



ON THE THEORY OF MAGNETIC SUSCEPTIBILITY OF METALS AT LOW TEMPERATURES

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The magnetic properties of electrons in a metal are investigated for the case of an arbitrary dispersion law. The energy levels of a quasiparticle for an arbitrary dispersion law in a magnetic field are found, and the magnetic moment of a gas of such quasiparticles is computed, spin paramagnetism being taken into account. It is shown that the periods and amplitudes of oscillations are determined by the form of the Fermi boundary surface. Knowledge of these quantities allows one to reconstruct the form of the Fermi surface and the values of velocities on it.

Introduction

The question of the electron energy spectrum is of central importance in the construction of a quantum theory of metals. There is every reason to suppose that the electron spectrum for metals is of the Fermi type. This implies that, at low temperatures, the electrons in the metal, interacting with one another and with the lattice, may be replaced for thermodynamic purposes by an ideal Fermi gas of charged particles following some dispersion law $\mathcal{E} = \mathcal{E}(p_x, p_y, p_z)$. The majority of the thermodynamic and kinetic properties of a degenerate Fermi gas, however, are highly insensitive to the dispersion law, as a consequence of which their investigation does not allow one to draw any conclusions concerning the form of the law.

Substantially different in this respect is the behavior of certain magnetic properties of metals — in particular, oscillations of the magnetic susceptibility — which, it appears, depend strongly on the electron energy spectrum and may serve to distinguish it uniquely.

The periodic dependence of the magnetic susceptibility on the field at low temperatures (the de Haas – van Alphen effect) has by now been observed for a large number of metals (Bi, Sb, Hg, Zn, Cd, Be, C, Mg, Ga, In, Sn, Tl, and Al) [1] and can be regarded as a property common to all metals. At the same time, the quantitative theory of this phenomenon had been

worked out till now only for the case of an electron gas following a quadratic dispersion law [2a, 2].

The quadratic dispersion law is correct for an electron in a metal only in the lower part of the appropriate energy band and can be used to investigate the magnetic properties of metals having a small number of conduction electrons (such as Bi). In general, however, there is no justification for the use of a quadratic dispersion law, as a consequence of which it is essential to determine to just what extent the peculiarities of the effect are to be attributed to the electronic dispersion law. Certain qualitative considerations associated with this circumstance have been presented earlier by Onsager [3]. A quantitative theory has been offered in a paper by the present authors [4].

The present article contains a detailed presentation of the results published earlier in the brief communication [4], with, in addition, a treatment of the spin paramagnetism (a treatment of spin paramagnetism for the case of a quadratic dispersion law has been given elsewhere [2a]).

1. Energy Levels of Quasiparticles in a Magnetic Field

Let us consider the motion of a charged quasiparticle under a general dispersion law

$$\mathcal{E} = \mathcal{E}(p_x, p_y, p_z) \quad (1.1)$$

in a homogeneous magnetic field.

If the magnetic field \mathbf{H} is directed along the z -axis, the Hamiltonian for such a particle in the magnetic field is obtained formally by replacing the momentum components p_i in (1.1) by components of the kinetic momentum operator \tilde{P}_i , which are interrelated by the commutation relations

$$[\tilde{P}_y, \tilde{P}_x] = \frac{e}{c} H, \quad [\tilde{P}_y, \tilde{P}_z] = [\tilde{P}_x, \tilde{P}_z] = 0. \quad (1.2)$$

This relation between \check{P}_x and \check{P}_y corresponds to the commutation relation between the generalized coordinate and the generalized momentum: $[\check{P}_y, \check{P}_x] = 1$.

The role of the generalized coordinate operator \check{Q}_y is played here by the operator $(c/eH)\check{P}_x$. Therefore, the quasiclassical quantization condition

$$\frac{1}{2\pi} \oint P_y dQ_y = (n + \gamma)\hbar$$

can be written in the form

$$(c/2\pi eH) \oint P_y dP_x = (n + \gamma)\hbar \quad (0 < \gamma < 1) \quad (1.3)$$

(for the case of a quadratic dispersion law, $\gamma = 1/2$; in the general case, γ can differ from $1/2$).

The integral $\oint P_y dP_x$ defines the area bounded by a plane closed curve

$$\mathcal{E}(P_x, P_y, P_z) = E = \text{const}, \quad P_z = p_z = \text{const}, \quad (1.4)$$

which allows relation (1.3) to be written in the more symmetric form

$$S(E, p_z) \equiv \iint dP_x dP_y = (n + \gamma)2\pi\hbar \frac{eH}{c}, \quad (1.5)$$

the double integral being taken over the region bounded by the curve (1.4). Here, $S(E, p_z)$ is the area intercepted on the surface of constant energy

$$\mathcal{E}(P_x, P_y, P_z) = E \quad (1.6)$$

by a plane perpendicular to the direction of the magnetic field.

Condition (1.5) specifies, in the quasiclassical approximation, the implicit dependence of the energy of a quasiparticle in a magnetic field on the quantum number n :

$$E = E_n(p_z; H). \quad (1.7)$$

In accordance with (1.5), the distance between the energy levels will be

$$\Delta E_n = E_{n+1} - E_n = 2\pi\hbar eH / (c \partial S / \partial E).$$

If the quasiparticle possesses spin $1/2$ and has a magnetic moment $\frac{1}{2}\mu_0 = \frac{1}{2}(e\hbar/m_0c)$, then the two possible orientations of the spin relative to the direction of the magnetic field \mathbf{H} must be taken into account in the expression for the energy of such a particle:

$$E = E_n(p_z; H) \pm \frac{1}{2}\mu_0 H. \quad (1.8)$$

Thus, the energy levels in the magnetic field of a quasiparticle having an arbitrary dispersion law and spin $1/2$, which we shall henceforth refer to as an electron, are given by expression (1.8); m_0 which appears in the definition of μ_0 represents the mass of the electron.

