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Magnetic Surface Levels in a Tipped Magnetic Field*

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The wave functions and spectrum for metallic electrons skipping along a surface in a magnetic field are calculated for general orientation of field and surface relative to the crystal axes of the material. Unlike the case in which the field is parallel to the surface, the energy levels form a continuum rather than a discrete set of bound magnetic surface levels. Nevertheless, except for rather extreme tip angles, no broadening or change of shape of the observed signals should be observed. In general there will be a rescaling of the field variable which can be used to measure Fermi-surface quantities inaccessible by other techniques. The analysis of the data is somewhat more complex than in the parallel-field case, however.

I. INTRODUCTION

The experimental study of magnetic surface levels[1–5] has proved to be extraordinarily useful in determining a wide variety of parameters characterizing a metallic system. These include Fermi-surface parameters (velocities, radii of curvature, and masses[6] as a function of temperature[7]), lifetimes (also as a function to temperature),[8] and properties of the metal-vacuum interface.[9] The latter includes static and dynamic roughness (Rayleigh waves)[10] and the probability of specular reflection as a function of glancing angle.[11,12]

One reason for the great interest in these measurements is that the observed properties, in a given experiment, are associated with a given point on the Fermi surface (or more accurately, with a given small region of the Fermi surface). Thus, for example, one is able to measure lifetimes as a function of position on the Fermi surface.[8]

Various modification of these experiments have been proposed,[13] and some of them have been carried out.[14,15] These have led to new results.

The purpose of this paper is to analyze another modification of the experiment which is easy to carry out experimentally, although it is surprisingly difficult to attack theoretically.

The basic experiment is a measurement of the surface impedance as a function of magnetic field when that field is applied parallel to the surface. The crucial electrons are those at the Fermi surface which are travelling nearly parallel to the real surface (assumed to be the plane $z=0$) and of maximal (or extremal) velocity perpendicular to the magnetic field (say, in the y direction). Thus the important electrons are those of energy E at the Fermi energy E_F, velocity $V_z \sim 0$, and the maximum V_x consistent with the previous conditions.[16]

These electrons are curved into the surface repeatedly by the Lorentz force $F_z = -eV_x B/c$ and skip repeatedly in very shallow hops along the surface (see Fig. 1). Thus their motion is periodic

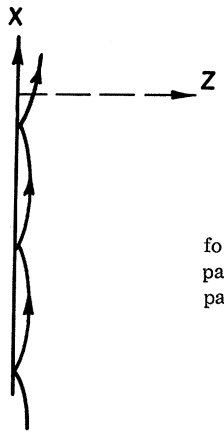

FIG. 1. Classical skipping orbit for the case of a magnetic field parallel to the surface (out of the paper).

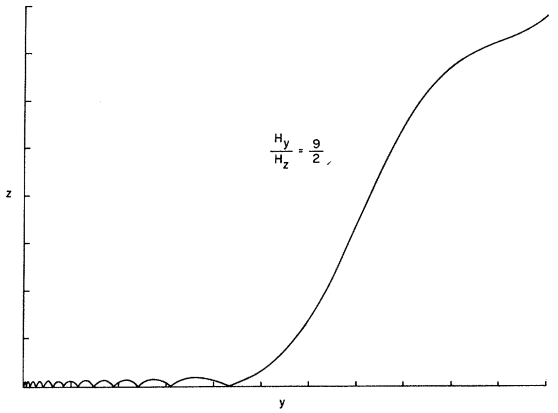

FIG. 3. Projection onto the $y-z$ plane of a classical orbit of an electron in a tipped magnetic field. The electron spirals in from large z and y, strikes the surface, makes a series of skips of gradually changing period, reverses itself, and spirals back into the bulk.

in the z coordinate and must be quantized. The electromagnetic microwave field in the surface impedance experiment causes resonant transitions between the levels. These are observed as peaks in the surface absorption.

All electrons in a narrow band on the Fermi surface defined by $V_z = 0$ (and not only those with the maximal V_x) will make their quantized skips. However the Lorentz force differs from one electron to the next so that the skipping period differs, as we consider the entire range of possible velocities. At an extremal velocity V_x, however, there will be a relatively large number of electrons with nearly the same Lorentz force, so this set of resonances will dominate the response. (This kind of consideration is familiar in the theory of Azbel-Kaner cyclotron resonance or the de Haas–van Alphen effect.) We show in Fig. 2 the orbits in momentum space of the electrons.

The effect of this distribution of V_x values on the signal is twofold. The resonance peaks will be broadened because of the spread of resonant frequencies, and skewed because this spread is entirely to one side of the dominant resonance. (Because the observed signal will be a superposition of many resonances whose tails overlap, a numerical evaluation is necessary to see in detail the result of this effect.[8])

The purpose of the present work is to study the case in which the magnetic field is tipped into the sample. The introduction of a field component normal to the surface introduces a Lorentz force $eV_x B_z/c$ in the y direction and since there is nothing to impede the motion, the electron will steadily increase its y momentum p_y, perforce changing its value of V_x.

