OF STATES

The density $\nu(\epsilon)$ of the electronic states per unit energy interval is given for a layer of thickness L by

$$\nu(\epsilon) = \frac{gV}{(2\pi\hbar)^2 L} \sum_{n=1}^{\infty} \left| \frac{\partial S(\epsilon, n)}{\partial \epsilon} \right|, \quad (1)$$

where $g = 2s + 1$, s —spin of the quasiparticle, V —volume of the layer,

$$\left| \frac{\partial S(\epsilon, n)}{\partial \epsilon} \right| = \int \delta[\epsilon - \epsilon(\mathbf{p}_{\perp}, n)] d^2\mathbf{p}_{\perp}, \quad (2)$$

$\mathbf{p}_{\perp} = ip_x + jp_y$, $\delta(x)$ is the Dirac δ -function, the quantum energy levels $\epsilon(\mathbf{p}_{\perp}, n)$ are determined by formulas (5) and (5') of^[2], and

$$S(\epsilon, n) = \int \theta[\epsilon - \epsilon(\mathbf{p}_{\perp}, n)] d^2\mathbf{p}_{\perp}, \quad (3)$$

$$\theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0 \end{cases}. \quad (3')$$

In those cases when only one pair of roots occurs in the quantization of Eq. (4) of^[2], the quantity $S(\epsilon, n)$ has an intuitive geometrical interpretation. Let the equal-energy surface $\mathcal{E}(\mathbf{p}) = \epsilon$ bound in \mathbf{p} -space a certain volume with energy smaller than ϵ . Projecting on the plane $p_z = \text{const}$ the points at which the given surface cuts off from the lines parallel to the p_z axis segments of length $2\pi\hbar n/L$, we obtain a line bounding a certain figure. The area of this figure is equal to $S(\epsilon, n)$. In the particular case when the quasimomentum component

$p_{zn} = \pi\hbar n/L$ is quantized, the quantity $S(\epsilon, n)$ is equal to the area of intersection of the equal-energy surface with the plane $p_z = p_{zn}$, and $\partial S/\partial \epsilon = 2\pi m^*$, where m^* is the effective mass of the electron for the given cross section.

Just as a change in the topology of the equal-energy surfaces leads to singularities in the volume density of states^[1], the corresponding changes in the topology of the curves bounding $S(\epsilon, n)$ also leads to unique singularities in the state density (1). In this respect, a characteristic example is the two-dimensional analog of the "break in the neck," when the curves bounding $S(\epsilon, n)$ have a hyperbolic point (see Fig. 1). In the vicinity of the hyperbolic point, the equation for the corresponding curves is

$$p_y^2/2m_2 - p_x^2/2m_1 = \varphi(\epsilon, n), \quad (4)$$

where $\varphi(\epsilon, n)$ is a certain sign-alternating function which vanishes at the hyperbolic point:

$$\varphi(\epsilon_n, n) = 0, \quad (5)$$

the exact form of which can be obtained only under certain assumptions concerning the dispersion law.

Calculating the profile S bounded by curves (4) and the lines $p_x = \pm P_x$, and differentiating with respect to the energy, we obtain

$$\frac{\partial S(\epsilon, n)}{\partial \epsilon} = -2\sqrt{m_1 m_2} \frac{\partial \varphi}{\partial \epsilon} \ln |\varphi(\epsilon, n)| + \frac{\partial \tilde{S}}{\partial \epsilon}, \quad (6)$$

where $\partial \tilde{S}/\partial \epsilon$ is a continuous function. From (1) and (6) it follows that

$$v(\epsilon) = -\frac{gV\sqrt{m_1 m_2}}{2L(\pi\hbar)^2} \sum_{n=1}^{\infty} \frac{\partial \varphi}{\partial \epsilon} \ln |\varphi(\epsilon, n)| + \tilde{v}(\epsilon). \quad (7)$$

At energy values $\epsilon = \epsilon_n$ satisfying (5), the density of the states goes to infinity logarithmically.

