Theory of Magnetic Susceptibility in 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 are found for a quasi-particle under an arbitrary dispersion law in a magnetic field, and the magnetic moment of a gas of such quasi-particles is computed, spin paramagnetism being taken into account. It is shown that the periods and amplitudes of the oscillations are determined by the form of the Fermi boundary surface. Knowledge of these quantities permits one to reconstruct the form of the Fermi surface and the values of the velocities upon it.

INTRODUC'TION

HE 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 $\mathcal{E} = \mathcal{E}(\mathbf{p}_x, \mathbf{p}_y, \mathbf{p}_z)$. 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 permit 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 upon the electron energy spectrum and may serve to distinguish it uniquely.

The periodic dependence of the magnetic susceptibility upon the field at low temperatures (the De Hass - 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, Al)¹

and may be regarded as a property common to all metals. At the same time, the quantitative theory of this phenomenon had until recently been worked out only for the case of an electron gas following a quadratic dispersion law^{2, 2a}.

The quadratic dispersion law is correct for an electron in a metal only in the lower part of the appropriate energy zone, and may 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 Onsager³. A qualitative theory has been offered in a paper by the present authors⁴.

The present article contains a detailed presentation of the results published earlier in the brief communication⁴, 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. ENE RGY LEVELS OF A QUASI-PARTICLE IN A MAGNETIC FIELD

We investigate the motion of a charged quasi-

^{2a} A. Akhiezer, Dokl. Akad. Nauk SSSR 23, 872 (1939);
Iu. Rumer, J. Exper. Theoret. Phys. USSR 18, 1081 (1948);
G. Zil'berman, J. Exper. Theoret. Phys. USSR 21, 1209 (1951);
E. Sondheimer, A. Wilson, Proc. Roy. Soc. (London) 210A, 173 (1951).

¹ B. Verkin, B. Lazarev, N. Rudenko, J. Exper. Theoret. Phys. USSR **20**, 93, 995 (1950); **21**, 658(1951); Dokl. Akad. Nauk SSSR **80**, 45 (1951); the collection "In Memory of Sergei Ivanovich Vavilov", Acad. Sci. USSR Press, 1952. B. Verkin, Dokl. Akad. Nauk SSSR **81**, 529 (1951); B. Verkin, I. Mikhailov, J. Exper. Theoret. Phys. USSR **24**, 324 (1953); **25**, 471 (1953).

² L. Landau, Z. f. Phys. **64**, 629 (1930); Supplement to the article: D. Shoenberg, Proc. Roy. Soc. **170A**, 341 (1939).

³ L. Onsager, Phil. Mag. **43**, 1006 (1952)

⁴ I. Lifshitz and A. Kosevich, Dokl. Akad. Nauk SSSR 96, 963 (1954).

particle under a general dispersion law

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

in a homogeneous magnetic field.

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If the magnetic field H is directed along the z - axis, the Hamiltonian for such a particle in the magnetic field is obtained formally by replacing in (1.1) the momentum component p_i by the linear momentum operator P_i^{\vee} , the latter being interrelated by the commutation rules:

$$[P_{y}, P_{x}] = \frac{e}{c} H, \ [\check{P}_{y}, \check{P}_{z}] = [\check{P}_{x}, \check{P}_{z}] = 0$$
(1.2)

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

 $[\check{P}_{\gamma}, \check{Q}_{\gamma}] = 1$. The role of the generalized coordinate operator is played here by the operator $(c/eH)\check{P}_{\chi}$. Therefore the quasi-classical quantization condition

$$\frac{1}{2\pi} \oint P_{\mathbf{y}} dQ_{\mathbf{y}} = (n+\gamma)\hbar$$

may be written in the form:

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

(for the case of a quadratic dispersion law $y = \frac{1}{2}$; in the general case, however, y may differ from $\frac{1}{2}$).

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

which allows (1.3) to be written in the more symmetrical 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

$${\mathop{\oplus}\limits_{C}} \left(P_x, P_y, P_z \right) = E$$
 (1.6)

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

The condition (1.5) specifies, in the quasiclassical approximation, the implicit dependence of the energy of a quasi-particle in a magnetic field upon the quantum number n:

$$E = E_n(p_z; H). \tag{1.7}$$

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

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

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

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

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

It should be remarked that the components p_i in (1.1) for electrons in a metal are components of a quasi-momentum. This fact, however, does not affect the results obtained, provided that the surface (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 M of the electron gas is found by taking the derivative of the thermodynamic potential Ω with respect to the field : $M=-\partial\Omega/\partial H$. To determine the thermodynamic potential Ω we make use of the usual formula of statistical mechanics:

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

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 with given p_z , n, and direction of spin is given by the expression (1.8).