It is worth to note that the components p_i in (1.1) for electrons in a metal are components of a quasimomentum. This fact, however, does not affect the results obtained, provided that the surface given by (1.6) does not intersect itself, and that each of the curves (1.4) is located within one of the cells of the reciprocal lattice. In addition, the radius of curvature of the electron trajectory must clearly be assumed to be large compared to the lattice constant.

2. Calculation of the Magnetic Moment

The magnetic moment \mathbf{M} of the electron gas is calculated as the derivative of the thermodynamic potential Ω with respect to the field: $\mathbf{M} = -\partial\Omega/\partial\mathbf{H}$. To determine the thermodynamic potential Ω , we make use of the usual formula of statistical physics

$$\Omega = -\Theta \sum_s \ln \left\{ 1 + \exp \frac{\zeta - E(s)}{\Theta} \right\}, \quad (2.1)$$

where $E(s)$ is the energy of the electron in the state s , ζ is the chemical potential, $\Theta = kT$, and the summation is performed over all of the possible states s of the individual electron. The energy $E(s)$ for an electron in a state, where p_z , n , and the direction of spin are set, is given by expression (1.8).

Since, in computing the number of states, the commutation relations (1.2) rather than the dispersion law for electrons are the essential factor, the number of states is calculated by the same method as that used by Landau for free electrons [2]. In particular, it is possible to assert that the number of states with momentum p_z in the interval $(p_z, p_z + \Delta p_z)$ for a given n and a given spin orientation is equal to

$$V \frac{eH}{4\pi^2 \hbar^2 c} \Delta p_z.$$

Therefore, relation (2.1) can be rewritten in the form

$$\Omega = -V \frac{eH}{4\pi^2 \hbar^2 c} \sum_{\text{spin}} \sum_{n=0}^{\infty} \Theta \int_{-\infty}^{\infty} dp_z \times \ln \left\{ 1 + \exp \frac{\zeta - E_n(p_z; H) \mp \frac{1}{2}\mu_0 H}{\Theta} \right\}. \quad (2.2)$$

Denoting the expression following the summation sign in (2.2) by $\varphi(n)$, we use the Poisson formula for the summation over n [5]:

$$\Omega = -V \frac{eH}{4\pi^2 \hbar^2 c} \sum_{\text{spin}} \left\{ \frac{1}{2} \varphi(0) + \int_0^\infty dn \varphi(n) + 2 \sum_{k=1}^\infty \int_0^\infty dn \varphi(n) \cos 2\pi kn \right\}.$$

Inasmuch as $\gamma \rightarrow 1/2$ for $E_n \rightarrow E_0$, it can be readily shown that the thermodynamic potential can be written in the form

$$\Omega = -V \frac{eH}{4\pi^2 \hbar^2 c} \sum_{\text{spin}} \left\{ \int_{-1/2}^\infty dn \varphi(n) + 2 \operatorname{Re} \sum_{k=1}^\infty \int_{-1/2}^\infty dn \varphi(n) e^{2\pi kin} \right\}. \quad (2.3)$$

The first term inside the curly brackets corresponds to the continuous energy spectrum. It can easily be shown that this term will contribute only to the spin paramagnetism of the electron gas. Introducing the symbol $\varepsilon = \zeta \mp \frac{1}{2} \mu_0 H$, we obtain

$$J_1 = \int_{-1/2}^\infty dn \varphi(n) = \Theta \int_{-1/2}^\infty dn \int_{-\infty}^\infty dp_z \ln \left\{ 1 + e^{(\varepsilon - E_n)/\Theta} \right\} = \Theta \int_0^\infty dE \ln \left\{ 1 + e^{(\varepsilon - E_n)/\Theta} \right\} \int_{S>0} dp_z \left(\frac{\partial n}{\partial E} \right),$$

where $S = S(E, p_z)$.

The relation between E and n is given by expression (1.5). Hence,

$$\frac{\partial n}{\partial E} = \frac{c}{2\pi e \hbar H} \frac{\partial S}{\partial E}; \quad (2.4)$$

$$J_1 = \frac{\Theta c}{2\pi e \hbar H} \int_0^\infty dE \ln \left\{ 1 + e^{(\varepsilon - E_n)/\Theta} \right\} \int_{S>0} dp_z \left(\frac{\partial S}{\partial E} \right). \quad (2.5)$$

Taking the specificity of the limits of integration for the inner integral in (2.5) into consideration, we write

$$J_1 = \frac{\Theta c}{2\pi e \hbar H} \int_0^\infty dE \times$$

$$\begin{aligned} & \times \ln \left\{ 1 + e^{(\varepsilon - E)/\Theta} \right\} \frac{d}{dE} \int_{S>0} dp_z S(E, p_z) = \\ & = \frac{c}{2\pi e \hbar H} \int_0^\infty \frac{dE}{e^{(E-\varepsilon)/\Theta} + 1} \int_{S>0} S(E, p_z) dp_z. \end{aligned} \quad (2.6)$$

We now note that the inner integral in (2.6) gives the volume bounded by the surface of constant energy E in the momentum space. Representing this volume by $U(E)$ and introducing the notation

$$W(\varepsilon) = \int_0^\infty \frac{U(E) dE}{e^{(E-\varepsilon)/\Theta} + 1},$$

we obtain

$$J_1 = \frac{c}{2\pi e \hbar H} W(\varepsilon). \quad (2.7)$$

Making use of the fact that $\mu_0 H \ll \zeta$, we can expand $W(\varepsilon)$ in powers of $\mu_0 H$, stopping with the second-order terms. If we insert this expansion into (2.3) and sum over the two possible spin orientations, it is seen that the corresponding part of the thermodynamic potential Ω is equal to

$$\Omega_1 = -\frac{V}{8\pi^3 \hbar^3} \left[2W(\zeta) + \left(\frac{\mu_0 H}{2} \right)^2 \frac{d^2 W(\zeta)}{d\zeta^2} \right]. \quad (2.8)$$

Therefore, J_1 actually contributes only to the spin paramagnetism of the electron gas:

$$M_{1z} = \mu_0 V \frac{1}{16\pi^3 \hbar^3} \frac{d^2 W(\zeta)}{d\zeta^2} \mu_0 H. \quad (2.9)$$