Following^[3], we separate the oscillating part of (7), summing over the Poisson formula:

$$v(\epsilon) = v_0 + v_{osc};$$

$$v_{osc}(\epsilon) = -\frac{gV\sqrt{m_1 m_2}}{2L(\pi\hbar)^2} \frac{\partial \varphi}{\partial \epsilon} \ln |2 \sin \pi \rho(\epsilon)|, \quad (8)$$

where $v_0(\epsilon)$ is a smooth function and $\rho(\epsilon)$ is defined by

$$\varphi[\epsilon, \rho(\epsilon)] = 0. \quad (9)$$

The logarithmic singularities occur at $\rho(\epsilon_n) = n$, $n = 1, 2, 3, \dots$

The presence of logarithmic singularities in the density of states is intrinsically connected with a definite form of the equal-energy surfaces.

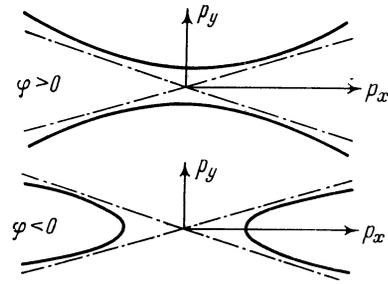


FIG. 1. Change in the topology of the curves bounding the figure $S(\epsilon, n)$ in the vicinity of the hyperbolic point.

A characteristic attribute of surfaces of this type are saddle points. Near the saddle point $(0, 0, p_{z0})$, the dispersion law $\mathcal{E}(\mathbf{p})$ takes the form^[7]:

$$\mathcal{E}(\mathbf{p}) = \epsilon_0(p_{z0}) + \frac{\partial \epsilon_0}{\partial p_{z0}} (p_z - p_{z0}) + \frac{1}{2} \left(\frac{p_y^2}{m_2} - \frac{p_x^2}{m_1} \right).$$

From this, in the case of quantization $p_{zn} = \pi\hbar n/L$, we have for the function $\varphi(\epsilon, n)$

$$\varphi(\epsilon, n) = \epsilon - \epsilon_0 - v_0(\pi\hbar n/L - p_{z0}),$$

where ϵ_0 and v_0 are respectively the energy and velocity at the saddle point. From the formulas obtained it follows that the density of states (7) becomes logarithmically infinite if the plane $p_z = p_{zn}$ is tangent to the equal-energy surface at the saddle point.

The next characteristic examples are the equal-energy surfaces in the vicinity of a conical point. In the corresponding coordinate system, the dispersion law near a conical point is defined by

$$\mathcal{E}(\mathbf{p}) = \epsilon_0 + \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} - \frac{p_z^2}{2m_3}. \quad (10)$$

Let $N(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ be a normal to the surface of the film in the given system of coordinates, and θ the angle between the axis of the neck and the normal N . Determining by means of formulas (5) and (5') of^[2] the corresponding quantum energy levels from (10), we obtain by straightforward but somewhat cumbersome calculations

$$v(\epsilon) = -\frac{gV}{2(\pi\hbar)^2 L} \left(\frac{m_1 m_2 m_3}{M} \right)^{1/2} \times \sum_{n=1}^{\infty} \ln \left| \epsilon - \epsilon_0 - \frac{\pi^2 \hbar^2 n^2}{2ML^2} \right| + v(\epsilon), \quad (11)$$

where

$$M^{-1} = \sin^2 \theta \left(\frac{\cos^2 \varphi}{m_1} + \frac{\sin^2 \varphi}{m_2} \right) - \frac{\cos^2 \theta}{m_3}. \quad (12)$$

The logarithmic singularities in the density of states are missing if $M^{-1} \leq 0$.

Summing (11), we obtain

$$v(\varepsilon) = v_0 + \delta v, \quad (13)$$

$$\delta v(\varepsilon) = -\frac{gV}{2(\pi\hbar)^2 L} \left(\frac{m_1 m_2 m_3}{M} \right)^{1/2} \times \left[\ln \left| 2 \sin \frac{L}{\hbar} (2M(\varepsilon - \varepsilon_0))^{1/2} \right| - \frac{1}{2} \ln |\varepsilon - \varepsilon_0| \right], \quad (13')$$

where $\nu_0(\varepsilon)$ is a certain continuous function. Logarithmic singularities arise at $\varepsilon = \varepsilon_n$, where

$$\varepsilon_n = \varepsilon_0 + \pi^2 \hbar^2 n^2 / 2ML^2, \quad n = 1, 2, 3, \dots \quad (14)$$

In the limit as $L \rightarrow \infty$ there follows from (13') the well known^[1] root singularity

$$\delta v(\varepsilon) = -\alpha(\varepsilon_0 - \varepsilon)^{1/2} \theta(\varepsilon_0 - \varepsilon), \quad (15)$$

$$\alpha = \frac{g\sqrt{2}}{2\pi^2} \frac{V}{\hbar^3} \sqrt{m_1 m_2 m_3}, \quad (15')$$

here $\theta(x)$ is defined by (3').