Since, in computing the number of states, the commutation relations (1.2) rather than the dispersion law for the electrons are the essential factor, the number of states is calculated by the same method as that used by Landau for free electrons²; in particular, it is possible to state that the number of states of 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

$$V \frac{e\bar{H}}{4\pi^2\hbar^2 c} \,\Delta p_z.$$

Therefore, (2.1) may be rewritten in the form:

$$\Omega = -V \frac{eH}{4\pi^2 \hbar^2 c} \sum_{spin} \sum_{n=0}^{\infty} \Theta \int_{-\infty}^{\infty} dp_z \qquad (2.2)$$

$$\times \ln \left\{ 1 + \exp \frac{\zeta - E_n (p_z; H) \mp \frac{1}{2} \mu_0 H}{\Theta} \right\}.$$

Representing the expression following the summation sign in (2.2) by $\varphi(n)$, we use for the summation over *n* the Poisson formula⁵:

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

Inasmuch as $\gamma \rightarrow \frac{1}{2}$ for $E_n \rightarrow E_0$, it may readily be shown that the thermodynamic potential can be written in the following form:

$$\Omega = -V \frac{eH}{4\pi^2 \hbar^2 c} \sum_{\overline{spin}} \left\{ \int_{-i/s}^{\infty} dn \varphi(n) + 2 \operatorname{Re} \sum_{h=1}^{\infty} \int_{-i/s}^{\infty} dn \varphi(n) e^{2\pi k i n} \right\}.$$
(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
$$\epsilon = \zeta \pm \frac{1}{2}\mu H$$
, we obtain

$$\begin{split} & U_1 = \int_{-1/2}^{\infty} dn \,\varphi(n) \\ &= \Theta \int_{-1/2}^{\infty} dn \int_{-\infty}^{\infty} dp_z \ln \{1 + e^{(\varepsilon - E_n)/\Theta}\} \\ &= \Theta \int_{0}^{\infty} dE \ln \left\{1 + e^{(\varepsilon - E_n)/\Theta}\right\} \int_{S>0} dp_z \left(\frac{\partial n}{\partial E}\right), \end{split}$$

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

The relation between E and n is given by the expression (1.5), and hence

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

$$J_1 = \frac{\Theta c}{2\pi e\hbar H} \int_0^\infty dE \tag{2.5}$$

×
$$\ln \{1 + e^{(z-E)/\Theta}\} \int_{S>0} dp_z \left(\frac{\partial S}{\partial E}\right)$$

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

$$J_{1} = \frac{\Theta c}{2\pi e \hbar H} \int_{0}^{\infty} dE \qquad (2.6)$$

$$\times \ln \{1 + e^{(\varepsilon - E)/\Theta}\} \frac{d}{dE} \int_{S>0} dp_{z} S(E, p_{z})$$

$$= \frac{c}{2\pi e \hbar H} \int_{0}^{\infty} \frac{dE}{e^{(E - \varepsilon)/\Theta} + 1} \int_{S>0} S(E, p_{z}) dp_{z}$$

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

$$W(\varepsilon) = \int_{0}^{\infty} \frac{U(E) dE}{e^{(E-\varepsilon)/\Theta} + 1},$$

we obtain

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

Making use of the fact that $\mu_0 H \ll \zeta$, we can expand $W(\epsilon)$ in powers of $\mu_0 H$, stopping with the second-order terms. If we insert this expansion

 $^{^5}$ Courant and Hilbert, "Methods of Mathematical Physics", v. I.