Relation (2.9) has a simple physical interpretation. Under the condition $\Theta \ll \zeta$, which we consider to be fulfilled always, one can set

$$W(\zeta) \approx \int_0^\zeta U(E) dE,$$

which yields

$$\frac{d^2 W(\zeta)}{d\zeta^2} \approx \frac{dU(\zeta)}{d\zeta}.$$

The product

$$\frac{V}{8\pi^3 \hbar^3} \frac{dU(\zeta)}{d\zeta} = \rho(\zeta) \quad (2.10)$$

gives the number of states per unit energy interval near the Fermi boundary energy. Therefore, relation (2.9) can be written in the form

$$M_{1z} = \frac{1}{2} \mu_0 \rho(\zeta) \mu_0 H. \quad (2.11)$$

The diamagnetism of the electron gas and the de Haas–van Alphen effect are described by the second term in the curly brackets in (2.3). Using (1.5) and (2.4), we can transform the integrals entering into this term:

$$\begin{aligned} J(k) &= \int_{-1/2}^{\infty} dn \varphi(n) e^{2\pi k i n} = \\ &= \Theta \int_{-1/2}^{\infty} dn \int_{-\infty}^{\infty} dp_z \ln \left\{ 1 + \exp \frac{\varepsilon - E_n}{\Theta} \right\} e^{2\pi k i n} = \\ &= \frac{\Theta c}{2\pi e \hbar} \int_0^{\infty} dE \ln \left\{ 1 + \exp \frac{\varepsilon - E_n}{\Theta} \right\} \times \\ &\times \int_{s>0} dp_z \left(\frac{\partial S}{\partial E} \right) \exp \left\{ \frac{kc}{e\hbar H} S(E, p_z) - 2\pi k i \gamma \right\}. \end{aligned}$$

Integration by parts leads to the expression

$$\begin{aligned} J(k) &= \frac{c}{2\pi e \hbar H} \int_0^{\infty} dE f \left(\frac{E - \varepsilon}{\Theta} \right) \times \\ &\times \int_0^{\infty} dE' \int_{s>0} dp_z \frac{\partial S(E', p_z)}{\partial E'} \times \\ &\times \exp \left\{ i \frac{kc}{e\hbar H} S(E', p_z) - 2\pi k i \gamma \right\}; \quad (2.12) \end{aligned}$$

where $f(x)$ represents the Fermi distribution function: $f(x) = (1 + e^x)^{-1}$.

While computing the inner double integral in (2.12), we used the fact that $(c/2\pi e \hbar H)S = n + \gamma$ is a very large number, by assumption. This allows us to use the method of stationary points for the asymptotic evaluation of the integral. It turns out that the major contribution to $J(k)$ comes, first, from the integration in a vicinity of the extremum point $S(E', p_z)$ for $E' = E$, i.e., the point at which $\partial S(E, p_z)/\partial p_z = 0$. Second, it comes from the integration in a vicinity of the vertices of the region of integration: $E' = E$, $S(E, p_z) = 0$. As for the integration in a vicinity of the stationary point, it yields the oscillating part of $J(k)$ (cf. Appendix) corresponding to the oscillating part of the magnetic moment. The integration in a vicinity of the vertex

$E' = E$, $S(E, p_z) = 0$, yields the nonperiodic part of $J(k)$ which determines the diamagnetism of the electron gas. The neighborhood of $S(E, p_z) = 0$ corresponds, however, to small values of the quantum number n [cf. (1.5)], for which the energy levels calculated in the quasiclassical approximation (Section 1) are, generally speaking, incorrect. Therefore, the nonperiodic part of $J(k)$, the expression for which is given in Appendix, can give the correct value for the diamagnetism of the electron gas only in the special case where the quasiclassical energy levels coincide with the true levels for all n (for instance, in the case of a quadratic dispersion law).

The principal term in the asymptotic expansion of the inner double integral in a vicinity of the stationary point leads to the following expression:

$$\begin{aligned} J(k) &= \frac{1}{\sqrt{2\pi}} \left(\frac{e\hbar H}{c} \right)^{1/2} \frac{1}{k^{3/2}} \times \\ &\times \exp \left\{ -2\pi k i \gamma \mp i \frac{\pi}{4} - i \frac{\pi}{2} \right\} \times \\ &\times \int_0^{\infty} dE f \left(\frac{E - \varepsilon}{\Theta} \right) \left| \frac{\partial^2 S(E, p_z)}{\partial p_z^2} \right|_m^{-1/2} \times \\ &\times \exp \left\{ i \frac{kc}{e\hbar H} S_m(E) \right\}. \quad (2.13) \end{aligned}$$

By $S_m(E)$, we denote the extremal value of $S(E, p_z)$ for E to be constant. If $S_m(E)$ represents a maximum for the intercepted area, then the phase $i\pi/4$ takes the minus sign in (2.13). Whereas, if $S_m(E)$ is a minimum area, the phase $i\pi/4$ takes the plus sign. The derivative $(\partial^2 S/\partial p_z^2)_m$ is taken at the extremal point.

To compute the integral in (2.13), we use the fact that, under the assumption that $dS_m(E)/dE \neq 0$ and for the evident inequality $\Theta \ll \varepsilon$, the major contribution to the integral comes from the integration about the point, at which the function $f[(E - \varepsilon)/\Theta]$ varies most rapidly; i.e., about $E = \varepsilon$. Therefore, expanding $S_m(E)$ in powers of $E - \varepsilon$ and integrating, we obtain

$$\begin{aligned} &\int_0^{\infty} dE f \left(\frac{E - \varepsilon}{\Theta} \right) \left| \frac{\partial^2 S}{\partial p_z^2} \right|_m^{-1/2} \exp \left\{ i \frac{kc}{e\hbar H} S_m(E) \right\} \approx \\ &\approx \frac{e\hbar H}{kc} \Psi(k) \frac{\exp \left\{ -i \frac{\pi}{2} + i \frac{kc}{e\hbar H} S_m(\varepsilon) \right\}}{\left| \partial^2 S/\partial p_z^2 \right|_m^{1/2} dS_m(\varepsilon)/d\varepsilon}, \quad (2.14) \end{aligned}$$

where $\Psi(z) = z/\sinh z$, and $\lambda = (\pi c \Theta / e \hbar H) \times (dS_m(\varepsilon)/d\varepsilon)$.

