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# DENSITY ATTENUATION OF SURFACE MAGNETIC STATES

L. A. FAL'KOVSKIĬ

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences

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The attenuation and shift of the levels of electrons moving in a magnetic field and being reflected from the rough surface of a metal are related to the microscopic characteristics of the surface. The results describe an electron for which the component of the wavelength normal to the surface is large in comparison with the average roughness. An expression is obtained for the density of states.

## 1. INTRODUCTION

It is well known that Landau levels exist in a constant magnetic field H, the distance between these levels being determined by the frequency of revolution $\Omega = eH/mc$ of an electron in a cyclotron orbit. In a finite sample, together with the electrons moving in such orbits there are also electrons which collide with the surface. Under suitable conditions, for example, in a magnetic field parallel to the surface, upon specular reflection of the electrons from the surface their motion is periodic, and a new system of levels appears. Such quantization was first considered by I. Lifshitz and Kosevich.[1]

A trajectory of an electron undergoing collisions with the surface is shown in Fig. 1. The metal occupies the half-space $x > 0$, the magnetic field is parallel to the z axis, and the dotted line indicates the part of the orbit located outside of the metal. The period of motion along a trajectory lying inside the metal is given by

$$T=\frac{\varphi}{\Omega}=\frac{2}{\Omega}\operatorname{arc\,tg}\frac{v_x}{v_y},$$

where $v_x$ and $v_y$ denote the components of the electron's velocity after its reflection from the surface.

Expressing $v_x$ and $v_y$ in terms of the tangential components of the momentum, which are integrals of the motion, for small values of the ratio $v_x/v_y$ we obtain:

$$T = 2(2m\varepsilon - p^2)^{1/2}/\Omega p_y, \quad p^2 = p_y^2 + p_z^2.$$

In the quasiclassical case the period T determines the distance between neighboring quantum levels

$$\delta\varepsilon / \delta n = \pi\hbar\Omega p_y (2m\varepsilon - p^2)^{-1/2}.$$

The dependence itself of $\epsilon$ on n is obtained after integration:

$$\varepsilon=\left[\frac{3\pi\hbar\Omega p_y}{2\sqrt{2m}}\left(n-\frac{1}{4}\right)\right]^{2/3}+\frac{p^2}{2m}, \qquad (1.1)$$
$$n = 1,2,\ldots, \quad 0 < p_y / (2m\varepsilon - p_z^2)^{1/2} \ll 1.$$

Experimentally the existence of the levels (1.1) appears in oscillations of the surface impedance, which were first observed by Khaĭkin.[2] The origin of these oscillations was explained by Nee and Prange.[3] The oscillations arise as a result of transitions of an electron between levels with different values of n. The basic condition for the existence of surface levels is the specular nature of the surface. A real surface, of course, does not satisfy this condition. As a consequence of the roughnesses, after a collision an electron crosses into another cyclotron orbit, which leads to a broadening and a shift of the levels. This question was discussed qualitatively in articles[4,5].

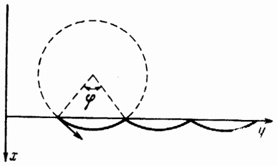

Fig. 1. Electron orbit.

In the present article it is shown that in certain cases a relatively simple theory can be constructed, making it possible to relate the width and shift of the levels to certain characteristics of the surface. An expression is also obtained for the density of the levels.

## 2. BOUNDARY CONDITION. DENSITY MATRIX

Let the equation of the surface have the form $x = \xi(\mathbf{s})$ where s is the point with coordinates y and z. We shall regard $\xi(\mathbf{s})$ as a random quantity and average observable quantities over an ensemble of the functions $\xi$. In this connection the average value of any observable quantity can be expressed in terms of the average of a certain number of products of the functions $\xi$.

The average value $\langle\xi(\mathbf{s})\rangle$, and also the average of the product of an arbitrary odd number of functions $\xi$ can be regarded as equal to zero since the result of averaging should not change upon changing the sign of $\xi$. In virtue of the uniformity of the surface the binary correlation function should only depend on the difference of coordinates:

$$\langle\xi(\mathbf{s})\xi(\mathbf{s}_1)\rangle = \xi_2(\mathbf{s}-\mathbf{s}_1). \qquad (2.1)$$

We require the Fourier components

$$\xi(\mathbf{p}) = \int d^2s\, \xi(\mathbf{s})\, e^{i\mathbf{p}\mathbf{s}},$$

where **p** is a two-dimensional vector with components $p_y$ and $p_z$. Let us rewrite Eq. (2.1) in terms of Fourier components:

$$\langle\xi(\mathbf{p})\xi(\mathbf{p}_1)\rangle = \xi_2(\mathbf{p})\,(2\pi)^2\delta(\mathbf{p}+\mathbf{p}_1). \qquad (2.2)$$

We require that the single-particle wave function on the true surface should satisfy the following boundary condition:

$$\psi(x\mathbf{s})\,|_{x=\xi(\mathbf{s})}=0. \tag{2.3}$$

We shall assume the characteristic period of variation of $\psi$ with respect to the variable x to be large in comparison with the average magnitude a of a roughness:

$$\alpha\equiv a(2m\varepsilon-p^2)^{1/2}/\hbar\ll 1 \tag{2.4}$$

and we expand condition (2.3) in powers of $\xi$:

$$\psi(0\mathbf{s})+\xi(\mathbf{s})\,\partial\psi(0\mathbf{s})/\partial x=0. \tag{2.5}$$

In the approximation under consideration the attenuation and shift of the levels are proportional to $\xi_2(\mathbf{p})$, i.e., quadratic in $\xi$, as will be shown below. The latter means that in condition (2.5) it is necessary to keep the term of second order in $\xi$. However, one can show that it leads to a quantity of the next order of smallness in $\alpha$. Condition (2.4) will be regarded as satisfied everywhere in this article. The opposite limiting case may be treated by the method of geometrical optics.