3. OSCILLATIONS OF ELECTRONIC THERMODYNAMIC QUANTITIES

Logarithmic singularities of the density of states are manifest strongly in the thermodynamic properties of metal films.

Calculating the free energy F in the case of state density (8) under the assumption that

$$2\pi^2 \rho' T \ll 1, \quad (16)$$

we obtain

$$F = \int_0^{\varepsilon_F} v_0(\varepsilon) \varepsilon d\varepsilon - \frac{\pi^2}{6} T^2 v_0(\varepsilon_F) + F_{\text{osc}},$$

$$F_{\text{osc}} = -\beta \left\{ \int_0^{\varepsilon_F} \varepsilon \frac{\partial \varphi}{\partial \varepsilon} \ln |2 \sin \pi \rho(\varepsilon)| d\varepsilon + \frac{T}{2\rho' \partial \varepsilon_{F,k=1}} \sum_{k=1}^{\infty} \frac{\cos(2\pi k \rho)}{k^2} \Phi(2\pi^2 k \rho' T) \right\}, \quad (17')$$

where

$$\beta = \frac{V}{L} \frac{\sqrt{m_1 m_2}}{(\pi\hbar)^2}, \quad \Phi(x) = \frac{1}{x} - \frac{1}{\text{sh } x} \quad (18)*$$

and $\rho'(\varepsilon) = d\rho/d\varepsilon \sim 1/\Delta\varepsilon$, $\Delta\varepsilon$ is the distance between the energy levels.

The Fermi ε_F is determined from the condition that the number of conduction electrons N is constant:

$$N = \int_0^{\varepsilon_F} v_0(\varepsilon) d\varepsilon - \beta \int_0^{\varepsilon_F} \frac{\partial \varphi}{\partial \varepsilon} \ln |2 \sin \pi \rho(\varepsilon)| d\varepsilon. \quad (19)$$

Summing the series in (17') under the condition (16), we obtain

$$F_{\text{osc}} = -\beta \int_0^{\varepsilon_F} \varepsilon \frac{\partial \varphi}{\partial \varepsilon} \ln |2 \sin \pi \rho(\varepsilon)| d\varepsilon + \frac{\pi^2}{6} T^2 \beta \frac{\partial \varphi}{\partial \varepsilon_F} \times \begin{cases} \ln(2\pi^2 \rho'(\varepsilon_F) T), & \varepsilon_F = \varepsilon_n \\ \ln |2 \sin \pi \rho(\varepsilon_F)|, & \varepsilon_F \neq \varepsilon_n \end{cases}. \quad (20)$$

We see therefore that there is a characteristic oscillatory dependence of the free energy F on the shift of the Fermi level ε_F . The amplitude of the oscillations decreases with increasing temperature, and the oscillations vanish when $2\pi^2 \rho' T \gg 1$.

Substituting in the condition (16) $\rho' = \varepsilon_F/L_0$, where L_0 is the number of atomic layers in the film, we obtain the equivalent condition

$$L_0 T / \varepsilon_F \ll 1, \quad (16')$$

which is more convenient for estimates.

The formulas obtained for the free energy allow us to consider the behavior of the thermodynamic quantities under deformation of the film.