Inserting expression (2.14) in (2.13), we obtain

$$J(k) = -\frac{1}{\sqrt{2\pi}} \left(\frac{e\hbar H}{c} \right)^{3/2} \times \\ \times \frac{1}{k^{5/2}} \frac{\Psi(k\lambda) \exp \left\{ i \frac{kc}{e\hbar H} S_m(\varepsilon) \mp i \frac{\pi}{4} - 2\pi k i \gamma \right\}}{\left| \partial^2 S(\varepsilon, p_z) / \partial p_z^2 \right|_m^{1/2} dS_m(\varepsilon) / d\varepsilon}. \quad (2.15)$$

We compute the second term in the curly brackets of (2.3) by summing over k :

$$2\text{Re} \sum_{k=1}^{\infty} J(k) = \\ = -\frac{2}{\sqrt{2\pi}} \left(\frac{e\hbar H}{c} \right)^{3/2} \left| \frac{\partial^2 S(\varepsilon, p_z)}{\partial p_z^2} \right|_m^{-1/2} \left(\frac{dS_m(\varepsilon)}{d\varepsilon} \right)^{-1} \times \\ \times \sum_{k=1}^{\infty} \frac{1}{k^{5/2}} \Psi(k\lambda) \cos \left[\frac{kc}{e\hbar H} S_m(\varepsilon) \mp \frac{\pi}{4} - 2\pi k \gamma \right]. \quad (2.16)$$

In summing over the two spin orientations, it is possible, in all of the expressions in (2.16) except the argument of the cosine, simply to replace ε by ζ . In the argument of the cosine, however, it is necessary to expand $S_m(\varepsilon)$ in powers of $\mu_0 H$, stopping with the first power of $\mu_0 H$:

$$S_m(\varepsilon) = S_m(\zeta) \pm \frac{1}{2} \mu_0 H \frac{dS_m(\zeta)}{d\zeta}.$$

Taking this into account in the summation, we obtain the final expression for the oscillating part of the thermodynamic potential Ω corresponding to the second term in the curly brackets of (2.3) as

$$\Omega_2 = \frac{V}{\pi^2 \sqrt{2\pi} \hbar^3} \left(\frac{e\hbar H}{c} \right)^{5/2} \left| \frac{\partial^2 S}{\partial p_z^2} \right|_m^{-1/2} \left(\frac{dS_m}{d\zeta} \right)^{-1} \times \\ \times \sum_{k=1}^{\infty} \frac{\Psi(k\lambda)}{k^{5/2}} \cos \left[\frac{kc}{e\hbar H} S_m(\zeta) \mp \frac{\pi}{4} - 2\pi k \gamma \right] \times \\ \times \cos \left[\frac{k}{2m_0} \frac{dS_m(\zeta)}{d\zeta} \right]. \quad (2.17)$$

In order to determine that part of the magnetic moment which is contributed by (2.17), we must differentiate Ω_2 with respect to the magnetic field intensity. In this differentiation, the factors preceding the cosine, which vary slowly with H , need not be differentiated at all; it is necessary only to differentiate the cosine, whose argument depends on H . We have, therefore, for the component of the moment in the

direction of the magnetic field¹:

$$M_{\text{osc}} = -\frac{V}{\pi^2 \sqrt{2\pi} \hbar^3} \left(\frac{e\hbar}{c} \right)^{3/2} \frac{S_m(\zeta) \sqrt{H}}{\left| \partial^2 S / \partial p_z^2 \right|_m^{1/2} dS_m / d\zeta} \times \\ \times \sum_{k=1}^{\infty} \frac{1}{k^{3/2}} \Psi(k\lambda) \sin \left[\frac{kc}{e\hbar H} S_m(\zeta) \mp \frac{\pi}{4} - 2\pi k \gamma \right] \times \\ \times \cos \left[\frac{k}{2m_0} \frac{dS_m(\zeta)}{d\zeta} \right]. \quad (2.18)$$

Combining (2.8) and (2.17), as well as (2.11) and (2.18), and taking the diamagnetism of the electron gas into consideration, we write the final expressions for the thermodynamic potential Ω and the magnetic moment:

$$\Omega = -\frac{V}{4\pi^3 \hbar^3} W(\varepsilon) - V \frac{1}{2} (\chi_1 + \chi_2) H^2 + \\ + \frac{V}{\pi^2 \sqrt{2\pi} \hbar^3} \left(\frac{e\hbar H}{c} \right)^{5/2} \left| \frac{\partial^2 S}{\partial p_z^2} \right|_m^{-1/2} \left(\frac{dS_m}{d\zeta} \right)^{-1} \times \\ \times \sum_{k=1}^{\infty} \frac{\Psi(k\lambda)}{k^{5/2}} \cos \left[\frac{kc}{e\hbar H} S_m(\zeta) \mp \frac{\pi}{4} - 2\pi k \gamma \right] \cos \left[\frac{k}{2m_0} \frac{dS_m(\zeta)}{d\zeta} \right]; \quad (2.19)$$

$$M = V(\chi_1 + \chi_2) H - \\ - \frac{4V}{\hbar^3 (2\pi)^{5/2}} \left(\frac{e\hbar}{c} \right)^{3/2} \frac{S_m(\zeta) \sqrt{H}}{\left| \partial^2 S(\zeta, p_z) / \partial p_z^2 \right|_m^{1/2} dS_m(\zeta) / d\zeta} \times \\ \times \sum_{k=1}^{\infty} \frac{\Psi(k\lambda)}{k^{3/2}} \sin \left[\frac{kc}{e\hbar H} S_m(\zeta) \mp \frac{\pi}{4} - 2\pi k \gamma \right] \cos \left[\frac{k}{2m_0} \frac{dS_m(\zeta)}{d\zeta} \right]. \quad (2.20)$$

Here, χ_1 represents the spin paramagnetic susceptibility of the electron gas determined from (2.11), and χ_2 is the constant part of the diamagnetic susceptibility (cf. Appendix).