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

$$\Omega_{1} = -\frac{V}{8\pi^{3}\hbar^{3}} \Big[2W(\zeta) + \left(\frac{\mu_{0}H}{\chi^{2}}\right)^{2} \frac{d^{2}W(\zeta)}{d\zeta^{2}} \Big].$$
(2.8)

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

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

The expression (2.9) has a simple physical interpretation. Under the condition $\mathfrak{S} \ll \zeta$, which we shall consider always to be fulfilled, one can set

$$W(\zeta) \approx \int_{0}^{\zeta} U(E) \, dE$$

which implies

$$rac{d^2 W(\zeta)}{d\zeta^2} pprox rac{dU(\zeta)}{d\zeta}.$$

The product

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

gives the number of states per unit energy interval at the Fermi boundary energy; (2.9) may therefore be written in the form

$$M_{1z} = \frac{1}{2} \,\mu_0 \rho \left(\zeta\right) \,\mu_0 H. \tag{2.11}$$

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:

$$J(k) = \int_{-1/s}^{\infty} dn \,\varphi(n) \, e^{2\pi k i n}$$

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

Integration by parts leads to the expression

$$J(k) = \frac{c}{2\pi e\hbar H} \int_{0}^{\infty} dE f\left(\frac{E-\varepsilon}{\Theta}\right) \times \int_{0}^{E} dE' \int_{S>0} dp_{z} \frac{\partial S(E',p_{z})}{\partial E'} \times \exp\left\{i \frac{kc}{e\hbar H} S(E', p_{z}) - 2\pi ki\gamma\right\};$$

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

In computing the inner double integral in (2.12) we make use of the fact that under the assumption of very large numbers $(c/2\pi e\hbar H)S = n + \gamma$. This permits the use of the method of stationary points for the asymptotic evaluation of the integral. It is found that the major contribution to J(k) comes. first, from integration in the vicinity of the peaks in the extremum point of S (E', p_z), for E' = E - i.e., the point at which $\partial S(E, p_z) / \partial p_z = 0$ - and second, from integration in the vicinity of the region of integration: E' = E, $S(E, p_z) = 0$. As regards the integration about the stationary point, this yields the oscillating part of J(k) (cf. Appendix), corresponding to the oscillating part of the magnetic moment. Integration about the peak 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 $S(E, p_{z}) = 0$, however, corresponds to small values of the quantum number n [cf. Eq. (1.5)], for which the energy levels calculated in the quasi-classical approximation (Section 1) are, generally speaking, incorrect. Therefore the nonperiodic part of J(k), an expression for which is given in the Appendix, can give the correct figure for the diamagnetism of the electron gas only in the special case for which the guasi-classical energy levels coincide with the true levels for all n (for instance, in the case of a quadratic dispersion law).

The first term in the asymptotic expansion of the inner double integral about the stationary point leads to the following expression for J(k):

$$J(k) = \frac{1}{V2\pi} \left(\frac{e\hbar H}{c}\right)^{1/2} \frac{1}{k^{3/2}}$$

$$\times \exp\left\{-2\pi k i \gamma \mp i \frac{\pi}{4} - i \frac{\pi}{2}\right\}$$

$$\times \int_{0}^{\infty} dE f\left(\frac{E-\varepsilon}{\Theta}\right) \left|\frac{\partial^{2}S\left(E, p_{z}\right)}{\partial p_{z}^{2}}\right|_{m}^{-1/2}$$

$$\times \exp\left\{i \frac{kc}{e\hbar H} S_{m}(E)\right\}.$$

We have represented by $S_m(E)$ the extremal value of $S(E, p_z)$ for constant E. If $S_m(E)$ represents a maximum for the intercepted area, then the phase $i\pi/4$ takes the minus sign in (2.13), while if $S_m(E)$ is a minimum area, the phase $i\pi/4$ takes the plus sign. The derivative $(\partial^2 \underline{S}/\partial p_z^2)_m$ is taken at the extremal point.

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

$$\int_{0}^{\infty} dE f\left(\frac{E-\varepsilon}{\Theta}\right) \left| \frac{\partial^{2}S}{\partial p_{z}^{2}} \right|_{m}^{-1/s} \exp\left\{ i \frac{kc}{e\hbar H} S_{m}(E) \right\}$$
$$\approx \frac{e\hbar H}{kc} \Psi(k\lambda) \frac{\exp\left\{ -i \frac{\pi}{2} + i \frac{kc}{e\hbar H} S_{m}(\varepsilon) \right\}}{\left| \frac{\partial^{2}S}{\partial p_{z}^{2}} \right|_{m}^{1/s} dS_{m}(\varepsilon) / d\varepsilon}, (2.14)$$