A. Fermi level. The dependence of the Fermi level ε_F on the deformation tensor u can be obtained from the condition that the number of conduction electrons (19) be constant. Differentiating (19) with respect to the components u_{ik} , we obtain

$$\frac{\partial \varepsilon_F}{\partial u_{ik}} = -\alpha_{ik} + \beta_{ik} \frac{a \ln |2 \sin \pi \rho(\varepsilon_F, u)|}{1 - a \ln |2 \sin \pi \rho(\varepsilon_F, u)|}, \quad (21)$$

where

$$\alpha_{ik} = \frac{1}{v_0} \frac{\partial \tilde{\mathcal{N}}_0}{\partial u_{ik}}, \quad \beta_{ik} = -\frac{1}{v_0} \frac{\partial \tilde{\mathcal{N}}_0}{\partial u_{ik}} + \frac{\partial \varepsilon_F}{\partial \rho} \frac{\partial \rho}{\partial u_{ik}},$$

$$\frac{\partial \tilde{\mathcal{N}}_0}{\partial u_{ik}} = \int_0^{\varepsilon_F} \frac{\partial}{\partial u_{ik}} v_0(\varepsilon, u) d\varepsilon - \frac{\partial}{\partial u_{ik}} \Big|_{\rho(\varepsilon_F, u) = \text{const}} \frac{V}{L} \frac{\sqrt{m_1 m_2}}{(\pi\hbar)^2} \quad (22)$$

$$\times \int_{\rho(0, u)}^{\rho(\varepsilon_F, u)} \frac{\partial \varphi}{\partial \varepsilon} \ln |2 \sin \pi \rho| \frac{\partial \varepsilon(\rho, u)}{\partial \rho} d\rho, \quad (22')$$

$$a = \frac{V}{L} \frac{\sqrt{m_1 m_2}}{(\pi\hbar)^2} \frac{1}{v_0} \frac{\partial \varphi}{\partial \varepsilon_F} \quad (23)$$

In order of magnitude, $a \sim 1/L_0$. As follows from (21), the linear dependence of the Fermi level ε_F on the deformation tensor u is strongly violated near the singular values of the energy $\varepsilon_F(u) = \varepsilon_n(u)$, i.e., $\rho(\varepsilon_F, u) = n$.

*sh \equiv sinh.

The other thermodynamic quantities are calculated in similar fashion.

B. Electronic part of the elastic moduli λ_{iklm} :

$$\lambda_{iklm} = \left(\frac{\partial^2 F(T, u)}{\partial u_{ik} \partial u_{lm}} \right)_{T=0} \\ = \tilde{\lambda}_{iklm} + \nu_0 \beta_{ik} \beta_{lm} \frac{a \ln |2 \sin \pi \rho(\epsilon_F, u)|}{1 - a \ln |2 \sin \pi \rho(\epsilon_F, u)|}, \quad (24)$$

where $\tilde{\lambda}_{iklm}$ is a smooth function of u . From (24) it follows that the amplitude of the oscillations is $\sim \nu_0 \beta_{ik} \beta_{lm}$, i.e., of the order of the smooth part.

C. Electronic heat capacity C :

$$\frac{C}{T} = \frac{\pi^2}{3} \nu_0 - \frac{V \sqrt{m_1 m_2}}{L 3 \hbar^2} \\ \times \frac{\partial \varphi}{\partial \epsilon_F} \begin{cases} \ln(2\pi^2 \rho' T), & \epsilon_F = \epsilon_n \\ \ln |2 \sin \pi \rho(\epsilon_F, u)|, & \epsilon_F \neq \epsilon_n \end{cases} \quad (25)$$

The ratio of the amplitude of the oscillations of the heat capacity to its smooth part is $\sim L_0^{-1} |\ln(TL_0/\epsilon_F)|$. For a film of thickness $L \sim 10^{-6}$ cm at helium temperatures, this amounts to $\sim 10\%$.

D. Electronic part of the stress tensor σ_{ik} :

$$\frac{1}{T} \frac{\partial \sigma_{ik}}{\partial T} = \frac{1}{T} \frac{\partial^2 F(T, u)}{\partial T \partial u_{ik}} = \left(\frac{1}{T} \frac{\partial \sigma_{ik}}{\partial T} \right)_0 \\ + \frac{\pi^3}{3} \beta_{ik} \nu_0 \frac{(\partial \rho / \partial \epsilon_F) a \cot(\pi \rho(\epsilon_F, u))}{1 - a \ln |2 \sin \pi \rho(\epsilon_F, u)|} \quad (26)$$