The boundary condition (2.5) helps to explain the meaning of the function $\xi_2(\mathbf{p})$. For this purpose let us consider a free electron gas in the absence of fields and expand $\psi(x\mathbf{s})$ in eigenfunctions corresponding to a given energy $\epsilon$:

$$\begin{aligned}\psi(x\mathbf{s})&=\int\frac{d^3p}{(2\pi)^2}\psi(p_x\mathbf{p})\,\delta\left(\varepsilon-\frac{p_x^2+p^2}{2m}\right)\exp(ip_xx+i\mathbf{ps})\\&=\int\frac{d^2p}{(2\pi)^2|v_x|}\,[\psi(p_x\mathbf{p})e^{ip_xx}+\psi(-p_x\mathbf{p})e^{-ip_xx}]\,e^{i\mathbf{ps}},\end{aligned} \tag{2.6}$$

where $p_x = (2m\epsilon - p^2)^{1/2}$. The boundary condition (2.5) gives

$$\psi(p_x\mathbf{p})+\psi(-p_x\mathbf{p})=-ip_x\int\frac{d^2q}{(2\pi)^2}\xi(\mathbf{p}-\mathbf{q})\,[\psi(q_x\mathbf{q})-\psi(-q_x\mathbf{q})]. \tag{2.7}$$

Let us consider the solution corresponding to a given value for the amplitude of the incident wave $\psi(-p_x\mathbf{p})$. To within quadratic terms in $\xi$ we find

$$\begin{aligned}\psi(p_x\mathbf{p})&=-\psi(-p_x\mathbf{p})+2ip_x\int\frac{d^2q}{(2\pi)^2}\xi(\mathbf{p}-\mathbf{q})\psi(-q_x\mathbf{q})\\&\quad-2p_x\int\frac{d^2q\,d^2q'}{(2\pi)^4}q_x\xi(\mathbf{p}-\mathbf{q})\xi(\mathbf{q}-\mathbf{q}')\psi(-q_x\mathbf{q}).\end{aligned} \tag{2.8}$$

Now let us construct the density matrix in the described representation:

$$\rho(\mathbf{pp}')=\langle\psi^*(p_x\mathbf{p})\psi(p_x'\mathbf{p}')\rangle. \tag{2.9}$$

Setting up the bilinear combination of the functions (2.8) and averaging, we find

$$\begin{aligned}\rho(\mathbf{pp}')&=(2\pi)^2\delta(\mathbf{p}-\mathbf{p}')\,\langle|\psi(p_x\mathbf{p})|^2\rangle,\\ \langle|\psi(p_x\mathbf{p})|^2\rangle&=|\psi(-p_x\mathbf{p})|^2\left[1-p_x\int\frac{d^2q}{\pi^2}q_x\xi_2(\mathbf{p}-\mathbf{q})\right]\\&\quad+p_x^2\int\frac{d^2q}{\pi^2}\xi_2(\mathbf{p}-\mathbf{q})\,|\psi(-q_x\mathbf{q})|^2.\end{aligned} \tag{2.10}$$

The diagonal matrix elements of the density matrix determine the probability density in the reflected wave averaged over the roughnesses. One can uniquely relate this quantity to the distribution function which appears in classical kinetic theory. Therefore, with the aid of (2.10) one obtains the boundary condition which the distribution function f(p) must satisfy:

$$\begin{aligned}f(p_x\mathbf{p})&=f(-p_x\mathbf{p})\left[1-p_x\int\frac{d^2q}{\pi^2}\xi_2(\mathbf{p}-\mathbf{q})q_x\right]\\&\quad+p_x\int\frac{d^2q}{\pi^2}\xi_2(\mathbf{p}-\mathbf{q})q_xf(-q_x\mathbf{q});\qquad q_x=\sqrt{2m\varepsilon-q^2}.\end{aligned} \tag{2.11}$$

Here the difference in the normalization of f(p) and $\psi(p_x\mathbf{p})$ has been taken into account. The condition (2.11) automatically guarantees that the flow of particles through the "reduced" surface x = 0 is equal to zero. It differs substantially from the phenomenological boundary condition which is usually required in the kinetic theory of metals.

## 3. DENSITY OF STATES

As is well known, the density of states is determined by the Green's function $G(\mathbf{r}, \mathbf{r}'; \epsilon)$:

$$\frac{dz}{d\varepsilon}=-\frac{1}{\pi}\int d^3r\,\mathrm{Im}\,\langle G(\mathbf{r},\mathbf{r};\varepsilon)\rangle. \tag{3.1}$$

Here it exists in the form of a retarded Green's function, which corresponds to the addition to the energy variable (which we shall not write down in what follows) of an infinitesimal correction with a positive imaginary part. The angular brackets denote averaging over the roughnesses. The Green's function satisfies the well-known equation

$$(\hat{H}(\mathbf{r})-\varepsilon)G(\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}') \tag{3.2}$$

and the boundary condition (2.5):

$$G(0\mathbf{s},x'\mathbf{s}')+\xi(\mathbf{s})\frac{\partial}{\partial x}G(0\mathbf{s},x'\mathbf{s}')=0. \tag{3.3}$$

Let us expand the function G in a Fourier integral with respect to the variables s and s′:

$$G(x\mathbf{s},x'\mathbf{s}')=\int\frac{d^2p\,d^2p'}{(2\pi)^4}G(x\mathbf{p},x'\mathbf{p}')\exp\{i(\mathbf{ps}-\mathbf{p}'\mathbf{s}')\}. \tag{3.4}$$