Thus, we will not have periodic motion in any direction, so no discrete set of quantum levels results.

Typical classical orbits in both real space and momentum space are plotted in Figs. 3, 4, and 5 for the case of a tipped field.

This kind of result is typical of the introduction of a magnetic field. For example, it is well known that in the absence of surfaces a constant magnetic field, however small, will give rise to discretely quantized levels (Landau levels) instead of a continuum of energy levels, thus changing remarkably and discontinuously the mathematical characterizations of the wave function, even though physical quantities must be continuous as the field vanishes. Here the reverse happens in that a small component B_z destroys the discreteness of the energy spectrum.

We calculate the effects of a "small" component of the magnetic field normal to the surface (B_z). The main result is that the surface impedance for a spherical Fermi surface (and certain similar cases) is unaffected by the component B_z until an electron with velocity $V_z = 0$ would, under the influence of B_z alone, transverse a significant fraction of the entire distance around the Fermi surface in a mean free time τ. In fact, corrections are of the order of $(\omega_z \tau)^2$, where $\omega_z = eB_z/m_{12}c$, with m_{12} being the mass associated with motion normal to the z direction.

It is to be emphasized that a value of B_z small in this sense can be quite large as compared with the values of B_y needed for resonance (which is typically 10 G).

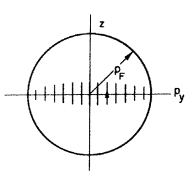

FIG. 2. Semiclassical orbits of electrons in momentum space. Each electron is on the Fermi surface and with each skip follows a trajectory which crosses the great circle $V_z = 0$. The periods are stationary as a function of p_y at $p_y = 0$.

In more general Fermi surface geometry, the effect of a normal component B_z can be described by an effective $B_y^{\text{eff}} = B_y - \gamma B_z$, where γ depends on certain Fermi-surface parameters. Although in the most general case γ is quite complicated, in certain special cases (as, for example, bismuth) γ has a simple geometrical significance. In any case, a proposed band structure can be used to calculate γ and can thus be checked by experiment.

We predict that there will be *no* broadening of the observed level structure until $\omega_z\tau \sim 1$. This is in spite of the fact that a given electron level will not be sharply quantized, since there is no periodic motion. Rather, each electron classically skips along the surface with a hop time that changes from one hop to the next. Kaner, Makarov, and Fuks[17] have predicted such a broadening. However, we find to an excellent approximation that this broadening is identical to that predicted from the distribution of V_x values for $B_z = 0$. In fact one can say that each electron in its orbit samples all values of V_x with approximately the same weight as occurs in summing over these values in the case of parallel field.

In Sec. II we develop the theory to deal with the spherical Fermi surface. In Sec. III we deal with the general quadratic Fermi surface, and in Sec. IV with an arbitrary Fermi surface. An Appendix is used to discuss some of the mathematical approximations made.

II. SPHERICAL FERMI SURFACE

A. Wave Functions

We may choose the field to be in the y-z plane. A convenient choice of vector potential is

$$\vec{A} = (B_y z, B_z x, 0) \ . \tag{1}$$

Thus, the Hamiltonian will be

$$H = \frac{[p_x + (e/c)B_y z]^2}{2m} + \frac{[p_y + (e/c)B_z x]^2}{2m} + \frac{p_z^2}{2m} \tag{2}$$

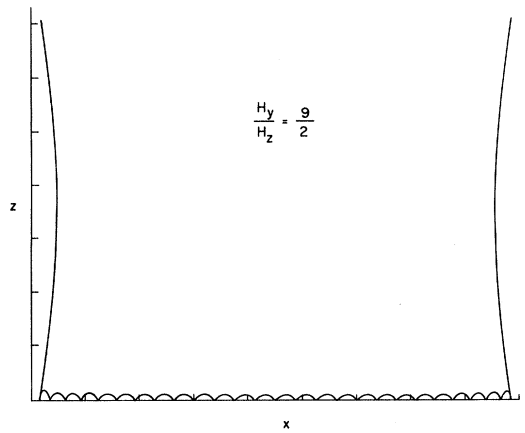

FIG. 4. The same orbit as in Fig. 3, as projected onto the x-z plane.

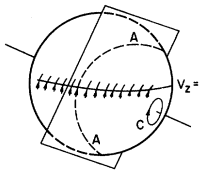

FIG. 5. A schematic drawing of the orbit of Figs. 3 and 4 in momentum space. Each skip traverses the band $V_z = 0$, following a circle on the Fermi surface of constant $p \times H$, as shown by the curve A – A. It gradually works its way around the Fermi surface, and after leaving the real surface, follows the helical path C.

together with the condition that the wave function vanish at $z = 0$. Unlike the case for which $B_z = 0$, p_x and p_y cannot be simultaneously constants of the motion. In fact, if we put $\hat{p}_i = p_i + (e/c)A_i$, we have

$$[\hat{p}_i, \hat{p}_j] = \epsilon_{ijk} \frac{\hbar e}{c} B_k \ . \tag{3}$$

Thus, $[p_x, \hat{p}_y] = (\hbar e/c)B_z$ and we cannot simultaneously diagonalize p_x, $\hat{p}_y$. Rather, the uncertainty principle tells us that at best there is an uncertainty that satisfies

$$\Delta p_x \Delta \hat{p}_y = \frac{e\hbar}{c} B_z \ . \tag{4}$$

Since this relation has dimensions, we must know how small B_z has to be in order that we can neglect the uncertainties in p_x and $\hat{p}_y$. The following analysis shows we must have $\Delta p_x \Delta \hat{p}_y \ll \hbar m/\tau$.