for $\epsilon_F \neq \epsilon_n$, i.e., $\rho \neq n$, $n = 1, 2, 3, \dots$. The zero denotes here the smooth part of a given function. In the vicinity of the point $\rho(\epsilon_F, u) = n$ for $\rho = n \pm (2\pi^2 \rho' T)$, the function $T^{-1} \partial \sigma_{ik} / \partial T$ reaches an extremal value

$$\left(\frac{1}{T} \frac{\partial \sigma_{ik}}{\partial T} \right)_{\text{extr}} = \left(\frac{1}{T} \frac{\partial \sigma_{ik}}{\partial T} \right)_0 \\ \pm \frac{\pi^3}{3} \beta_{ik} \nu_0 \frac{\partial \rho}{\partial \epsilon_F} \frac{G(\xi)}{(2\pi^2 \rho' T) |\ln(2\pi^2 \rho' T)|} \quad (27)$$

where ξ is determined from

$$\int_0^\infty \frac{x \operatorname{cth} x - 1}{\operatorname{sh} x} \cos(x\xi) dx = 0, \quad (28)^*$$

and the function $G(\xi)$ is defined by

$$G(\xi) = 6 \int_0^\infty \frac{x \operatorname{cth} x - 1}{x \operatorname{sh} x} \sin(x\xi) dx. \quad (29)$$

* $\operatorname{cth} \equiv \operatorname{coth}$.

At the point $\rho(\epsilon_F, u) = n$ we have

$$\frac{1}{T} \frac{\partial \sigma_{ik}}{\partial T} = \left(\frac{1}{T} \frac{\partial \sigma_{ik}}{\partial T} \right)_0 \quad (30)$$

E. Paramagnetic susceptibility χ :

$$\chi = \chi_0 - \frac{\mu^2}{2} \frac{V \sqrt{m_1 m_2}}{L (\pi \hbar)^2} \left\{ \frac{\partial \varphi(\epsilon_F + \mu H, u)}{\partial \epsilon_F} \right. \\ \left. - \ln |2 \sin \pi \rho(\epsilon_F + \mu H, u)| \right. \\ \left. + \frac{\partial \varphi(\epsilon_F - \mu H, u)}{\partial \epsilon_F} \ln |2 \sin \pi \rho(\epsilon_F - \mu H, u)| \right\}. \quad (31)$$

Formula (31) determines the dependence of the paramagnetic susceptibility on the external magnetic field H and the deformation tensor u .

4. ANOMALIES OF THE THERMODYNAMIC CHARACTERISTICS OF A METAL FILM IN THE VICINITY OF THE ELECTRONIC TRANSITION POINT

In considering the anomalies of thermodynamic quantities of a metal film near the point of electronic transition, we confine ourselves to the most interesting case, when the Fermi-surface topology is altered via rupture of a neck. For simplicity, and also for comparison of the obtained results with the corresponding results in^[1,2], we shall take hydrostatic compression to be the external perturbation that shifts the chemical potential.

At low temperatures

$$T / |\epsilon_F - \epsilon_n| \ll 1, \quad (32)$$

the free energy F is determined by the well known expression^[8]

$$F(T, V) = N \epsilon_F - \int_0^{\epsilon_F} \mathcal{N}(\epsilon, V) d\epsilon - \frac{\pi^2}{6} T^2 \nu(\epsilon_F, V), \quad (33)$$

and the Fermi energy ϵ_F is determined from the condition

$$\mathcal{N}(\epsilon_F, V) \equiv \int_0^{\epsilon_F} \nu(\epsilon, V) d\epsilon = N, \quad (33')$$

where the density of states ν is given by formulas (13) and (13').