Later on we will need the function $G_\infty(\mathbf{r}, \mathbf{r}')$ which satisfies Eq. (3.2) over all space. In order to calculate $G_\infty(\mathbf{r}, \mathbf{r}')$ we extend the definition of the Hamiltonian $\hat{H}(\mathbf{r})$ to the region x < 0, having chosen it in the same manner as if no surface were present. Since in this case the conditions of the problem are homogeneous in the variables s and s′, one can find a representation in which the dependence of $G_\infty$ on s and s′ is determined by only the difference s − s′. Then

$$G_\infty(x\mathbf{s},x'\mathbf{s}')=\int\frac{d^2p}{(2\pi)^2}G_\infty(xx',\mathbf{p})\exp\{i\mathbf{p}(\mathbf{s}-\mathbf{s}')\}.$$

The function $G_\infty(xx', \mathbf{p})$ satisfies the one-dimensional equation which is obtained from Eq. (3.2):

$$\left\{\frac{1}{2m}\left[\hat{p}_x^2+\left(p_y-\frac{eHx}{c}\right)^2+p_z^2\right]-\varepsilon\right\}G_\infty(xx',\mathbf{p})=-\delta(x-x'); \tag{3.5}$$

the vector-potential of the uniform field is chosen in the form A = {0, Hx, 0}. Here a term which depends on the spin has been omitted. Taking it into account reduces to the replacement $\epsilon \to \epsilon \pm \mu H$ and to a summation over the two spin states in all final formulas.

One can write down the Green's function $G_\infty(xx', \mathbf{p})$ in the form of a series in eigenfunctions of the corresponding homogeneous equation, which are the Hermite functions $\psi_n(x - p_yc/eH)$:

$$G_\infty(xx',\mathbf{p})=\sum_{n=1}^{\infty}\frac{1}{\varepsilon-\varepsilon_n}\psi_n\left(x-\frac{p_yc}{eH}\right)\psi_n\left(x'-\frac{p_yc}{eH}\right), \tag{3.6}$$

$$\varepsilon_n=\hbar\Omega(n-{}^1\!/_2)+p_z^2/2m,\quad n=1,2,\ldots \tag{3.7}$$

The function $G_\infty(xx', \mathbf{p})$ may be represented in a different form which is more convenient for calculations.

As is well known, the solution of an inhomogeneous equation with a δ-shaped right hand side can be sought in the form of a bilinear combination of two linearly independent solutions of the homogeneous equation, for which we choose the parabolic cylinder functions $D_{l-1/2}(\zeta)$ and $D_{l-1/2}(\zeta)$, where

$$l=\left(\varepsilon-\frac{p_z^2}{2m}\right)\frac{1}{\hbar\Omega},\quad \zeta=\left(x-\frac{cp_y}{eH}\right)\frac{1}{x_0},\quad x_0=\left(\frac{c\hbar}{2eH}\right)^{1/2}. \tag{3.8}$$

The function $D_{l-1/2}(\zeta)\rightarrow 0$ as $\zeta\rightarrow+\infty$. Then we obtain

$$G_\infty(xx',\mathrm{p})=-\frac{\Gamma(-l-1/2)}{\sqrt{2\pi}}\begin{cases}D_{l-1/2}(\zeta)D_{l-1/2}(-\zeta'), & x>x'\\ D_{l-1/2}(\zeta')D_{l-1/2}(-\zeta), & x'>x\end{cases}. \tag{3.9}$$

The gamma function $\Gamma(-l-1/2)$ arises upon joining the solutions together at the point $x = x'$. Its tending to infinity corresponds to the volume Landau levels given by Eq. (3.7).

In the next section we proceed to solve Eqs. (3.2) and (3.3), but here we present the almost obvious solution for $G(\mathrm{xp}, \mathrm{x'p'})$ in the case of specular reflection ($\xi = 0$):

$$G_0(x\mathrm{p},x'\mathrm{p}')=(2\pi)^2\delta(\mathrm{p}-\mathrm{p}')\left[G_\infty(xx',\mathrm{p})-\frac{G_\infty(x0,\mathrm{p})G_\infty(0x',\mathrm{p})}{G_\infty(00,\mathrm{p})}\right]. \tag{3.10}$$

Expression (3.10) satisfies Eq. (3.2) and vanishes for $x, x' = 0$. The poles of the second term in (3.10), which determine the surface levels, are the zeros of the function $G_\infty(00, \mathrm{p})$. This circumstance can be easily understood with the aid of Eq. (3.9) if it is taken into account that the eigenfunctions of Eq. (3.5), without anything on the right hand side, must vanish on the surface.

Formula (3.10) enables us to obtain the density of states associated with specular reflection ($\xi = 0$). For this purpose it is necessary to substitute (3.10) and (3.6) into (3.1) and integrate over the half-space $x > 0$. Since the integrand does not depend on the coordinate s, the integration over s gives the area of the surface, S. After integration over $p_y$ (with the aid of the orthogonality relations) the first term in (3.10) turns out to not depend on x and one obtains, on the whole a factor proportional to the volume. The integration of the second term in (3.10) is carried out by using the evenness property of the Hermite functions, as a consequence of which $G_\infty(xx', \mathrm{p}) = G_\infty(-x, -x', -\mathrm{p})$. One can therefore extend the integration over $x > 0$ to an integration over the entire axis, but then again use the orthogonality of the Hermite functions. Thus we obtain

$$\frac{dz}{d\varepsilon}=\frac{eHV}{c}\sum_{n=1}^{\infty}\int\frac{dp_z}{(2\pi\hbar)^2}\delta(\varepsilon-\varepsilon_n)-\frac{S}{2\pi}\int\frac{d^2p}{(2\pi\hbar)^2}\,\mathrm{Im}\frac{\partial}{\partial\varepsilon}\ln G_\infty(00,\mathrm{p}). \tag{3.11}$$

The first term leads to the well-known expression for the density of the Landau levels:

$$\frac{dz^{(V)}}{d\varepsilon}=\frac{VeHm^{1/2}}{2^{3/2}\pi^2\hbar^2c}\sum_{n=1}^{\infty}\left[\varepsilon-\hbar\Omega\left(n-\frac{1}{2}\right)\right]^{-1/2}.$$

The poles and zeros of the function $G_\infty(00, \mathrm{p})$ introduce a contribution to the second term in Eq. (3.11). We denote the values of $\epsilon$ for which $G_\infty(00, \mathrm{p})$ has poles and zeros by $\epsilon_n^{(V)}(\mathrm{p})$ and $\epsilon_n^{(S)}(\mathrm{p})$, respectively.