Returning to Eq. (2), we note that p_y may be chosen constant and p_z may be represented as $(\hbar/i)\partial/\partial z$. We choose to represent

$$x = i\hbar\, \partial/\partial p_x - (c/eB_z)\, p_y \quad \text{so that } [x, p_x] = i\hbar \ .$$

Then (2) becomes

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial p_x^2} + \frac{1}{2m}\left(p_x + \frac{e}{c} B_y z\right)^2 \ . \tag{5}$$

Here

$$M = m(c/eB_z)^2 \ , \tag{6}$$

as B_z is "small" M will be "large" and we have a Schrödinger equation in two variables with a small and a large "mass." The Born-Oppenheimer or adiabatic approximation is designed to deal with this. Clearly, the physical basis for the Born-Oppenheimer approximation to be valid is that the p_x "motion" be slow compared with that in z. That is, p_x is required to remain nearly constant in one hop of the electron along the surface. We treat this in more detail in an Appendix.

We thus may approximate the eigensolutions to (5) by

$$\psi_{nE}(p_x, z) = \phi_{nE}(p_x) u_{np_x}(z) \ . \tag{7}$$

In (7), $u_{np_x}(z)$ is to satisfy

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+\frac{1}{2m}\left(p_x+\frac{e}{c}B_y z\right)^2\right]u_{np_x}(z)=\epsilon_n(p_x)u_{np_x}\ , \tag{8}$$

where p_x is treated as a parameter. The equation for $\phi_{nE}(p_x)$ is

$$\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial p_x^2}+\epsilon_n(p_x)\right)\phi_n=E\phi_n\ . \tag{9}$$

Let us first note that (8) is exactly the equation to be solved in the case $B_z=0$. We anticipate from the study of that case that the important values of p_x will be large (of order p_F) and thus we may replace

$$(2m)^{-1}(p_x+e/cB_y z)^2\cong p_x^2/2m+\frac{e}{c}V_x B_y z\ , \tag{10}$$

i.e., we have a linear potential. Therefore the solution can be written as an Airy function:

$$u_{np_x}\propto \mathrm{Ai}(\alpha z-a_n)\ , \tag{11}$$

$$\epsilon_n(p_x)=\frac{\hbar^2\alpha^2}{2m}a_n+\frac{p_x^2}{2m}\ , \tag{12}$$

where $\mathrm{Ai}(-a_n)=0$,

$$\alpha=(2e/\hbar^2 cF)^{1/3} \tag{13}$$

and

$$F=mV_x B_y\ . \tag{14}$$

The wave number α, which enters also the energy levels (12) is central to the results. In typical cases $\alpha\sim 10^5\ \mathrm{cm}^{-1}$.

The equation for ϕ_n cannot be solved exactly, but since M is large we may use the WKB method, expecially if we are careful near the classical turning point, where Airy functions are again encountered as an approximation to ϕ. We shall not bother to show the solution just at the turning point, but shall just quote the solution in WKB approximation. This is

$$\phi_{nE}(p_x)=\frac{1}{(\hbar eB_z/c)^{1/2}}\frac{1}{[E-\epsilon_n(p_x)]^{1/4}}\,2\,\mathrm{Re}\exp\left(-i\int_{p_0}^{p_x}\frac{\{2m[E-\epsilon_n(p')]\}^{1/2}dp'}{\hbar eB_z/c}-i\frac{\pi}{4}\right), \tag{15}$$

where $\epsilon_n(p_0)=E$ and solution applies only in the classical accessible region.

B. Surface Impedance

To make a quantitative calculation we adopt the formulation used in Ref. 5. The formula we use for the change in the surface impedance δZ due to the surface levels is

$$\delta Z=\frac{e^2}{i}\frac{eB_z}{c}\sum_{nm}\int dE\int dE'\int\frac{dp_x dp_x'}{(2\pi)^3}V_x V_x'\,\alpha_{nm}(p_x)\alpha_{nm}(p_x')\phi_{nE}(p_x)\phi_{mE'}(p_x)\phi_{nE}(p_x')\phi_{mE'}(p_x')$$
$$\times\int\frac{d\omega_1 d\omega_2}{(2\pi)^2}\frac{\gamma_{nE}(\omega_1)\gamma_{mE'}(\omega_2)}{\omega-(\omega_1-\omega_2)+i\eta}\frac{f(\omega_1)-f(\omega_2)}{\omega_2-\omega_1}\ . \tag{16}$$

Here

$$\alpha_{nm}(p_x)=\int_0^\infty dz\,\frac{E(z)}{E'(0)}u_{np_x}(z)u_{mp_x}(z) \tag{17}$$

is a normalized matrix element of the microwave electric field $E(z)$ (assumed to be nearly the same as at zero magnetic field); and

$$\gamma_{nE}(\omega)=\frac{\Gamma}{(\omega-E/\hbar)^2+(\Gamma/2)^2} \tag{18}$$

is the spectral function connecting the actual energy $\hbar\omega$ with the nominal energy E. The lifetime $\tau=1/\Gamma$. The Fermi function is denoted by f.