We put $z = \epsilon_F - \epsilon_0$. Substituting (13) and (13') in (33') and differentiating them over the volume V , we obtain

$$\frac{dz}{dV} = \gamma \left[1 - a \left(\ln \left| 2 \sin \frac{L}{\hbar} \sqrt{2Mz} \right| - \frac{1}{2} \ln |z| \right) \right]^{-1}, \quad (34)$$

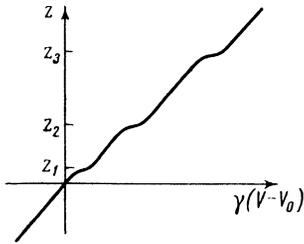


FIG. 2. Displacement of the Fermi level $\epsilon_F = z + \epsilon_0$ upon deformation of a metal film.

where

$$\gamma = -\frac{1}{v_0} \left(\frac{\partial \tilde{N}_0}{\partial V} + v_0 \frac{d\epsilon_0}{dV} \right), \quad a = \frac{V \sqrt{m_1 m_2 m_3}}{L(\pi \hbar)^2 \sqrt{M} v_0}. \quad (34')$$

\tilde{N}_0 is defined by an expression similar to (22'), and differs from the smooth volume part of the number of states N_0 in having a smooth surface part $\sim 1/L_0$. γ coincides in order of magnitude with the corresponding quantity in^[1].

When $z \neq z_n$, where

$$z_n = \pi^2 \hbar^2 n^2 / 2ML^2, \quad (35)$$

we have $z \sim \gamma(V - V_0)$ (here V_0 is the volume at which the rupture of the neck occurs). The derivative dz/dV vanishes at the points $z = z_n$, as follows from (34), so that the dependence of z on V is of the form shown in Fig. 2.

For the coefficient of electronic compressibility $\partial p / \partial V$ we obtain as a result of the calculations

$$\frac{\partial p}{\partial V} = -\frac{\partial^2 F}{\partial V^2} = \left(\frac{\partial p}{\partial V} \right)_0 + \delta \left(\frac{\partial p}{\partial V} \right);$$

$$\delta \left(\frac{\partial p}{\partial V} \right) = -\frac{v_0 \gamma^2 a (\ln |2 \sin L \hbar^{-1} \sqrt{2Mz}| - 1/2 \ln |z|)}{1 - a (\ln |2 \sin L \hbar^{-1} \sqrt{2Mz}| - 1/2 \ln |z|)}. \quad (36)$$

Here and below the subscript zero denotes the continuous part of the corresponding quantities. Under the conditions

$$z < 0, \quad L \frac{1}{\hbar} \sqrt{2M|z|} \gg 1 \quad (37)$$

we set from (36) the well known expression^[1]

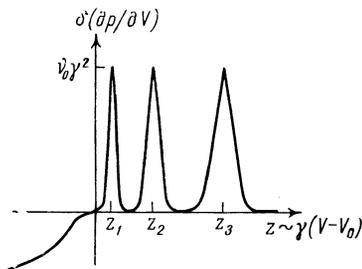


FIG. 3. Oscillation of the coefficient of electronic compressibility of a metal film near the transition point.

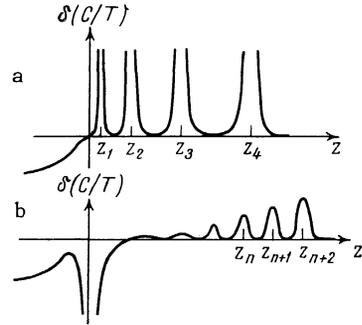


FIG. 4. Anomaly of the electronic heat capacity of a metal film near the point of transition (as a function of $z \sim \gamma(V - V_0)$): a- $T = 0$; b- $T/\Delta \epsilon \geq 1, T/|z| \ll 1$.

$$\delta \left(\frac{\partial p}{\partial V} \right) = -\alpha \gamma^2 |z|^{1/2}.$$

When $z > 0$, oscillations of electronic compressibility take place (Fig. 3).

The electronic heat capacity C is given by

$$C = C_0 + \delta C; \quad \frac{\delta C}{C_0} = -a \left(\ln \left| 2 \sin \frac{L}{\hbar} \sqrt{2Mz} \right| - \frac{1}{2} \ln |z| \right). \quad (38)$$

Under condition (37), it follows from (38) that

$$\delta C / C_0 = -(\alpha / v_0) |z|^{1/2},$$

and the oscillations shown in Fig. 4a take place when $z > 0$.