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

Inserting the expression (2.14) into (2.13), we obtain:

$$J(k) = -\frac{1}{\sqrt{2\pi}} \left(\frac{e\hbar H}{c}\right)^{s/s}$$

$$\chi \frac{1}{k^{s/s}} \frac{\Psi(k\lambda) \exp\left\{i \frac{kc}{e\hbar H} S_m(\varepsilon) \mp i \frac{\pi}{4} - 2\pi ki\gamma\right\}}{\left|\partial^2 S(\varepsilon, p_2) / \partial p_2^2\right|_m^{1/s} dS_m(\varepsilon) / d\varepsilon}.$$
(2.15)

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

$$2\operatorname{Re}\sum_{k=1}^{\infty} J(k) \qquad (2.16)$$

$$= -\frac{2}{V2\pi} \left(\frac{e\hbar H}{c}\right)^{*/*} \left| \frac{\partial^2 S(\varepsilon, p_2)}{\partial p_2^2} \right|_m^{-1/*} \left(\frac{dS_m(\varepsilon)}{d\varepsilon}\right)^{-1}$$

$$\times \sum_{k=1}^{\infty} \frac{1}{k^{*/*}} \Psi(k\lambda) \cos\left[\frac{kc}{e\hbar H} S_m(\varepsilon) \mp \frac{\pi}{4} - 2\pi k\gamma\right].$$

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 $S_m(\epsilon)$ 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 as the final expression for the oscillating part of the thermodynamic potential Ω , corresponding to the second term in the curly brackets of (2.3):

$$\Omega_{2} = \frac{V}{\pi^{2} V 2\pi \hbar^{3}} \left(\frac{e\hbar H}{c}\right)^{s/_{2}} \left|\frac{\partial^{2}S}{\partial p_{z}^{2}}\right|_{m}^{-1/_{4}} \left(\frac{dS_{m}}{d\zeta}\right)^{-1} \qquad (2.17)$$

$$\times \sum_{k=1}^{\infty} \frac{\Psi(k\lambda)}{k^{s/_{2}}} \cos\left[\frac{kc}{e\hbar H} S_{m}(\zeta) \mp \frac{\pi}{4} - 2\pi k\gamma\right]$$

$$\times \cos\left[\frac{k}{2m_{0}} \frac{dS_{m}(\zeta)}{d\zeta}\right].$$

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 upon H. We have, therefore, for the component of the moment in the direction of the magnetic field*:

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

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

$$\Omega = -\frac{V}{4\pi^3\hbar^3} W(\varepsilon) - V \frac{1}{2} (\chi_1 + \chi_2) H^2 \quad (2.19)$$

^{*} Throughout what follows, the values given are those of the component M_z of the momentum in the direction of 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).

$$+ \frac{V}{\pi^{2} \sqrt{2\pi} \hbar^{3}} \left(\frac{e\hbar H}{c}\right)^{*/2} \left|\frac{\partial^{2}S}{\partial p_{z}^{2}}\right|_{m}^{-1/2} \left(\frac{dS_{m}}{d\zeta}\right)^{-1} \\ \times \sum_{k=1}^{\infty} \frac{\Psi(k\lambda)}{k^{*/2}} \cos\left[\frac{kc}{e\hbar H} S_{m}(\zeta)\right] \\ \mp \frac{\pi}{4} - 2\pi k\gamma \cos\left[\frac{k}{2m_{0}} \frac{dS_{m}(\zeta)}{d\zeta}\right];$$

$$M = V(\chi_{1} + \chi_{2}) H$$

$$(2.20)$$

$$\frac{4 V}{\hbar^{3} (2\pi)^{s/s}} \left(\frac{e\hbar}{c}\right)^{s/s} \frac{S_{m}(\zeta) V\overline{H}}{\left|\partial^{2} S(\zeta, p_{z}) / \partial p_{z}^{2}\right|_{m}^{1/s} dS_{m}(\zeta) / d\zeta}$$

$$\times \sum_{k=1}^{\infty} \frac{\Psi(k\lambda)}{k^{s/s}} \sin\left[\frac{kc}{e\hbar H} S_{m}(\zeta) - \frac{k}{d\zeta}\right]$$

$$= \frac{\pi}{4} - 2\pi k\gamma \cos\left[\frac{k}{2m_{0}} \frac{dS_{m}(\zeta)}{d\zeta}\right]$$

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 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.