Some details of the derivation of this formula are in the Appendix.

This formula differs from that finally derived in Ref. 5 in that there are two p_x integrals and two E integrals, since p_x is not conserved in this case. A connection between p_x and p_x', etc., is nevertheless approximately maintained through the wave functions ϕ, which for $B=0$ are oscillatory δ functions. However, one cannot simply examine the broadening of the functions ϕ, since their oscillations beat against one another.

We now embark on the p_x integrals. To do these we note that the phase factor in (15) is rapidly varying for B_z small, so that the integrals may be done by the method of stationary phase, and the other factors vary slowly (typically variations $\delta p_x\sim p_F$ must be considered to make appreciable changes in the other factors). The main contribution thus comes when p_x satisfies

$$[E-\epsilon_n(p_x)]^{1/2}=[E'-\epsilon_m(p_x)]^{1/2} \tag{19}$$

or

$$E-E'=\epsilon_n(p_x)-\epsilon_m(p_x)\ . \tag{20}$$

In order for the WKB solution to be valid we must have $E-\epsilon_n(p_x) \gg (\hbar e/cm)B_z$ for the value of p_x satisfying (20), but a more detailed analysis allows us to extend the results through the turning point. It is easily checked that the stationary phase approximation is excellent, because of the very slow variation of all factors other than the exponential.

These integrals may then be performed, with the result

$$\delta Z = \frac{e^2}{i}\sum_{n,m}\int dE\int dE'\, V_x^2\,\frac{\alpha_{nm}^2(p_x)}{\epsilon_n'(p_x)-\epsilon_m'(p_x)} \times \frac{1}{\{2m[E-\epsilon_n(p_x)]\}^{1/2}} \times \int \frac{d\omega_1 d\omega_2}{(2\pi)^2}\,\frac{\gamma_{nE}(\omega_1)\gamma_{mE'}(\omega_2)}{\omega-(\omega_1-\omega_2)+i\eta}\,\frac{f(\omega_1)-f(\omega_2)}{\omega_2-\omega_1}, \tag{21}$$

and p_x is determined from (20) as a function of $E-E'$.

The following steps are now carried out. We transform from the variable E' to p_x by means of (20). Then put $\omega_1=\omega_1'+E/\hbar$, $\omega_2=\omega_2'+E/\hbar$ to achieve a factor

$$\frac{f(\omega_1''+E/\hbar)-f(\omega_2'+E/\hbar)}{\omega_2'-\omega_1'}$$

inside the integral. For the important values of $\omega_1'\omega_2'$, this factor acts as a spread-out δ function requiring $E\sim E_F\pm kT$. After taking these steps and doing the E integration we may carry out the ω_1' and ω_2' integrations. The final result is

$$\delta Z = \frac{e^2}{i}\sum_{mn}\int_0^\infty \frac{dp_x}{(2\pi)^2}\frac{dp_y}{dp_x} \times V_x\,\frac{\alpha_{nm}^2(p_x)}{\hbar\omega-[\epsilon_n(p_x)-\epsilon_m(p_x)]+i\Gamma\hbar}\ . \tag{22}$$

This result is precisely that obtained earlier.[5] The factor

$$\frac{dp_y}{dp_x}=\frac{p_x}{(p_F^2-p_x^2)^{1/2}} \tag{23}$$

is just the singular factor which ensures that a dominating contribution will come from $p_x=p_{x_{\max}}=p_F$.

The complete analysis which is valid at the classical turning point (corresponding to $p_x\sim p_F$) replaces the factor dp_y/dp_x by

$$2p_x\lambda_{nm}^{1/2}\,\pi\{\mathrm{Ai}[-\lambda_{nm}(p_F^2-p_x^2)]\}^2\ , \tag{24}$$

where

$$\lambda_{nm}=\frac{1}{p_F^2}\left(\frac{(\epsilon_n(p_F)-\epsilon_m(p_F))^2}{(6\hbar eB_z/mc)^2}\right)^{1/3}\ . \tag{25}$$

The factor (24) oscillates rapidly about its mean which is $p_x/(p_F^2-p_x^2)^{1/2}$. The degree to which it is a good approximation to replace (24) by (23) depends on how rapidly the multiplying factors vary. The most rapid variation is in the energy denominator where a smearing of p_x values over a range $\Delta p_x \lesssim p_F\hbar\Gamma/(\epsilon_n-\epsilon_m)$ can be tolerated. A study of (24) reveals that the first corrections are smaller than the main result by a factor of order

$$\frac{1}{200}(p_x\Delta p_x\lambda_{nm})^{-3}\sim\frac{1}{10}\left(\frac{\hbar\Gamma^3}{(\epsilon_n-\epsilon_m)(eB_z/mc)^2}\right)^{-1}\ ;$$

since $\epsilon_n-\epsilon_m\sim\hbar\omega$ we have the criterion mentioned in the introduction, i.e., corrections go as $(\omega_z\tau)^2(\omega\tau/10)$.