The regular part of the logarithmic derivative does not give any contribution since the Green's function (3.9) is real (in spite of the complex nature of the asymptotic expression (3.15)) for real values of its arguments. One obtains

$$\frac{dz}{d\varepsilon}=\frac{dz^{(V)}}{d\varepsilon}+S\sum_n\int\frac{d^2p}{(2\pi\hbar)^2}\left[\delta(\varepsilon-\varepsilon_n^{(S)})-\frac{1}{2}\delta(\varepsilon-\varepsilon_n^{(V)})\right] \tag{3.12}$$

which is essentially an expansion in powers of $V^{-1/3}$; the summation is carried out over all poles of $\Gamma(-l-1/2)$ and over the zeros of $D_{l-1/2}(\zeta)$.

One can easily find the position of the zeros by using the quasiclassical asymptotic expressions for $D_{l-1/2}(\zeta)$ which have been studied by Fok:[6]

$$D_{l-1/2}(\zeta)=\frac{C_l}{(t^2-1)^{1/4}}\exp\left\{-2l\int_1^t dt\sqrt{t^2-1}\right\},\quad t>1, \tag{3.13}$$

$$D_{l-1/2}(\zeta)=\frac{2C_l}{(1-t^2)^{1/4}}\cos\left(2l\int_1^t dt\sqrt{1-t^2}+\frac{\pi}{4}\right),\quad 1>t>-1. \tag{3.14}$$

$$D_{l-1/2}(\zeta)=\frac{C_l}{(t^2-1)^{1/4}}\left\{\exp\left[i\pi\left(l-\frac{1}{2}\right)-2l\int_1^{-t}dt\sqrt{t^2-1}\right]\right.$$
$$\left.-2\sin\pi\left(l-\frac{1}{2}\right)\exp\left[2l\int_1^{-t}dt\sqrt{t^2-1}\right]\right\},\quad t<-1, \tag{3.15}$$

where

$$C_l=2^{-1/2}\exp\left\{-\frac{l}{2}+\frac{1}{2}\left(l-\frac{1}{2}\right)\ln l\right\},\quad t=\frac{\zeta}{2\sqrt{l}}. \tag{3.16}$$

The condition for the validity of expressions (3.13)–(3.15) is

$$l|1-t^2|^{3/2}\gg|t|. \tag{3.17}$$

The cited asymptotic expressions pertain to the case $l > 0$ since the zeros of $D_{l-1/2}(\zeta)$ only lie in this region.

It is convenient to picture the position of the zeros in terms of the dependence of t on $l$ for a given number n, where

$$t=\frac{p_y}{(2m\varepsilon-p_z^2)^{1/2}},\quad l=\left(\varepsilon-\frac{p_z^2}{2m}\right)\frac{1}{\hbar\Omega}$$

(see Fig. 2). This dependence is determined by the equations

$$l[\arccos t-t(1-t^2)^{1/2}]=\pi(n-1/4),\ -1<t<1, \tag{3.18}$$

$$l=n-1/2+(2\pi)^{-1}\exp\{-2(n-1/2)[|t|(t^2-1)^{1/2}-\mathrm{Arch}\,t]\},\ t<-1. \tag{3.19}$$

If t is close to unity, then by expanding $\cos^{-1}t$ in powers of $(1-t^2)^{1/2}$ we arrive at Eq. (1.1).

Equations (3.18) and (3.19) have a simple physical meaning. If the electron does not collide with the surface, then $t < -1$ and the spectrum (3.19) to within an exponential term is simply the spectrum of the Landau levels (3.7). Let us begin to let the center of the orbit approach the surface. The condition when it first touches the surface is $t = -1$, and we arrive in the region described by relation (3.18). If $t > 0$ the center of the orbit

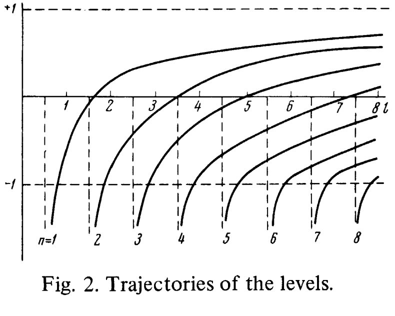

Fig. 2. Trajectories of the levels.

lies outside the surface of the metal, but for t > 1 the orbit does not have any sections lying inside the metal.