We may remark that the nonperiodic part of the magnetic moment [the first two terms in (2.20)] is of little interest, inasmuch as it is obscured in metals by the other effects (for example, by the atomic magnetism). The oscillating part of the magnetic moment, to the analysis of which we now turn, is of primary interest.

¹Throughout what follows, the values given are those of the component M_z of the momentum in the direction of \mathbf{H} . The corresponding oscillating component M_x of the momentum in the perpendicular direction is obtained by multiplying (2.18) by $(1/S_m)(\partial S_m / \partial \vartheta)$ (ϑ being the angle in the $x-z$ plane).

3. Analysis of Results

From the formula for the magnetic moment (2.20), it can be seen that the amplitude and the period of oscillations in the magnetic moment are fully determined by the extremal value of the area on the Fermi boundary surface intercepted by the plane $\mathbf{P} \times \mathbf{H} = \text{const}$ and by the derivatives of the area intercepted on the Fermi surface at the extremal point.

For a quadratic dispersion law

$$\mathcal{E} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2), \quad (3.1)$$

we have

$$\begin{aligned} S(E, p_z) &= 2\pi m(E - (p_z^2/2m)); \\ S_m(E) &= 2\pi mE, \quad dS_m(E)/dE = 2\pi m, \\ |\partial^2 S/\partial p_z^2| &= 2\pi; \quad \gamma = 1/2. \end{aligned}$$

In this case, expression (2.20) goes over into the usual formula for the magnetic moment of a gas of free electrons [2].

For a temperature of absolute zero or for very strong magnetic fields, in which case $\lambda \ll 1$, the function $\Psi(k\lambda)$ can be replaced by unity in (2.20). Then the oscillating part of the magnetic moment is given by the formula

$$\begin{aligned} M_{\text{osc}} &= -\frac{4V}{\hbar^3(2\pi)^{5/2}} \left(\frac{e\hbar}{c}\right)^{3/2} \times \\ &\times \frac{S_m(\zeta)\sqrt{H}}{|\partial^2 S(\zeta, p_z)/\partial p_z^2|_m^{1/2} dS_m(\zeta)/d\zeta} \times \\ &\times \sum_{k=1}^{\infty} \frac{1}{k^{3/2}} \sin\left[\frac{kc}{e\hbar H} S_m(\zeta) \mp \frac{\pi}{4} - \right. \\ &\left. - 2\pi k\gamma\right] \cos\left[\frac{k}{2m_0} \frac{dS_m(\zeta)}{d\zeta}\right]. \end{aligned} \quad (3.2)$$

For small fields, $\lambda \gg 1$ and $\Psi(k\lambda) \approx 2k\lambda e^{-k\lambda}$. Therefore, only one term (for $k=1$) of the summation in expression (2.20) need be taken, which yields

$$M_{\text{osc}} = -A(H, \zeta) \sin\left[\frac{c}{e\hbar H} S_m(\zeta) \mp \frac{\pi}{4} - 2\pi\gamma\right], \quad (3.3)$$

where

$$\begin{aligned} A(H, \zeta) &= \frac{4V}{\hbar^3(2\pi)^{3/2}} \left(\frac{e\hbar}{c}\right)^{1/2} \times \\ &\times \frac{\Theta S_m(\zeta)e^{-\lambda}}{|\partial^2 S(\zeta, p_z)/\partial p_z^2|_m^{1/2} \sqrt{H}} \cos\left[\frac{1}{2m_0} \frac{dS_m(\zeta)}{d\zeta}\right]. \end{aligned}$$

Since we used the thermodynamic potential Ω in calculating the magnetic moment, the quantities ζ

and H must be regarded, as a result, as independent variables. In specific applications of formulas (2.20), (3.2), and (3.3), one must take into consideration, however, the dependence of ζ on H determined by the constancy of the number of particles

$$N = -\partial\Omega(\zeta, H)/\partial\zeta = \text{const.}$$

This dependence is, however, sufficiently weak that it can be neglected. It is easy to convince oneself of this by evaluating the part of ζ which depends on the magnetic field. The expression for $\Omega(\zeta, H)$ is given by formula (2.19); on differentiating this with respect to ζ , we retain, as before, only the first few terms in the expansion in powers of H . Then

$$\begin{aligned} N &= \frac{V}{4\pi^3\hbar^3} \frac{dW(\zeta)}{d\zeta} - \\ &- \frac{V}{2\pi^3\hbar^3} \left(\frac{e\hbar H}{c}\right)^{3/2} \frac{\sqrt{2\pi}}{|\partial^2 S(\zeta, p_z)/\partial p_z^2|_m^{1/2}} \times \\ &\times \sum_{k=1}^{\infty} \frac{1}{k^{3/2}} \Psi(k\lambda) \sin\left[\frac{kc}{e\hbar H} S_m(\zeta) \mp \right. \\ &\left. \mp \frac{\pi}{4} - 2\pi k\gamma\right] \cos\left[\frac{k}{2m_0} \frac{dS_m(\zeta)}{d\zeta}\right]. \end{aligned} \quad (3.4)$$

Under the assumptions we have made ($\Theta \ll \zeta$), $dW(\zeta)/d\zeta = U(\zeta)$; this is the volume in the momentum space enclosed by the Fermi boundary surface. If we introduce this notation into formula (3.4) and, for simplicity, designate the summation in the second term of this formula by $G(\zeta, H)$, we obtain

$$U(\zeta_0) = U(\zeta) - \left(\frac{e\hbar H}{c}\right)^{3/2} \frac{2\sqrt{2\pi}G(\zeta, H)}{|\partial^2 S(\zeta, p_z)/\partial p_z^2|_m^{1/2}}, \quad (3.5)$$

where ζ_0 is the chemical potential at $H=0$.