Physically, this means that during the several skips an electron makes in its lifetime, the electron progresses a significant distance around the Fermi surface. Since the adiabatic approximation is based on the slow motion of p_x in a single skip, it is clear that this approximation breaks down simultaneously thus making it difficult to estimate the correction in more detail.

III. GENERAL QUADRATIC SURFACE

In general, a quadratic energy surface can be reduced to a normal form by appropriate choice of coordinate axes. We shall deal with two cases, distinguished by whether or not the z axis is a principal direction.

Principal direction normal to the sample surface. In this case, at zero field, the energy function is

$$H=\frac{p_x^2}{2m_1}+\frac{p_y^2}{2m_2}+\frac{p_z^2}{2m_3}\ , \tag{26}$$

where the m's may be either positive or negative.

In fact, the case of all positive masses may be reduced to the spherical case by the introduction of rescaled variables (denoted by the same symbols written with a bar) according to substitutions

$$p_x\to\bar{p}_x(m_1)^{1/2},\ \text{etc.};\quad B_y\to\bar{B}_y(m_1m_3)^{1/2},\ \text{etc.}$$

Since this is quite trivial we shall just list the results, which are the same as for the spherical case with the following interpretation of the symbols:

(a) Let the field be in the $y-z$ plane [so (26) will not in general be diagonal in this coordinate system].

(b) Replace F of Eq. (14) by $m_3(\vec{V}\times\vec{B})_z$. [Note $m_3V_x=\hbar K$. (K is the radius of curvature of intersection of the Fermi surface with the plane $p_y=\text{const.}$)]

(c) In Eq. (22), we may regard the integration as being over p_y, where p_x is a function of p_y computed as follows. Solve the simultaneous equations $H(p_xp_yp_z)=E_F$ and $V_z=\partial H/\partial p_z=0$ for p_x as a function of p_y.

In the quadratic case this is simple: The prescription in (c) is still more general.

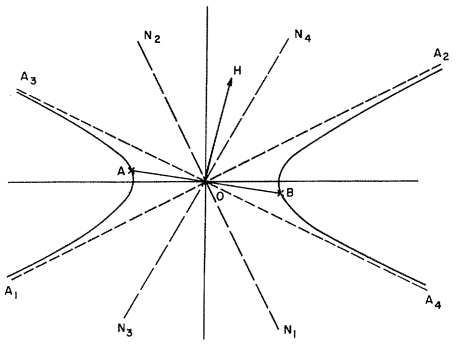

FIG. 6. Construction to locate the contributing point for a quadratic Fermi surface. The projection onto the $p_x - p_y$ plane of the curve $V_z = 0$ is, in this case, assumed to be a hyperbola. A line normal to the field H is passed through the origin, and its intersection with hyperbola at one of the points A or B is the contributing point. In order for this point to exist, H must lie between the lines N, normal to the asymptotes.

(d) The contributing point will be the point where $\epsilon_n - \epsilon_m$ is stationary as a function of p_y, which, since m_3 is constant, is at the extremal value of $(\vec{V}\times\vec{B})_z$. This extremal value can be found by the following construction: For $V_z = 0 = p_z$, $H(p_x, p_y, 0)$ is an ellipse. A line passing through the center of the ellipse and normal to the magnetic field will intersect the ellipse at the contributing value of p_x and p_y.

(e) The criterion for the applicability of the result is $\omega_z \tau \ll 1$, where $\omega_z = (e/c)B_z/(|m_1 m_2|)^{1/2}$.

If m_2 is negative relative to m_1, a scale change does not reduce things to the spherical case, but to a hyperbolic case where matters are equally simple. The only difference is that $(\vec{V}\times\vec{B})_z$ will have a minimum instead of a maximum. The construction of part (d) is still correct, except that $H(p_x, p_y, 0)$ is a hyperbola. As a result, for certain field directions, there is no minimum $(\vec{V}\times\vec{B})_z$ and one would not expect distinct oscillations (see Fig. 6).

General quadratic surface. We see that for a quadratic energy function, the equation $V_z = 0$ defines a plane. By an appropriate choice of coordinates, we may bring the Hamiltonian H into the form

$$H = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{(p_z + \gamma_x p_x + \gamma_y p_y)^2}{2m_3} + \text{const} \ . \quad (27)$$

Note that m_1, m_2, m_3 are *not* the principal masses of the quadratic form, although they are easily related to them. The vector $(\gamma_x, \gamma_y, 1) = \vec{\Gamma}$ is normal to the plane defined by $V_z = 0$.