Now let us return to the density of states (3.12). The contribution of the zeros and poles to the density of the surface states depends on the region in which the appropriate integrand is being considered. For large negative values of t the zeros and poles merge together, essentially canceling each other. For $-1 < t < 1$ the contribution of a pole may be combined with the corresponding term in the density of Landau levels, its relative magnitude is of the order of $R/L_x$, where $R = (2\epsilon/m)^{1/2}/\Omega$ is the Larmor radius, and $L_x$ is the extent of the metal in the x direction.[2] Then, what remains in the n-th term in the expression for the density of surface levels after integration over $p_z$ with the utilization of Fig. 2, has the following form:

$$\left(\frac{dz}{d\varepsilon}\right)_n^{(S)} = \frac{mS}{(2\pi\hbar)^2}\left\{\theta\left(\delta_n - \frac{1}{4}\right)\right.$$
$$\times \int\limits_{n-1/4}^{\varepsilon/\hbar\Omega} \frac{dl}{(\varepsilon/\hbar\Omega - l)^{1/2}} \frac{|\pi(n - 1/4) + lt(1-t^2)^{1/2}|}{(1-t^2)\,l^{3/2}} + \frac{\theta(\delta_n)}{2\,[n-1/2]^{1/2}\,\delta_n^{1/2}}$$
$$\left.\times \int\limits_0^{\min\{\delta_n,\, 1/2\pi\}} dl\,(t^2-1)^{-1/2}(\delta_n - l)^{-1/2}(\sqrt{\delta_n} + \sqrt{\delta_n - l})^{-1}\right\}, \tag{3.20}$$

where the dependence t(*l*) in the first term is described by formula (3.18), and in the second term by (3.19); $\delta_n = \epsilon/\hbar\Omega - n + 1/2$.

The integral I appearing inside the curly brackets in (3.20) can be estimated in the following way ($a_i \sim 1$):

$$I = \frac{a_1\mathcal{R}}{\delta_n^{3/2}(n - 1/2)^{1/2}}, \qquad \mathcal{R} = \left[\frac{2(n-1/2)}{\ln(1/2\pi\delta_n)}\right]^{1/2} \ll 1, \tag{3.21}$$

$$I = \frac{a_2}{\delta_n^{3/2}(n-1/2)^{1/2}} + a_3\left(\frac{n}{\delta_n - 1/4}\right)^{1/6}, \quad 1 \lesssim \delta_n - 1/4 \ll n - 1/4, \tag{3.22}$$

$$I = \frac{a_2}{\delta_n^{3/2}(n-1/2)^{1/2}} + a_4\left[\frac{2\delta_n}{3\pi(n-1/4)}\right]^{1/3}, \quad \delta_n \gg n - 1/4. \tag{3.23}$$

The singularities of the density of surface states lie at $\delta_n = 0$, i.e., at those points which are also the singularities of the density of the volume states. The nature of these singularities is given by formulas (3.21)–(3.23).

For $\epsilon/\hbar\Omega \gg 1$ the last term in Eq. (3.23) carries the major contribution to the nonsingular part of the density of surface states. In this connection the number of terms in the sum (3.12) is large and, digressing from the singularities of the density of states, one can replace the summation by an integration. We obtain[7]

$$\left(\frac{dz}{d\varepsilon}\right)^{(S)} \sim \frac{Sm}{\hbar^2}\left(\frac{\hbar\Omega}{\varepsilon}\right)^{2/3}, \quad \frac{\varepsilon}{\hbar\Omega} \gg 1. \tag{3.24}$$

This quantity is inversely proportional to the magnetic field, and its ratio to the smooth part of the density of volume states is of the order of

$$\left(\frac{dz}{d\varepsilon}\right)^{(S)} \Big/ \left(\frac{dz}{d\varepsilon}\right)^{(V)} \sim \frac{\hbar}{L_x(2m\varepsilon)^{1/2}}\left(\frac{\varepsilon}{\hbar\Omega}\right)^{4/3}$$

## 4. ATTENUATION OF THE LEVELS

Let us calculate the Green's function satisfying Eq. (3.2) and the boundary condition (3.3). Just as is assumed for the solution of boundary value problems, we shall seek the solution in the form

$$G(\mathbf{r}, \mathbf{r}') = G_\infty(\mathbf{r}, \mathbf{r}') + \int ds'' G_\infty(\mathbf{r}, \mathbf{s}'')\,\mu(\mathbf{s}'', \mathbf{r}'), \tag{4.1}$$

where the unknown function $\mu(\mathbf{s}, \mathbf{r}')$, playing the role of the density of surface charges, must satisfy only condition (3.3) since the right hand side of Eq. (4.1) satisfies Eq. (3.2) for arbitrary $\mu$.

Let us expand $\mu(\mathbf{s}'', \mathbf{s}'x')$ in a Fourier integral with respect to $\mathbf{s}''$ and $\mathbf{s}'$, and we introduce a new function $\nu(\mathbf{pp}')$ which is related to $\mu(\mathbf{p}, \mathbf{p}'x')$ by the equation

$$\mu(\mathbf{p}, \mathbf{p}'x') = \frac{\nu(\mathbf{pp}')}{G_\infty'(00, \mathbf{p})} - \frac{G_\infty'(0x', \mathbf{p})}{G_\infty'(00, \mathbf{p})}(2\pi)^2\,\delta(\mathbf{p} - \mathbf{p}'). \tag{4.2}$$

Here and below

$$G_\infty'(0x', \mathbf{p}) = \lim_{x\to 0+} \frac{\partial}{\partial x} G_\infty(xx', \mathbf{p});$$

among the arguments of $\nu$ we do not write down the variable $x'$, which plays the role of a parameter. For the determination of $\nu(\mathbf{pp}')$, from Eq. (3.3) we obtain the equation

$$\frac{\nu(\mathbf{pp}')}{\varphi(\mathbf{p})} = (2\pi)^2\,\delta(\mathbf{p} - \mathbf{p}')\,\psi(\mathbf{p}) + \int \frac{d\mathbf{q}}{(2\pi)^2}\,\xi(\mathbf{p} - \mathbf{q})\,\nu(\mathbf{qp}'), \tag{4.3}$$

whose solution has been well investigated in the theory of alloys.[8] The difference is associated with the fact that instead of averaging over the positions of the impurities here it is necessary to average over the random functions $\xi$, which was done for H = 0 by Chaplik and Éntin.[9] The functions $\varphi(\mathbf{p})$ and $\psi(\mathbf{p})$ are determined by the expressions

$$\varphi(\mathbf{p}) = -\frac{G_\infty'(00, \mathbf{p})}{G_\infty(00, \mathbf{p})} = -\frac{1}{x_0}\frac{\partial D_{l-1/2}(\zeta)}{\partial\zeta}\frac{1}{D_{l-1/2}(\zeta)}\bigg|_{\zeta = 2p_y x_0/\hbar}, \tag{4.4}$$

$$\psi(\mathbf{p}) = G_\infty(0x', \mathbf{p}) - G_\infty'(0x', \mathbf{p})\,G_\infty(00, \mathbf{p})\,/\,G_\infty'(00, \mathbf{p}). \tag{4.5}$$

Equation (4.3) is solved by iterations in $\xi$, which corresponds to an expansion in powers of $\alpha$ (see Eq. (2.4)), and at each stage averaging is carried out.