Assuming a small increment to ζ dependent on the magnetic field H , we can set

$$\zeta = \zeta_0(1 + \xi(H)), \quad \xi \ll 1.$$

Expanding the quantities in (3.5) which depend on ζ in powers of ξ and stopping after the first few terms, we have

$$\begin{aligned} U(\zeta_0) &= U(\zeta_0) + \xi\zeta_0 \frac{dU(\zeta_0)}{d\zeta_0} - \\ &- \left(\frac{e\hbar H}{c}\right)^{3/2} \frac{2\sqrt{2\pi}G(\zeta_0, H)}{|\partial^2 S(\zeta_0, p_z)/\partial p_z^2|_m^{1/2}}, \end{aligned}$$

whence it follows that

$$\xi(H) = \frac{2\sqrt{2\pi}}{\zeta_0 dU(\zeta_0)/d\zeta_0} \left(\frac{e\hbar H}{c} \right)^{3/2} \times \frac{G(\zeta_0, H)}{|\partial^2 S(\zeta_0, p_z)/\partial p_z^2|^{1/2}}. \quad (3.6)$$

Inasmuch as the summation $G(\zeta, H)$ appearing in (3.6) is of the order of unity, while $|\partial^2 S/\partial p_z^2|^{1/2}$ is a dimensionless quantity representing the anisotropy of the Fermi boundary surface (in the case of a spherical surface, it is equal to $\sqrt{2\pi}$), the quantity $\xi(H)$ is determined by the ratio $(e\hbar H/c)^{3/2}/\zeta_0(dU(\zeta_0)/d\zeta_0)$. If the cases in which the anisotropy of the Fermi surface is anomalously large are neglected, then it is possible to assume that $U(\zeta_0) \sim [S(\zeta_0)]^{3/2}$, where $S(\zeta_0)$ is the mean area intercepted on the Fermi surface by the planes $p_z = \text{const}$. This allows setting, by the order of magnitude,

$$\zeta_0 \frac{dU(\zeta_0)}{d\zeta_0} \sim U(\zeta_0) \sim [S(\zeta_0)]^{3/2} \sim \left[\zeta_0 \frac{dS}{d\zeta_0} \right]^{3/2},$$

and we can write

$$\xi(H) \sim \left(\frac{e\hbar H}{c} \right)^{3/2} \Big/ \zeta_0 \frac{dU(\zeta_0)}{d\zeta_0} \sim \left(\frac{e\hbar H}{\zeta_0 c} \Big/ \frac{dS(\zeta_0)}{d\zeta_0} \right)^{3/2}. \quad (3.7)$$

We note here that, as follows from (1.5), the mean distance between neighboring energy levels near the boundary energy is equal to

$$\Delta E = \frac{2\pi e\hbar H}{c} \Big/ \frac{dS(\zeta_0)}{d\zeta_0}.$$

The distance between the levels is assumed to be considerably less than the boundary energy ζ_0 ; from (3.7), therefore, we obtain the following estimation of $\xi(H)$:

$$\xi(H) \sim (\Delta E/\zeta_0)^{3/2} \ll 1. \quad (3.8)$$

Thus, the quantity $\xi(H)$ determined by expression (3.6) is actually small in magnitude. In the case of the quadratic dispersion law (3.1),

$$\xi(H) = \left(\frac{e\hbar H}{mc\zeta_0} \right)^{3/2} \frac{G(\zeta_0, H)}{2\pi\sqrt{2}} \sim \left(\frac{e\hbar H}{mc\zeta_0} \right)^{3/2} = \left(\frac{\mu H}{\zeta_0} \right)^{3/2} \ll 1.$$

As for the argument of the sine in (2.20), (3.2), or (3.3), its dependence on the magnetic field is incorporated in the expression

$$\begin{aligned} \frac{c}{e\hbar H} S_m(\zeta) &= \frac{c}{e\hbar H} \left[S_m(\zeta_0) + \xi\zeta_0 \frac{dS_m(\zeta_0)}{d\zeta_0} \right] = \\ &= \frac{c}{e\hbar H} S_m(\zeta_0) + \frac{2\sqrt{2\pi}}{dU(\zeta_0)/d\zeta_0} \left(\frac{e\hbar H}{c} \right)^{1/2} \times \\ &\times \frac{G(\zeta_0, H) \frac{dS_m(\zeta_0)}{d\zeta_0}}{|\partial^2 S(\zeta_0, p_z)/\partial p_z^2|^{1/2}}. \end{aligned} \quad (3.9)$$

The second term in (3.9) is equal in the order of magnitude to $(\Delta E/\zeta_0)^{1/2} \ll 1$; the periodic dependence of the magnetic moment on the magnetic field is therefore fully determined by the first term in (3.9):

$$\frac{c}{e\hbar H} S_m(\zeta) \approx \frac{c}{e\hbar H} S_m(\zeta_0). \quad (3.10)$$

It follows from (3.8) and (3.10) that ζ can be replaced by ζ_0 in (2.19) and (2.20), as well as in (3.2) and (3.3), and the period of oscillations can be represented in the form

$$\Delta \left(\frac{1}{H} \right) = \frac{2\pi e\hbar}{c S_m(\zeta_0)}. \quad (3.11)$$

If there are several unfilled zones, in which the classical motion of the electron is independent, i.e., when the Fermi surface is reduced to a few closed surfaces, then each group of electrons has its own $S_m(E)$ and makes its own oscillatory contribution to the magnetic moment. If, in this case, the boundary energy ζ is found to be placed near the bottom of the unfilled zone, we can restrict ourselves with the expansion

$$\mathcal{E}(P_x, P_y, P_z) = \varepsilon_0 + \left(\frac{P_x^2}{2m_1} + \frac{P_y^2}{2m_2} + \frac{P_z^2}{2m_3} \right).$$