3. ANALYSIS OF RESULTS

From the formula for the magnetic moment (2.20) it can be seen that the amplitude and period of the oscillations in the magnetic moment are fully determined by the extremal value of the area on the Fermi boundary surface intercepted by the plane

 $P \times H = \text{const.}$, and by the derivatives of the area intercepted on the Fermi surface at the extremal point.

For a quadratic dispersion law

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

we have

$$S(E, p_z) = 2\pi m (E - (p_z^2 / 2m));$$

$$S_m(E) = 2\pi mE, \ dS_m(E) / dE = 2\pi m,$$

$$|\partial^2 S / \partial p_z^2| = 2\pi; \ \gamma = 1/2.$$

In this case the expression (2.20) goes over into the usual formula for the magnetic moment of a gas of free electrons².

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

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

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

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

where

$$A(H, \zeta) = \frac{4 V}{\hbar^3 (2\pi)^{*/*}} \left(\frac{e\hbar}{c}\right)^{1/*}$$

$$\times \frac{\Theta S_m(\zeta) e^{-\lambda}}{\left| \partial^2 S(\zeta, p_z) / \partial p_z^2 \right|_m^{1/2} \sqrt{H}} \cos \left[\frac{1}{2m_0} \frac{dS_m(\zeta)}{d\zeta} \right].$$

Since we used the thermodynamic potential Ω in calculating the magnetic moment, ζ and II must in consequence be regarded as independent variables. In actual applications of Eqs. (2.20), (3.2), and (3.3), however, one must take into consideration the dependence of ζ upon II, determined by the constancy of the number of particles N:

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

This dependence is, however, sufficiently weak that it may be neglected. It is easy to convince oneself of this by evaluating the part of ζ which depends upon the magnetic field. The expression 642

for $\Omega(\zeta, H)$ is given by formula (2.19); in differentiating this with respect to ζ we retain, as before, only the first few terms in the expansion in powers of H. Then

$$N = \frac{V}{4\pi^{*}\hbar^{3}} \frac{dW(\zeta)}{d\zeta}$$
(3.4)

$$-\frac{V}{2\pi^{\circ}\hbar^{\circ}} \left(\frac{e\hbar H}{c}\right)^{*/*} \frac{V 2\pi}{\left|\partial^{2}S\left(\zeta, p_{z}\right)\partial^{2}p_{z}\right|_{m}^{1/*}} \\ \times \sum_{k=1}^{\infty} \frac{1}{k^{*/*}} \Psi\left(k\lambda\right) \sin\left[\frac{kc}{e\hbar H} S_{m}\left(\zeta\right)\right. \\ \left. \left. \left. \left. + \frac{\pi}{4} - 2\pi k\gamma\right] \cos\left[\frac{k}{2m_{0}} \frac{dS_{m}\left(\zeta\right)}{d\zeta}\right] \right] \right\}$$

Under the assumptions we have made $(\Theta \ll \zeta)$, $dW(\zeta)/d\zeta = U(\zeta)$; this is the volume in 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

$$U(\zeta_{0}) = U(\zeta)$$

$$-\left(\frac{e\hbar H}{c}\right)^{*/*} \frac{2V\overline{2\pi} G(\zeta, H)}{\left|\partial^{2}S(\zeta, p_{z}) / \partial p_{z}^{2}\right|_{m}^{1/*}}$$
(3.5)

where ζ_0 is the chemical potential at H = 0.

Assuming a small increment to ζ dependent upon the magnetic field H, we may set

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

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

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

whence it follows that

$$\xi (H)$$

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

Inasmuch as the summation $G(\zeta, H)$ appearing in (3.6) is of the order of unity, while $|\partial^2 S / \partial p_z^2|_m^{\chi}$ is a

nondimensional quantity representing the anisotropy of the Fermi boundary surface (for the case of a spherical surface it is equal to $\sqrt{2\pi}$), the quantity ξ (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 = const. This permits setting, in order of magnitude

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

and we can write

$$\varepsilon(H)$$

$$\sim \left(\frac{e\hbar H}{c}\right)^{s/s} / \zeta_0 \frac{dU(\zeta_0)}{d\zeta_0} \sim \left(\frac{e\hbar H}{\zeta_0 c} / \frac{dS(\zeta_0)}{d\zeta_0}\right)^{s/s}.$$

$$(3.7)$$

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

$$\Delta E = \frac{2\pi e\hbar H}{c} \left(\frac{dS\left(\zeta_{0}\right)}{d\zeta_{0}} \right)$$