The result of the zero-order approximation, $\nu_0(\mathbf{pp}') = (2\pi)^2\delta(\mathbf{p} - \mathbf{p}')\psi(\mathbf{p})\varphi(\mathbf{p})$, has already been used in Eq. (3.10).

In the first two approximations it is necessary to average the expressions which are shown graphically in Figs. 3 a and 3 b. The diagram shown in Fig. 3 a is equal to zero because $\langle\xi(\mathbf{p} - \mathbf{p}')\rangle = 0$. Averaging of the diagram shown in Fig. 3 b leads to the graph shown in Fig. 4 a, where the dotted lines indicate the binary correlation function. In this case one integration is removed with the aid of Eq. (2.1), and the result turns out to be given by

$$\nu_2(\mathbf{pp}') = (2\pi)^2\delta(\mathbf{p} - \mathbf{p}')\,\nu_2(\mathbf{p}), \tag{4.6}$$

where

$$\nu_2(\mathbf{p}) = \nu_0(\mathbf{p})\,\varphi(\mathbf{p}) \int \frac{d\mathbf{q}}{(2\pi)^2}\,\varphi(\mathbf{q})\,\xi_2(\mathbf{p} - \mathbf{q}). \tag{4.7}$$

Since the correction (4.7) turns out to be of the order

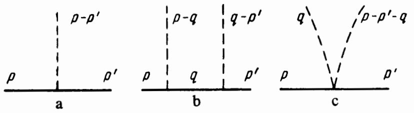

FIG. 3. Unaveraged diagrams of perturbation theory. The solid lines correspond to $G_\infty^{-1}(00, \mathbf{p})$, the dotted lines to $\xi(\mathbf{p})$.

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[2] Two surfaces, bounding the metal in the x direction, can be considered independently if $L_x \gg R$.

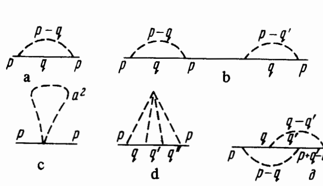

FIG. 4. Averaged diagrams of perturbation theory. A dotted segment corresponds to the binary correlation function $\xi_2(\mathbf{p})$, and four segments starting from a single point correspond to the fourth order correlation function.

of $\xi^2$, in the boundary condition (3.3) it would be necessary to also write down the terms of second order in $\xi$. In this connection, together with the vertex of the type shown in Fig. 3 a, the new vertex shown in Fig. 3 c appears. Averaging of this graph (see Fig. 4 c) gives the factor

$$\int \frac{d^2q}{(2\pi)^2}\xi_2(\mathbf{q})=a^2,$$

where $a^2$ denotes the value of the binary correlation function $\xi_2(\mathbf{s})$ for $s = 0$. Thus, taking account of the diagrams of the type shown in Fig. 4 c corresponds simply to a renormalization of the Green's function and does not shift its poles.

Since $\varphi(\mathbf{p})$ has poles corresponding to the zeros of $G_\infty(00, \mathbf{p})$, i.e., correspond to surface states, it is impossible to confine ourselves to the second-order correction (4.7). In subsequent approximations, together with diagrams of the type shown in Fig. 4 b, graphs appear containing higher-order correlation functions. Thus, a correlation function of fourth order is shown in Fig. 4 d. It is easy to see that, in comparison with Fig. 4 b, diagrams of the type shown in Figs. 4 d and 4 e do not contain a pole factor $\varphi(\mathbf{p})$.

Summation of all dangerous diagrams is accomplished by the equation

$$\nu(\mathbf{p})=\nu_0(\mathbf{p})+\nu(\mathbf{p})\varphi(\mathbf{p})\int\frac{d^2q}{(2\pi)^2}\frac{\nu(\mathbf{q})}{\psi(\mathbf{q})}\xi_2(\mathbf{p}-\mathbf{q}), \tag{4.8}$$

where $\nu(\mathbf{p})$ is related to $\langle \nu(\mathbf{pp}')\rangle$ by a relation of the type (4.6). The solution of Eq. (4.8) has the form

$$\nu(\mathbf{p})\,/\,\psi(\mathbf{p}) = [\varphi^{-1}(\mathbf{p})-\Sigma(\mathbf{p})]^{-1}, \tag{4.9}$$

and the self-energy part $\Sigma(\mathbf{p})$ satisfies the equation

$$\Sigma(\mathbf{p})=\int\frac{\xi_2(\mathbf{p}-\mathbf{q})}{\varphi^{-1}(\mathbf{q})-\Sigma(\mathbf{q})}\frac{d^2q}{(2\pi)^2}. \tag{4.10}$$

Using the formulas written down, we obtain the following answer for the Green's function:

$$\langle G(x\mathbf{p}, x'\mathbf{p}')\rangle = (2\pi)^2\delta(\mathbf{p}-\mathbf{p}')G(xx', \mathbf{p}),$$
$$G(xx', \mathbf{p})=G_\infty(xx', \mathbf{p})-\frac{G_\infty(x0, \mathbf{p})G_\infty(0x', \mathbf{p})}{G_\infty(00, \mathbf{p})-G_\infty'(00\ \mathbf{p})\Sigma(\mathbf{p})}. \tag{4.11}$$

Here only the pole part of G is written down, which is the only part which is essential for a determination of the damping.