For simplicity we shall at first assume that the magnetic field is in the $y - z$ plane in the coordinate system defined by (27). Starting with the same gauge as before, we obtain

$$H = \frac{[p_x + (e/c)B_y z]^2}{2m_1} + \frac{(p_y + (e/c)B_z x)^2}{2m_2} + \frac{1}{2m_3}(p_z + \gamma_x p_x + \gamma_y p_y + \frac{e}{c}\gamma_x B_y z + \frac{e}{c}\gamma_y B_z x)^2 \ . \quad (28)$$

The term $(e/c)\gamma_y B_z x$ can be eliminated by a guage transformation

$$\psi \to e^{-i(e/\hbar c)\gamma_y B_z x z}\psi \ , \quad p_x \to p_x - (e/c)\gamma_y B_z z \ , \quad p_z \to p_z - (e/c)\gamma_y B_z x \ . \quad (29)$$

A subsequent gauge transformation

$$p_z \to p_z - \gamma_y p_y - \frac{e}{c}\gamma_x B_y z + \frac{e}{c}\gamma_x \gamma_y B_z z \quad (30)$$

reduces (28) to

$$H = \frac{(p_x + (e/c)\tilde{B}_y z)^2}{2m_1} + \frac{(p_y + (e/c)B_z x)^2}{2m_2} + \frac{1}{2m_3}(p_z + \gamma_x p_x)^2 \ , \quad (31)$$

where

$$\tilde{B}_y = B_y - \gamma_y B_z \ . \quad (32)$$

Again we may make the adiabatic approximations, treating p_x as a constant, etc. Except for the fact that the breakdown of the adiabatic approximation occurs at somewhat lower fields [because of the $\gamma_x p_x$ term in (31)] everything is exactly as before, provided one replaces B_y by $\tilde{B}_y$.

If the field is in an arbitrary direction relative to the principal axes defined by (27) we may express the results as follows:

(c) The quantity F appearing in the wave number α (Eq. 14) must be replaced by

$$F = m_3(\vec{V}\times\vec{B})_z\left(1 - \frac{\vec{B}\cdot\overleftrightarrow{m}\cdot\vec{\Gamma}}{\vec{B}\cdot\overleftrightarrow{m}\cdot\vec{B}}B_z\right) \ , \quad (33)$$

where $\overleftrightarrow{m}$ is the 2×2 mass matrix. [This matrix was chosen to be diagonal and of the form $m_{ij} = \delta_{ij} m_i$ by choice of coordinate system (27).]

(d) The extremum of (33) is at the same point as that of $(\vec{V}\times\vec{B})_z$, since we have assumed m_3, $\overleftrightarrow{m}$, and $\vec{\Gamma}$ to be constant.

At that point the expression (33) takes on the simple form

$$F = m_3(\vec{V}\times\vec{B})\cdot\vec{\Gamma} \ . \quad (34)$$

The remaining remarks (c) and (e) remain the same, with $|m_1 m_2| = |\det \overleftrightarrow{m}|$.

Thus, for a quadratic Fermi surface we find that

for tipping fields small enough to satisfy (e), there is no broadening or change of shape of the signal and the contributing point on the Fermi surface does not change. However, the effective field which enters the expression α (and thus the energy and matrix elements) is given by (33), which can in this case be simplified to (34).

The most notable case of a quadratic energy surface which is suitable for this type of experiment is that of bismuth. The analysis of the tipped field effects in this case is straightforward in view of the simplicity of Eq. (34) and the construction of (d).

IV. GENERAL FERMI SURFACE

Unfortunately, energy surfaces which are globally quadratic are the exception rather than the rule. On the other hand, we know that it is only the electrons in the neighborhood of one point of the Fermi surface that contribute significantly to the observed resonant response, so that one can imagine making an expansion of the energy function near the point to second order. Since at least the energy surfaces are locally quadratic, one is tempted to apply the preceding arguments without further change.

This would presumably be satisfactory if we know in advance the correct point about which to expand. Often it is possible to obtain this point from symmetry considerations, but in general, it is part of our problem to determine the contributing point.

Unfortunately, in this case the quadratic approximation is surely not sufficient.

The reason is that, according to Eq. (22), the oscillatory part of the surface impedance is an integral over p_y of a function with a rapidly varying energy denominator. We expect, therefore, that the main contribution will arise when this energy denominator is extremal with respect to p_y. In other words, the condition is that $\epsilon_n - \epsilon_m$ be extremal, with respect to p_y (when p_x is considered to be a function of p_y). In general, however, the mass m_3, mass matrix $\overleftrightarrow{m}$, and the vector $\vec{\Gamma}$ must be considered to vary as p_y varies. Thus, in general, since (33) enters into the expression for the energy levels, the variation of all these quantities would have to be considered. In fact, one would guess that the correct condition [since m_3 explicitly enters Eq. (12) for ϵ_n] is that

$$F/m_3^{3/2} \tag{35}$$

be extremal and all parameters are to be regarded as functions of p_x and p_y, that is, of position on the Fermi surface.

Since to find the extremum it is only necessary to keep the linear dependence of (35) on p_y, one ought to retain at least the cubic terms in the expansion of the energy functions.