The maximum area intercepted on the ellipsoid $\mathcal{E}(P_x, P_y, P_z) = E$ by the plane $\mathbf{P} \times \mathbf{H} = \text{const}$ will be

$$S_m = 2\pi m(E - \varepsilon_0),$$

$$m = (m_1 m_2 m_3)^{1/2} / (m_1 \alpha_1^2 + m_2 \alpha_2^2 + m_3 \alpha_3^2)^{1/2},$$

where the α_i are the direction cosines of the magnetic field vector H in the system of the crystallographic axes. For the corresponding factor, this yields $\partial S_m/\partial E = 2\pi m$ and the period

$$\Delta \left(\frac{1}{H} \right) = \frac{\mu}{\zeta - \varepsilon_0} \quad \left(\mu = \frac{e\hbar}{mc} \right).$$

In the case of a nearly filled zone, the energy at the upper boundary has the form

$$\mathcal{E}(P_x, P_y, P_z) = \varepsilon'_0 - \left(\frac{P_x^2}{2m_1} + \frac{P_y^2}{2m_2} + \frac{P_z^2}{2m_3} \right),$$

which yields

$$\partial S_m / \partial E = -2\pi m \quad \text{and} \quad \Delta \left(\frac{1}{H} \right) = \frac{\mu^*}{\varepsilon'_0 - \zeta},$$

$$\mu^* = \frac{e\hbar}{m^*c},$$

$$m^* = (m_1^* m_2^* m_3^*)^{1/2} / (m_1^* \alpha_1^2 + m_2^* \alpha_2^2 + m_3^* \alpha_3^2)^{1/2}.$$

In the presence of strong mass anisotropy, even a slightly mosaic structure leads to the obscuration or complete obliteration of oscillations in the case where the number of electrons in the corresponding zone is large. This obscuration of the phase of the oscillatory term can be represented in the form

$$\Delta\varphi = \frac{\zeta - \varepsilon_0}{\mu H} \frac{\Delta m}{m} \sim \frac{\zeta - \varepsilon_0}{\mu H} \Delta\vartheta,$$

where $\Delta\vartheta$ is the angle of mosaicity. For $\Delta\varphi \ll 1$, the oscillations disappear. Therefore, only those groups of electrons or holes, in which the number of particles is extremely small, will participate in the effect. Oscillations having smaller periods can appear only for sufficiently high fields. Since, however, the curvature of the surface corresponding to an anomalously small number of electrons is, as a rule, extremely high (anomalously small electronic “masses”), there is no foundation, even in this case, for assuming a quadratic dispersion law.

Thus, the occurrence of the experimentally observable de Haas–van Alphen effect in a large group of metals provides grounds for assuming that the presence of zones having an anomalously small number of electrons is a general property of metals. It is possible that the appearance of these zones is related to the interaction between the electrons and the lattice. The discovery of an isotopic effect might serve to confirm such a supposition.

Finally, we turn our attention to the fact that the careful experimental measurement of the period of oscillations of the magnetic moment $\Delta(1/H)$, as well as of the amplitude of oscillations and the temperature dependence, would allow one to reconstruct the form of the Fermi boundary surface and to determine the velocity of electrons on this surface. That is, this

allows one to solve the problem inverse in some sense to that we have solved. The feasibility of this procedure is a consequence of the fact that the period of oscillations determines the extreme value $S_m(\zeta)$ of the area intercepted on the Fermi boundary surface by the planes perpendicular to the direction of the magnetic field, while the amplitude of oscillations and the temperature dependence determine $dS_m(\zeta)/d\zeta$ and $|\partial^2 S(\zeta, p_z) / \partial p_z^2|^{1/2}$. As has been demonstrated in a paper by Lifshits and Pogorelov [6], the knowledge of these quantities, under quite general assumptions, is adequate for the solution of the inverse problem.

If it is assumed that the Fermi boundary surface has a center of symmetry and that the extremal intercept is the central one, then the length of the radius vector \mathbf{r} , extending from the center to the surface in the direction \mathbf{e} (\mathbf{e} being the unit vector), is determined by the formula [6]

$$\pi r^2(\mathbf{e}) = X_{\mathbf{e}}(0) - \int_0^1 [X_{\mathbf{e}}(u) - X_{\mathbf{e}}(0)] \frac{du}{u^2}. \quad (3.12)$$

Here, we have introduced the notation

$$X_{\mathbf{e}}(u) = \frac{1}{2\pi} \int [S_m(\zeta)]_{\mathbf{n}} \delta(\mathbf{n}\mathbf{e} - u) d\Omega_{\mathbf{n}},$$

where $[S_m(\zeta)]_{\mathbf{n}}$ is the area intercepted on the boundary surface $\mathcal{E}(P_x, P_y, P_z) = \zeta$ by a plane passing through the center normally to a given unit vector \mathbf{n} , $\delta(z)$ is the delta-function, and $d\Omega_{\mathbf{n}}$ is the element of solid angle in the direction \mathbf{n} .

Having determined the form of the surface $r(\mathbf{e})$ and knowing the quantity $dS_m(\zeta)/d\zeta$, one can readily determine the velocity of electrons on the boundary surface.

For the magnetic fields at which the measurements of the de Haas–van Alphen effect have been conducted ($H \sim 10^4$ Oe), the periods observed experimentally for oscillations are determined, as we have pointed out, by the zones having an anomalously small number of electrons. For this reason, the method described above can be used to reconstruct the Fermi boundary surface only for these zones. Measurements in considerably stronger fields are needed before it will be possible to draw any conclusions regarding the form of the boundary surface for the normal energy zones.

APPENDIX

We will evaluate the integral

$$I = \int \int dE' dp_z \frac{\partial S(E', p_z)}{\partial E'} \exp \left\{ i \frac{kc}{e\hbar H} S(E', p_z) - 2\pi k\gamma i \right\},$$

in which the region of integration is bounded by the straight line $E' = E$ and the curve $S(E', p_z) = 0$. We shall not specify the extremely weak dependence of γ on E' and p_z .

Assuming that $\partial S(E', p_z)/\partial E' \neq 0$, we may conclude that the primary contribution to I is provided by the integration in the neighborhood of the point on the boundary of the region of integration $E' = E$ for which $\partial S(E, p_z)/\partial p_z = 0$, in the vicinity of the point $E' = p_z = 0$ for which $\partial S(0, p_z)/\partial p_z = 0$, and near the vertices of the region of integration [7].