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 evaluation of ξ (*H*):

$$\xi(H) \sim (\Delta E / \zeta_0)^{*/_2} \ll 1. \tag{3.8}$$

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

$$\xi(H) = \left(\frac{e\hbar H}{mc\zeta_0}\right)^{*/_2} \frac{G(\zeta_0, H)}{2\pi \sqrt{2}}$$
$$\sim \left(\frac{e\hbar H}{mc\zeta_0}\right)^{*/_2} = \left(\frac{\mu H}{\zeta_0}\right)^{*/_2} \ll 1.$$

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

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

μ

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

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

It follows from (3.8) and (3.9) that ζ may be

replaced by ζ_0 in Eqs. (2.19) and (2.20), as well as in (3.2) and (3.3), and the period of the oscillations may be represented in the form

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e\hbar}{cS_m(\zeta_0)} \qquad (3.11)$$

In the event that 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 — 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 distributed about the lower part of the unfilled zone, we may content ourselves with the representation

$${}_{O}^{O}(P_{x}, P_{y}, P_{z}) = \varepsilon_{0} + \left(\frac{P_{x}^{2}}{2m_{1}} + \frac{P_{y}^{2}}{2m_{2}} + \frac{P_{z}^{2}}{2m_{3}}\right)$$

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. This yields for the corresponding factor $\partial S_m / \partial E = 2\pi m$ and period

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

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

$${}_{C}^{O}(P_{x}, P_{y}, P_{z}) = \varepsilon_{0}' - \left(\frac{P_{x}^{2}}{2m_{1}} + \frac{P_{y}^{2}}{2m_{2}} + \frac{P_{z}^{2}}{2m_{3}}\right),$$

which yields

$$\partial S_m / \partial E = -2\pi m \text{ and } \Delta\left(\frac{1}{H}\right) = \frac{\mu^*}{\varepsilon_0' - \zeta}$$

* = $e\hbar / m^*c$,

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

In the presence of strong mass anisotropy even a slightly mosaic structure leads to obscuration or complete obliteration of the oscillations in the event that the number of electrons in the corresponding zone is large. This obscuration of the phase of the oscillatory term may 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 $\Delta \vartheta \gg 1$ 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''), even in this case there is no foundation for assuming a quadratic dispersion law.

Thus, the occurrence of the experimentally observable De Haas-Van Alphen 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 connected with interactions 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 careful experimental measurement of the period of the oscillations in the magnetic moment $\Delta(1/H)$, as well as of the amplitude of the oscillations and the temperature dependence, would permit the reconstruction of the form of the Fermi boundary surface, and would also permit the determination of the velocity of the electrons upon this surface – i.e., the problem may be solved in an inverse sense, so to speak, to that in which we have solved it. The feasibility of this procedure is a consequence of the fact that the period of the 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 the oscillations and the temperature dependence determine $dS_m(\zeta)/d\zeta$ and $|\partial^2 S(\zeta, p_z)/\partial_p^2|_m$. As has been demonstrated in a paper by Lifshitz and Pogorelov⁶, a 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 formula⁶

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

We have introduced here the representation

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

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 through the center normal to a given unit vector \mathbf{n} , $\partial(z)$ is the delta-function, and $d\Omega_{\underline{n}}$ 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 may readily determine the velocity of the electrons on the boundary surface.

For the magnetic fields under which the measurements of the De Haas-Van Alphen effect have been conducted ($H \sim 10^4$ gauss) the periods observed experimentally for the oscillations are determined, as we have pointed out, by those zones having an anomalously small number of electrons; for this reason the method described above can be used to reconstruct the Fermi boundary surface for these zones alone. 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 shall evaluate the integral

$$I = \iint dE' dp_z \frac{\partial S(E', p_z)}{\partial E'}$$

$$\times \exp\left\{i \frac{kc}{e\hbar H} S(E', p_z) - 2\pi k\gamma i\right\}$$

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 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 about the peaks of the region of integration⁷.