In one does so, however, a host of complications arises. For example, third-order differential equations will be encountered and difficulties with choice of boundary conditions might ensue.

However, one may ignore mathematical niceties and argue from the uncertainty principle of Eq. (4). We have seen that p_x and $\hat{p}_y$ can continue to be construed as constants of the motion so long as $\omega_z \tau \ll 1$. A detailed verification of this in the case of the cubic terms has been carried out[18] and it is found that the condition for the validity of the neglect of the uncertainties in p_x and $\hat{p}_y$ is unchanged.

In this case, the proper interpretation of the vector $(\gamma_x, \gamma_y, 1)$ is as follows: Solve the equation $V_z(p_x p_y p_z) = 0$ for p_z in the form $p_z + \Lambda(p_x p_y) = 0$. Then we have $\gamma_i = \partial\Lambda/\partial p_i$. Alternatively, the vector $\vec{\Gamma} = (\gamma_x, \gamma_y, 1)$ is normal to the surface (no longer a plane) defined by $V_z = 0$. Unfortunately, it does not appear that $\vec{\Gamma}$ has any necessary simple geometrical relationship to the Fermi surface geometry.

In this most general case, therefore, the expression (33) continues to be valid but the contributing point is not found so easily but is given by the extremum of (35) as a function of p_y. In particular the simplicity of Eq. (34) is lost. The experimentally measured quantities will therefore depend on the quadratic expansion of the energy function at the contributing point, but the determination of the contributing point is more complicated, unless particularly symmetric situations are envisaged. The expression (35) is complicated enough that it seems probable that for nonsymmetry points the best method of data analysis would require use of a hypothetical energy surface function to predict the contributing point and the value of (33).

It may be pointed out, however, that (33) depends on the mass matrix in a way never encountered in other types of Fermi surface experiments. In fact, in the quadratic expansion of the energy surfaces there are 9 parameters; the symmetric mass matrix and the velocity. Of these 9 one may be chosen as the magnitude of the velocity and five combinations of the others define the Fermi surface orientation and curvature at the point in question.

All experiments presently employed in the analysis of the energy level structure near the Fermi surface depend only in these six quantities, that is to say, on the *geometry* of the Fermi surface and the magnitude of the Fermi velocity.

The remaining three parameters can be regarded as being the components of the gradient of the magnitude of the Fermi velocity. These parameters appear in expression (33).

That the phenomenon of magnetic surface levels in a tipped field should depend on these additional parameters in an essential way of course adds greatly to the difficulty of data analysis, as we have

pointed out, but to some extent it would provide a motivation for that analysis in that it could provide a check on quantities not previously entering into consideration.

We remark that in many cases, a crystal face is chosen which is a plane of reflection symmetry. In this case it is to be expected that the band $V_z = 0$ lies in a plane $p_z = 0$. Then, even for a general Fermi surface there is no tipped field effect, if the normal component of B is ignored.

In the experiments so far carried out, B has been tipped an angle θ, so that $B_y = B\cos\theta$. Since peaks are observed for fixed values B^0_{mn} we see that the observed peaks should obey the simple scaling

$$B = B^0_{mn}/\cos\theta \ .$$

This has in fact been observed to be the case.[19] However, the observations made in cases with $\vec{\gamma} \neq 0$ have not thus far been analyzed. Nor have B_z values sufficiently large to cause a breakdown of the approximations made in this note been employed.

APPENDIX

Surface Impedance

The formula for the surface impedance Eq. (16) is obtained as follows: It is possible to show[4] that the change in surface impedance due to a small change in conductivity $\delta\sigma$ is

$$\delta Z = -\int_0^\infty dz \int_0^\infty dz' \ \frac{E(z)\delta\sigma(z,z')E(z')}{E'(0)^2} \ , \qquad \text{(A1)}$$

where $E(z)$ is the unperturbed electric field. For the paramagnetic part of $\delta\sigma$ we may use

$$\delta\sigma(z,z') = \frac{e^2}{\hbar\omega}\int_0^\infty d\tau\, e^{i(\omega+i\eta)\tau} \times \int dx'dy' \langle [J(\vec{x},\tau),\ J(\vec{x}',0)]\rangle \ , \qquad \text{(A2)}$$

where the intermediate states are restricted to the surface level states. The current operator J is expressed as usual in terms of creation and annihilation operators $\psi(x)$ and $\langle\ \rangle$ is the expectation value in the grand canonical ensemble.

The operator $\psi(x)$ may be expanded as

$$\psi(x) = \sum_n \int dE \int \frac{dp_2}{\sqrt{2\pi}}\, e^{ip_2 y} \int \frac{dq}{2\pi}\, e^{iq(x+\hbar p_2/B_z)} \times \phi_{nE}(q) u_{nq}(z)\ a_{nEp_2} \ , \qquad \text{(A3)}$$

where a_{nEp_2} destroys an electron in state n, E, p_2.