The thermal pressure coefficient $\partial p / \partial T$ is

$$\frac{1}{T} \frac{\partial p}{\partial T} = -\frac{1}{T} \frac{\partial^2 F}{\partial T \partial V} = \left(\frac{1}{T} \frac{\partial p}{\partial T} \right)_0 - \frac{\pi^2}{6} \frac{\gamma \alpha z^{-1/2} (\text{ctg } L \hbar^{-1} \sqrt{2Mz} - \hbar / L \sqrt{2Mz})}{1 - a (\ln |2 \sin L \hbar^{-1} \sqrt{2Mz}| - 1/2 \ln |z|)}, \quad (39)$$

from which it follows under condition (37) that

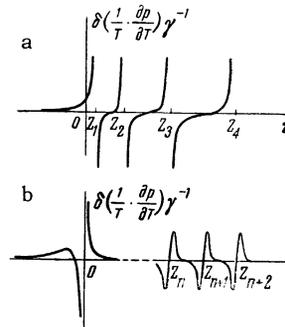


FIG. 5. Anomaly of thermal pressure coefficient of a metal film near the transition point (as a function of $z \approx \gamma(V - V_0)$): a- $T = 0$; b- $T/\Delta \epsilon \geq 1, T/|z| \ll 1$.

$$\delta \left(\frac{1}{T} \frac{\partial p}{\partial T} \right) = \frac{\pi^2}{6} \gamma \alpha |z|^{-1/2},$$

and when $z > 0$ we get the oscillations shown in Fig. 5a.

A similar expression determines also the coefficient of thermal expansion $\partial V / \partial T$.

For the paramagnetic susceptibility χ we have

$$\chi = \chi_0 + \delta\chi;$$

$$\begin{aligned} \delta\chi = & -\frac{\mu^2}{2} \frac{V \sqrt{m_1 m_2 m_3}}{L (\pi \hbar)^2 \sqrt{M}} \left\{ \ln \left| 2 \sin \frac{L}{\hbar} [2M(z + \mu H)]^{1/2} \right| \right. \\ & - \frac{1}{2} \ln |z + \mu H| + \ln \left| 2 \sin \frac{L}{\hbar} \sqrt{2M(z - \mu H)} \right| \\ & \left. - \frac{1}{2} \ln |z - \mu H| \right\}. \end{aligned} \quad (40)$$

The oscillations of the paramagnetic susceptibility are shown in Fig. 6.

In the case under consideration, as follows from the presented formulas, there are no singularities of the thermodynamic quantities at the point $z = 0$.

The obtained expressions for the free energy F and its derivatives are valid when $T \rightarrow 0$, with the exception of the vicinity of the singular points $\epsilon_F = \epsilon_n$. To consider the thermodynamic quantities near the singular points it is convenient to write the state density (13') in the form

$$\delta v(\epsilon) = \delta v_0 + v_{\text{osc}}; \quad (41)$$

$$\delta v_0(\epsilon) = -\alpha(\epsilon_0 - \epsilon)^{1/2} \theta(\epsilon_0 - \epsilon) + \frac{\alpha \hbar}{2L \sqrt{2M}} \ln |\epsilon - \epsilon_0|, \quad (42)$$

$$v_{\text{osc}}(\epsilon) = -\frac{\alpha \hbar}{L \sqrt{2M}}$$

$$\times \begin{cases} \ln |2 \sin [L \hbar^{-1} (2M(\epsilon - \epsilon_0))^{1/2}]|, & \epsilon \geq \epsilon_0 \\ \ln (1 - \exp[-2L \hbar^{-1} (2M(\epsilon_0 - \epsilon))^{1/2}]), & \epsilon \leq \epsilon_0 \end{cases}. \quad (43)$$

In the region $z > 0$, under the condition

$$\pi T \frac{L}{\hbar} \sqrt{\frac{2M}{z}} \ll 1 \quad (44)$$

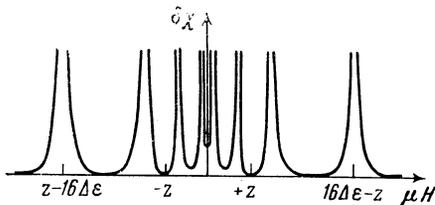


FIG. 6. Oscillations of paramagnetic susceptibility of a metal film near the transition point.