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

$$I_{1} = \frac{\partial S(E, p_{m})}{\partial E} \exp\left\{i\frac{kc}{e\hbar H}S(E, p_{m}) - 2\pi ki\gamma\right\}$$
$$\times \int_{E=0}^{E} dE \int_{P_{m}=0}^{P_{m}+0} dp_{z} \exp\left\{i\frac{kc}{e\hbar H}\left[(E'-E)\frac{\partial S}{\partial E} + \frac{1}{2}(p_{z}-p_{m})^{2}\frac{\partial^{2}S}{\partial p_{z}^{2}}\right\}$$

After further computation we obtain

$$I_{1} \sim \left(\frac{e\hbar H}{kc}\right)^{3/2} \frac{V 2\pi}{\left|\partial^{2}S / \partial p_{z}^{2}\right|_{m}^{1/2}} \exp\left\{i\frac{kc}{e\hbar H}S(E, p_{m})\right.$$
$$\left.-2\pi ki\gamma - i\frac{\pi}{2} \mp i\frac{\pi}{4}\right\}$$

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 following asymptotic formula:

$$\int_{x_0} f(x) \exp\left\{\pm i W(x-x_0)\right\} dx$$

$$\sim f_n \frac{\Gamma(n+1)}{W^{n+1}} \exp\left\{\pm i \frac{n+1}{2}\pi\right\}$$
 (W>>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 it is inserted into equation (2.12), setting $S_m(E) = S(E, p_m)$, the latter will yield (2.13).

2) Designating by $\pm p_0$ the values of p_z corresponding to the peaks in the region of integration, we investigate the integral in the

⁶ I. Lifshitz, and A. Pogorelov, Dokl. Akad. Nauk SSSR **96**, 1143 (1954).

⁷ J. Corput. Proc. Acad. Sci. (Amsterdam) **51**, 650 (1948).

vicinity of one of the peaks

$$I_{2} \approx \frac{\partial S(E, p_{0})}{\partial E} e^{-2\pi k i \gamma} \int_{p_{0} \to 0}^{p_{0}} dp_{z} \int_{0}^{E} dE'$$

$$\times \exp\left\{i \frac{kc}{e\hbar H} \left[(p_{z} - p_{0}) \frac{\partial S}{\partial p_{0}} + (E' - E) \frac{\partial S}{\partial E}\right]\right\}$$

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

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

With substitution of variables we have

$$I_2 \sim \left(\frac{e\hbar H}{kc}\right)^2 \frac{e^{-2\pi h i \gamma}}{\partial S(E, p_0)/dp_0} \int_0^\infty dx e^{-ix} \int_0^\infty dy e^{-iy}$$

Computing the integral using 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 l.

Inserting l_2 into (2.12) we obtain the corresponding contribution to the real part of J(k):

$$\operatorname{Re}\left\{J\left(k\right)\right\} \sim \frac{e\hbar H}{c} \frac{\sin 2\pi k\gamma - \cos 2\pi k\gamma}{2\pi k^{2}} \int_{0}^{\infty} \frac{f\left(\frac{E-\varepsilon}{\Theta}\right) dE}{\partial S\left(E, p_{0}\right) / \partial p_{0}}.$$

Noting that the region of integration has two symmetrical peaks, 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:

$$\Omega = -V \frac{1}{\hbar^3} \left(\frac{e\hbar H}{c}\right)^2 \frac{1}{\pi^3} \sum_{k=1}^{\infty} \frac{\sin 2\pi k\gamma - \cos 2\pi k\gamma}{k^2}$$

$$\times \int_{0}^{\infty} \frac{f\left(\frac{E-\zeta}{\Theta}\right) dE}{\partial S\left(E, p_0\right) / \partial p_0}$$
(P.1)

$$M = V \frac{2}{\pi^3} \frac{e^2}{\hbar c^2} H \sum_{k=1}^{\infty} \frac{\sin 2\pi k\gamma - \cos 2\pi k\gamma}{k^2}$$
(P.2)

$$\times \int_0^{\infty} \frac{f\left(\frac{E-\zeta}{\Theta}\right) dE}{\partial S\left(E, p_0\right) / \partial p_0}$$

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

In the general case, however, our formulas for the constant part of the diamagnetic susceptibility may turn out to be incorrect, since it is impossible to use the quasi-classical 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 surface⁸, while the expressions (P.1) and (P.2) are determined by all of the electrons together.

3). One can readily convince oneself that integration about the point $E' = p_z = 0$ yields a 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.

Translated by S. D. Elliot 267

⁸ R. Peierls , Physik. **80**, 763 (1933); A. Wilson, *Quantum Theory of Metals*.