The poles of the second term in (4.11) determine the spectrum of the surface states:

$$D_{l-1/2}(\zeta)-\frac{\partial D_{l-1/2}(\zeta)}{\partial\zeta}\frac{1}{x_0}\Sigma(\mathbf{p})=0; \tag{4.12}$$

the relation of $l$ and $\zeta$ with p and $\epsilon$ is given by relationship (3.8), where it is necessary to set $x = 0$.

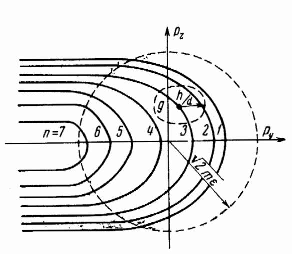

FIG. 5. Projection of the intersection of the energy bands with an equal-energy plane.

In order to analyze Eq. (4.10), let us turn to Fig. 5 on which the solid curves represent projections of intersections of the surfaces $\epsilon = \epsilon_n^{(S)}(\mathbf{q})$, on which $\varphi^{-1}(\mathbf{q})$ vanishes, with the plane $\epsilon = \text{const}$. The region bounded by the circle of radius $(2m\epsilon)^{1/2}$ corresponds to electrons colliding with the surface; in a circle of radius h/d with center at the point p is indicated a region g in which the function $\xi(\mathbf{p}-\mathbf{q}) \sim a^2d^2$ differs from zero. Let $\delta p(\epsilon pn)/\delta n$ denote the distance in the plane p between neighboring levels. This quantity is determined by differentiation of relations (3.18) and (3.19). In relatively weak magnetic fields, such that $\epsilon/\hbar\Omega \gg 1$, it will have a value $\delta p/\delta n \ll \sqrt{2m\epsilon}$.

Depending on the relation between $\delta p/\delta n$ and $\hbar/d$ there are two possibilities. For $\delta p/\delta n \ll \hbar/d$ the function $\varphi^{-1}(\mathbf{q})$ has many zeros in the range of integration in (4.10), and the basic assumption (2.4) means that

$$\Sigma(\mathbf{p})\,(2m\varepsilon-p^2)^{1/2}/\,\hbar \ll 1. \tag{4.13}$$

In this case in the integral (4.10) one should omit $\Sigma(\mathbf{q})$, understanding the integral in the sense of a principal value. For $\delta p/\delta n \gg \hbar/d$ the condition for the smallness of $\Sigma$ remains the previous condition (4.13) for $\hbar/d \gg \sqrt{2m\epsilon}$ and becomes more stringent for $\hbar/d \ll \sqrt{2m\epsilon}$. In this latter case one can omit $\Sigma(\mathbf{q})$ inside the integral in Eq. (4.10) only under the condition that

$$\Sigma(\mathbf{q}) \ll 2x_0^2\,/\,d. \tag{4.14}$$

We shall assume that conditions (4.13) and (4.14) are satisfied, and we calculate the displacement $\delta p_y^{(n)}(\epsilon p_z) \equiv p_y - p_y^{(n)}(\epsilon p_z)$ as a consequence of scattering on the surface ($p_y^{(n)}(\epsilon p_z)$ is the solution of Eq. (4.12) for $\Sigma(\mathbf{p}) = 0$). In this approximation one can expand Eq. (4.12) with respect to $\Sigma$ near $p_y^{(n)}(\epsilon p_z)$:

$$\delta p_y^{(n)}(\varepsilon p_z)=\sum_{n'}\int\frac{d^2q}{(4\pi x_0)^2}i\pi\delta(q_y-q_y^{(n')})\xi_2(p_y^{(n)}-q_y, p_z-q_z)$$
$$+\fint\frac{d^2q}{(4\pi x_0)^2}\frac{\partial}{\partial q_i}\left\{\ln D_{l-1/2}\left(\frac{2q_yx_0}{\hbar}\right)\right\}\xi_2(p_y^{(n)}-q_y, p_z-q_z). \tag{4.15}$$

The first term on the right hand side of (4.15) appears as a result of going around the poles of $\varphi(\mathbf{q})$, and the second term is the principal value of the integral. Formula (4.15) in essence represents the characteristic result of second order perturbation theory; the $\delta$-function expresses the law of conservation of the center of the orbit, and the last term takes into account transitions to volume states.

The integral (4.15) can be estimated with the aid of Fig. 5. First let us consider the case $\hbar/d \ll \delta p/\delta n$. Then only the single term with $n = n'$ remains in the sum (4.15), which only gives a contribution to the attenuation, while the last term of (4.15) only gives a contribution to the shift of the level:

$$\delta p_y^{(n)}(\varepsilon p_z) \sim i\frac{\pi\hbar a^2}{4x_0^2 d}\left[1+\left(\frac{\partial p_y^{(n)}(\varepsilon p_z)}{\partial p_z}\right)^2\right]^{-1/2} + C\frac{a^2}{x_0^2}(2m\varepsilon - p^2)^{1/2}. \tag{4.16}$$

Here C is a real constant. The derivative $\partial p_y/\partial p_z$ is taken along the trajectory $p_y^{(n)}(\epsilon p_z)$:

$$\frac{\partial p_y^{(n)}(\varepsilon p_z)}{\partial p_z} = \frac{p_z}{(2m\varepsilon - p_z^2)^{1/2}}\left(\frac{n - {}^1/_4}{\pi l(1-t^2)^{1/2}} + t\right), \quad -1 < t < 1.$$

For electrons which do not collide with the surface, the first term in (4.16) is exponentially small because $\partial p_y/\partial p_z \to \infty$ as $p_y \to -\infty$.