the free energy is $F = F_0 + \delta F_0 + F_{\text{osc}}$, where F_0 is a smooth function, δF_0 is determined by the density of states δv_0 (42) and was investigated in^[2], and

$$\begin{aligned} F_{\text{osc}} = & -\frac{\alpha \hbar}{L \sqrt{2M}} \int_0^z \ln \left| 2 \sin \frac{L}{\hbar} \sqrt{2Mx} \right| (\epsilon_0 + x) dx \\ & - \Delta \epsilon T \frac{\alpha \sqrt{z}}{\pi} \sum_{h=1}^{\infty} \frac{\cos(2kL \hbar^{-1} \sqrt{2Mz})}{k^2} \Phi \left(\pi k T \frac{L}{\hbar} \sqrt{\frac{2M}{z}} \right), \end{aligned} \quad (45)$$

where

$$\Delta \epsilon = \pi^2 \hbar^2 / 2ML^2,$$

and the function $\Phi(x)$ is defined by (18).

Summing the series in (45) we obtain

$$\begin{aligned} F_{\text{osc}} = & -\frac{\alpha \hbar}{L \sqrt{2M}} \int_0^z \ln \left| 2 \sin \frac{L}{\hbar} \sqrt{2Mx} \right| (\epsilon_0 + x) dx \\ & + \frac{\alpha \hbar}{L \sqrt{2M}} \frac{\pi^2}{6} T^2 \begin{cases} \ln \left(\frac{\pi^2 T}{n \Delta \epsilon} \right), & z = z_n \\ \ln \left| 2 \sin \frac{L}{\hbar} \sqrt{2Mz} \right| & z \neq z_n \end{cases} \end{aligned} \quad (46)$$

The dependence of z on V is determined from (33').

In the opposite limiting case

$$\pi T \frac{L}{\hbar} \sqrt{\frac{2M}{z}} \gg 1$$

we have

$$F_{\text{osc}} \sim O \left(\frac{1}{L_0^3}; \exp \left[-\pi T \frac{L}{\hbar} \sqrt{\frac{2M}{z}} \right] \right),$$

and z , which is given by the equation

$$N = \int_0^{z_0+z} (v_0 + \delta v_0) d\epsilon,$$

depends linearly on $V - V_0$. It follows therefore that if

$$T / \Delta \epsilon \gg 1, \quad T / |z| \ll 1 \quad (47)$$

the thermodynamic quantities have at the transition point $z = 0$ singularities due to their volume and surface parts^[1-2]; these singularities are not compensated by oscillating terms.

Knowing F from (45) and (46) we can obtain expressions for the thermodynamic quantities in the vicinity of the singular points z_n .

The heat capacity C at the points $z = z_n$ has a maximum equal to

$$C_{\text{max}} = C_0 + \frac{\alpha \hbar}{L \sqrt{2M}} \frac{\pi^2}{3} T \left| \ln \frac{\pi^2 T}{n \Delta \epsilon} \right|, \quad (48)$$

and when $z \neq z_n$ it is determined by formula (38).

Under condition (47), a logarithmic singularity of the electronic heat capacity occurs in the vicinity of the point $z = 0$ and is due to the surface part of the state density^[2], and oscillations, whose amplitude, given by (48), increases with increasing n (see Fig. 4b), occur in the region $z > 0$, at sufficiently large n , such that $T/n\Delta\epsilon \ll 1$. The ratio of the amplitude of the oscillations to the smooth part increases logarithmically with decreasing temperature.

The thermal coefficient of pressure $\partial p/\partial T$ reaches in the vicinity of the points z_n , at $z = z_n \pm (\pi^2 T/n\Delta\epsilon)\xi$, an extremal value

$$\left(\frac{1}{T} \frac{\partial p}{\partial T}\right)_{\text{extr}} = \left(\frac{1}{T} \frac{\partial p}{\partial T}\right)_0 - \frac{\pi}{6} \gamma v_0 \frac{\pm G(\xi)}{T |\ln(\pi^2 T/n\Delta\epsilon)|}, \quad (49)$$

where ξ and $G(\xi)$ are determined by (28) and (29) respectively. Outside the vicinity of the points $z = z_n$, the coefficient of thermal pressure is given by formula (39). Under condition (47), a strong singularity exists at the point $z = 0$ and is due to the volume and surface parts of the density of states (see Fig. 5b).

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