1) On integrating near the stationary point on the straight line $E' = E$, we expand $S(E', p_z)$ in a power series in $(E - E')$ and $(p_z - p_m)$ (p_m corresponds to the stationary point), stopping after the first nonvanishing terms:

$$I_1 = \frac{\partial S(E, p_m)}{\partial E} \exp \left\{ i \frac{kc}{e\hbar H} S(E, p_m) - 2\pi k i \gamma \right\} \times \\ \times \int_{E-0}^E dE \int_{p_m-0}^{p_m+0} dp_z \exp \left\{ i \frac{kc}{e\hbar H} \left[(E' - E) \frac{\partial S}{\partial E} + \right. \right. \\ \left. \left. + \frac{1}{2} (p_z - p_m)^2 \frac{\partial^2 S}{\partial p_z^2} \right] \right\}.$$

After the further computation, we obtain

$$I_1 \sim \left(\frac{e\hbar H}{kc} \right)^{3/2} \frac{\sqrt{2\pi}}{|\partial^2 S/\partial p_z^2|^{1/2}} \exp \left\{ i \frac{kc}{e\hbar H} S(E, p_m) - \right. \\ \left. - 2\pi k i \gamma - i \frac{\pi}{2} \mp i \frac{\pi}{4} \right\}.$$

The sign of the last term in the exponent agrees with the sign of $\partial^2 S(E, p_m)/\partial p_m^2$.

In computing the integral, we have made use of the asymptotic formula

$$\int_{x_0} f(x) \exp \{ \pm i W(x - x_0) \} dx \sim \\ \sim f_n \frac{\Gamma(n+1)}{W^{n+1}} \exp \left\{ \pm i \frac{n+1}{2} \pi \right\} \quad (W \gg 1),$$

assuming that, in the neighborhood of $x = x_0$, the function $f(x)$ has the form $f(x) \approx f_n(x - x_0)^n$.

The expression obtained for I_1 determines the oscillatory part of $J(k)$; if we insert it in (2.12) and denote $S_m(E) = S(E, p_m)$, we obtain (2.13).

2) Denoting the values of p_z corresponding to the vertices in the region of integration by $\pm p_0$, we investigate the integral in the vicinity of one of the vertices

$$I_2 \approx \frac{\partial S(E, p_0)}{\partial E} e^{-2\pi k i \gamma} \int_{p_0-0}^{p_0} dp_z \int_{p_0-0}^E dE' \times \\ \times \exp \left\{ i \frac{kc}{e\hbar H} \left[(p_z - p_0) \frac{\partial S}{\partial p_0} + (E' - E) \frac{\partial S}{\partial E} \right] \right\}.$$

The lower limit of the integral over E' lies on the curve $S(E', p_z) = 0$. Near the vertex, it is possible to make the substitution

$$E' = E + (p_0 - p_z) \left(\frac{\partial S}{\partial p_0} / \frac{\partial S}{\partial E} \right).$$

With the change of variables, we have

$$I_2 \sim \left(\frac{e\hbar H}{kc} \right)^2 \frac{e^{-2\pi k i \gamma}}{\partial S(E, p_0)/\partial p_0} \int_0 dx e^{-ix} \int_0^{-x} dy e^{-iy}.$$

Computing the integral with the use of the above formula, we obtain

$$I_2 \sim \left(\frac{e\hbar H}{kc} \right)^2 \frac{\sin 2\pi k \gamma - \cos 2\pi k \gamma}{\partial S(E, p_0)/\partial p_0} (1 + ia),$$

where a is some real quantity; its value is not important, since we shall be interested only in the real part of I .

Inserting I_2 in (2.12), we obtain the corresponding contribution to the real part of $J(k)$:

$$\text{Re}\{J(k)\} \sim \frac{e\hbar H}{c} \frac{\sin 2\pi k \gamma - \cos 2\pi k \gamma}{2\pi k^2} \int_0^\infty \frac{f\left(\frac{E-\varepsilon}{\Theta}\right) dE}{\partial S(E, p_0)/\partial p_0}.$$

Noting that the region of integration has two symmetric vertices, we write the expression for that part of the thermodynamic potential Ω and the magnetic moment M which is determined by the quantity I_2 in the form

$$\Omega = -V \frac{1}{\hbar^3} \left(\frac{e\hbar H}{c} \right)^2 \frac{1}{\pi^3} \sum_{k=1}^\infty \frac{\sin 2\pi k \gamma - \cos 2\pi k \gamma}{k^2} \times \\ \times \int_0^\infty \frac{f\left(\frac{E-\zeta}{\Theta}\right) dE}{\partial S(E, p_0)/\partial p_0}, \quad (\text{A.1})$$

$$M = V \frac{2}{\pi^3} \frac{e^2}{\hbar c^2} H \sum_{k=1}^\infty \frac{\sin 2\pi k \gamma - \cos 2\pi k \gamma}{k^2} \int_0^\infty \frac{f\left(\frac{E-\zeta}{\Theta}\right) dE}{\partial S(E, p_0)/\partial p_0}. \quad (\text{A.2})$$

These expressions describe the constant part of the diamagnetism of the electron gas. In the case of the quadratic dispersion law (3.1), $\partial S(E, p_0)/\partial p_0 = -2\pi\sqrt{2mE}$, and (A.2) passes into the known Landau formula.

In the general case, however, our formulas for the constant part of the diamagnetic susceptibility can turn out to be incorrect, since it is impossible to use the quasiclassical energy levels in the vicinity of $S(E, p) = 0$. The diamagnetic susceptibility of the electron gas is determined by the electrons near the Fermi boundary surface [8], while the expressions (A.1) and (A.2) are determined by all of the electrons together.

3) One can readily convince oneself that the integration about the point $E' = p_z = 0$ yields a contribution to the real part of I which is small in comparison with the real parts of I_1 and I_2 ; we shall not, therefore, investigate it.

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