If $\delta p/\delta n \ll \hbar/d$, then in the summation in (4.15) one should take many terms into account, and one can replace it by an integral. The damping and shift of a level turn out to be of the same order; however, their estimate for $\hbar/d \ll \sqrt{2m\epsilon}$ still depends on just how close the point **p** is to the right boundary of the region g. If **p** is located near the right boundary, so that $\hbar/d \gg m\epsilon/p - p/2$, then

$$\delta p_y^{(n)}(\varepsilon p_z) \sim \frac{a^2}{x_0^2}\left(\frac{p\hbar}{d}\right)^{1/2}. \tag{4.17}$$

In the other limiting case $\hbar/d \ll m\epsilon/p - p/2$ we obtain

$$\delta p_y^{(n)}(\varepsilon p_z) \sim a^2 x_0^{-2}(2m\varepsilon - p^2)^{1/2}. \tag{4.18}$$

Finally, let us estimate the shift and the attenuation for $\hbar/d \gg \sqrt{2m\epsilon}$ and $p < \sqrt{2m\epsilon}$. We have

$$\delta p_y^{(n)}(\varepsilon p_z) \sim \frac{a^2 d^2}{x_0^2\hbar^2}[2m\varepsilon]^{3/2} \tag{4.19}$$

It still remains to verify whether conditions (4.13) and (4.14) are satisfied. One can easily do this with the aid of formulas (4.16) and (4.19) if the relation

$$\Sigma = \frac{2x_0^2}{\hbar}\delta p_y^{(n)}(\varepsilon p_z).$$

is taken into account.

For practical estimates it is convenient to represent the formulas obtained here in another form, regarding the quantum numbers p and n as independent and expressing them in terms of the shift and attenuation of the n-th level, $\epsilon_n(\mathbf{p}) = \epsilon_n^{(S)}(\mathbf{p}) + \delta\epsilon_n(\mathbf{p})$. The required connection is obtained by simple differentiation of relations (3.18) and (3.19):

$$\delta\varepsilon = 2\Omega x_0 \sqrt{l}\,|(n - {}^1/_4)/\pi l(1-t^2)^{1/2} + t|^{-1}\,\delta p_y^{(n)}(\varepsilon p_z), \quad -1 < t < 1,$$

$$\delta\varepsilon = 4\Omega x_0(l - n + {}^1/_2)(n - {}^1/_2)^{1/2}(t^2 - 1)^{1/2}\,\delta p_y^{(n)}(\varepsilon p_z), \quad t > 1.$$

The relation of t and $l$ with **p** is given by formulas (3.18) and (3.19). In the case of skipping orbits, whose spectrum is described by expression (1.1), one finds

$$\delta\varepsilon = (2m\varepsilon - p_z^2)^{1/2}\delta p_y^{(n)}(\varepsilon p_z)\,/\,m.$$

## 5. DISCUSSION OF THE RESULTS

For a perfectly smooth surface the arrangement of the levels is described by relations (3.18) and (3.19) where $p_y$, $p_z$, and n serve as the quantum numbers. The distance between neighboring levels for skipping electron orbits is given by

$$\frac{\delta\varepsilon}{\delta n} \sim \frac{\hbar\Omega}{\pi}\left[\frac{2(\varepsilon - p_z^2/2m)}{3\pi\hbar\Omega n}\right]^{1/3}$$

for $(t^2 - 1)^{1/2} \ll 1$ and $\delta\epsilon/\delta n \sim \hbar\Omega$ in the general case, i.e., if $t^2 - 1 \sim 1$. The small parameter appearing here has a value

$$[3\pi\hbar\Omega\,/\,2(\varepsilon - p_z^2\,/\,2m)]^{1/3} \sim 10^{-1} \div 10^{-2}$$

in fields of the order of oersteds and for characteristic values of the Fermi energy. As a consequence of the unevenness of the surface the levels are displaced, and attenuation arises, which is described by the formulas presented in Section 4. The results obtained here are valid if the component of the electron's wavelength normal to the metal surface is large in comparison with the average size of a surface roughness: $a(2m\epsilon - p^2)^{1/2} \ll \hbar$.

The shift and attenuation of a level are maximal when the size d of the planar sections of the surface are so small that during collisions with the surface the electron may go into practically any quantum state. In this case $\delta\epsilon \sim a^2 d^2 \Omega(2m\epsilon)^{3/2}(2m\epsilon - p_z^2)^{1/2}/\hbar^3$ (see Eq. (4.19)). If the parameters a and d are of atomic dimensions, then for not overly large values of $p_z$ one will have $\delta\epsilon \sim \hbar\Omega$. This quantity is small in comparison with the distance between levels only for skipping electrons. Such a situation is also preserved for other values of the parameter d. Scattering from the surface essentially has no effect on the spectrum of skipping electrons, and for them the main effect is due to scattering by volume defects, for example, by impurities. If the gliding angles are not small, then scattering on the surface has a substantial effect on the spectrum of the surface states, and formulas (4.16)—(4.19) may serve, for example, as a means of investigating the surface and electronic properties. The corresponding experiment may be, for example, the observation of a cutting off of the cyclotron resonance.[10]

The density of surface states was calculated in Sec. 3 only for the specular case. It is easy to understand what happens when scattering on the surface is taken into account. Since the singularities of the states are related to levels, the distance between which is $\hbar\Omega$, scattering by a surface leads to an effective broadening of these singularities (here the fact that an electron moving in such an orbit "sees" the surface under a small angle is not essential). The smooth part of the density of the surface states (3.12) is primarily related to the levels of the skipping electrons. Therefore its dependence on the magnetic field remains the same as the previous dependence (3.25), provided that the characteristic wavelength is small in comparison with the mean free path associated with scattering by volume defects.

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