We then make the Hartree-Fock approximation in factoring (A2). Expressions such as

$$\int_{-\infty}^{\infty} \langle a_{nEp_2}(\tau) a^\dagger_{n'E'p_2'}(0)\rangle d\tau e^{+i\omega\tau} \qquad \text{(A4)}$$

are encountered and are set equal to

$$\delta_{nn'}\delta(E-E')\delta_{p_2,p_2'}\gamma_{nE}(\omega)[1-f(\omega)] \ ,$$

where $\gamma_{nE}(\omega)$ is defined in Eq. (18). Straightforward though tedious calculations then lead to Eq. (2).

Adiabatic Approximation

Using a time-dependent Schrödinger equation corresponding to Eq. (5), and putting the solution ψ

$$\psi(q,z,t) = \sum_m \phi_m(qt) u_{mq}(z) \ , \qquad \text{(A5)}$$

we may derive equations for ϕ

$$i\hbar\dot{\phi}_l = \epsilon_l(q)\phi_l - \hbar^2/2M\,\phi_l'' + \sum_m M'_{ml}\phi_m' + \sum_m M_{ml}\phi_m \ , \qquad \text{(A6)}$$

where

$$M'_{ml} = -\frac{\hbar^2}{M}\int u^*_{lq}(z)\,\frac{\partial}{\partial q}\,u_{mq}(z)dz \ , \qquad \text{(A7)}$$

$$M_{ml} = -\frac{\hbar^2}{2M}\int u^*_{lq}(z)\,\frac{\partial}{\partial q^2}\,u_{mq}(z)dz \ . \qquad \text{(A8)}$$

For our purposes we may assume $\epsilon_l(q)$ to be linear in q near $q = p_F$, which is the important region. If we put

$$\phi_l = a_l(t)e^{-i\epsilon_l(q)t/\hbar}e^{-i(\epsilon_l')^2t^3/6M\hbar} \ , \qquad \text{(A9)}$$

where $a_l(0) = \delta_{ln}$, then

$$\dot{a}_l(t) \simeq -\frac{2i\epsilon_F t}{\hbar p_F}M'_{ml} + \frac{iM_{ml}}{\hbar}\ e^{-i[\epsilon_m - \epsilon_l(p_F)]t/\hbar} \ . \qquad \text{(A10)}$$

Since the largest values of t are of order τ, we conclude that the term in M' dominates and we find that

$$|a_l(\tau)| \simeq \frac{2v_F\tau}{|\epsilon_n - \epsilon_l|}M'_{nl} \ , \qquad \text{(A11)}$$

where

$$M'_{nl} = \hbar^2/Mp_F(a_l - a_n)^3 \ . \qquad \text{(A12)}$$

Thus we may estimate that the condition for the validity of the adiabatic approximation is

$$[(\omega_2\tau)^2/\omega\tau](n-\tfrac{1}{4})^2 \ll 1 \ , \qquad \text{(A13)}$$

which for low states is somewhat less stringent than our previous condition, but for high states is a stronger condition.

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Energy Levels of Bloch Electrons in Magnetic Fields*

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From the calculation of the energy levels of conduction electrons in a simple model of a metal in a magnetic field three interesting results emerge. (a) Quantum corrections to Onsager's semiclassical quantization formula are found to be sufficiently small that the usual interpretation of the de Haas–van Alphen effect should provide an accurate measure of Fermi-surface cross sections in potassium. (b) The undetermined constant appearing in Onsager's formula is found to be $\frac{3}{4}$ for effects due to "lens" orbits in hexagonal metals when the magnetic field lies in the basal plane. (c) The quantization of energy levels in a variety of periodic open orbits is predicted to be observable in principle through cyclotron-resonance experiments in a suitable geometry in the intermediate magnetic-breakdown regime.

I. INTRODUCTION

One of the most useful concepts in the theory of metals is that of the quantization of the orbits of conduction electrons in a magnetic field. A semiclassical treatment due to Onsager[1] predicts that in the presence of a uniform magnetic field $\vec{B}$ the area $\vec{a}(\mathcal{E})$ in wave-number space of an allowed orbit is given by

$$\vec{a}(\mathcal{E}) = (n+\sigma)(2\pi e/\hbar c)\vec{B}\,, \tag{1}$$

where n is an integer and σ is an unspecified constant. These orbits are intersections of surfaces of constant energy with planes perpendicular to $\vec{B}$.

More recently it has been found[2] that if $\vec{B}$ is large enough, the phenomenon known as magnetic breakdown can occur, resulting in tunneling of electrons from one of the semiclassically allowed orbits to another such orbit. Although calculations using this tunneling concept have provided results consistent with most observations of the de Haas–van Alphen and similar effects, such work does not provide an entirely satisfying description from a theoretical point of view. The phenomena involved depend upon the energy-level structure of electrons in a constant lattice potential and a constant magnetic field, and hence are describable in terms of the eigenstates of a time-independent Hamiltonian. It accordingly is of interest to investigate the energy-level structure that corresponds in the time-independent picture to the interpretation in terms of tunneling between orbits in the time-dependent description.

The difficulty of solving the Schrödinger equation for this problem makes it convenient for us to consider what we will call the "sandwich" model,[3] in