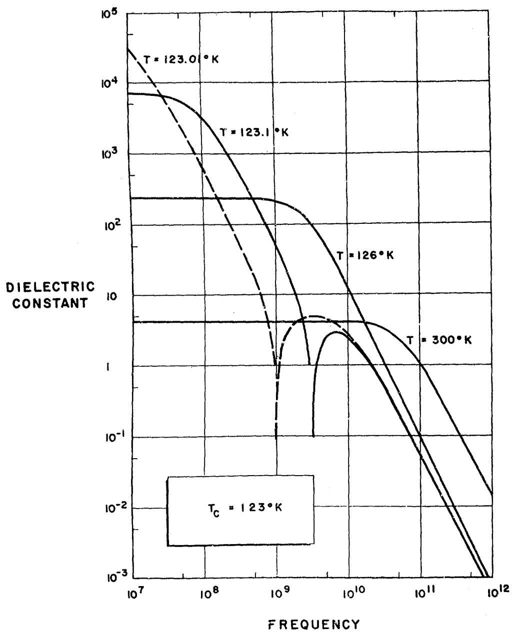

FIG. 2. Dielectric constant as a function of frequency.

ative before reaching a minimum, and then asymptotically approaches zero. In Fig. 2 the absolute value of the dielectric constant has been plotted.

There have been several experimental studies[6] of the frequency-dependent dielectric constant of deuterated and nondeuterated KH_2PO_4. Hill and Ichiki have measured the dielectric relaxation in deuterated KH_2PO_4 and have interpreted their results in terms of a Debye relaxation form for the dielectric constant that is averaged over a Gaussian distribution of relaxation times. One can obtain a similar expression to that of Hill and Ichiki by taking a Gaussian average over the relaxation time T_1, with the tunneling frequency set equal to zero. In any subseqent analysis of the results of experiment, the preceding theory can be generalized, if need be, by averaging over relaxation times and energy separations in the presence of finite tunneling frequencies.

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LANDAU LEVELS AT SADDLE POINTS AND MAGNETOACOUSTIC EFFECTS

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The calculation of Landau quantization in a magnetic field, near a singular point of the surface $\epsilon = \text{const}$, is of primary importance for the study of magnetoacoustic effects in solids. Certain aspects of this problem have been considered by several authors. Lifshitz[1] gives a semiclassical treatment for a saddle point with a particular direction of the magnetic field. More recently, Baldareschi and Bassani[2] reconsidered the problem in connection with magneto-optical effects. They predict the disappearance of the Landau quantization at a singular point when the magnetic field falls outside a cone of angle θ (θ being determined by the effective masses).[3]

In this Letter we shall consider the problem in a more general aspect, i.e., the Landau quantization either near a singular point or near a saddle point, for an arbitrary orientation of the magnetic field. We shall show also that, for H outside the θ cone, Landau levels exist, in general, except for very special combinations of values of the energy ϵ and momentum ζ.

We shall use a semiclassical treatment that, at present, is the only approximation that takes into account the actual shape of the surface $\epsilon = \text{const}$. As a consequence the cyclotron frequency, which is a property of the full orbit on these surfaces, is correctly determined.

For a discussion of the sound absorption in solids in a magnetic field, it will be stressed that the only electrons which may interact with phonons are those whose momentum ζ in the H direction takes the value $\zeta=\zeta_0=m^*u/\hbar\cos\beta$, where $\vec{u}$ is the sound velocity and β is the angle between $\vec{H}$ and $\vec{u}$. As a consequence, nonextremal Fermi-surface cross sections will be found from experiments.[4]

In the following we will use the term "saddle point" for a point belonging to a surface $\epsilon=\text{const}$ in which the total curvature is negative, reserving the term "singular point" to the point in k space in which the energy $\epsilon=\epsilon(\vec{k})$ becomes extremal (conic double point).

Labeling by k_1, k_2, k_3 a suitable frame of reference, in the neighborhood of the singular point the function $\epsilon=\epsilon(k)$ may be expanded as follows:

$$\epsilon=\epsilon_0+\frac{\hbar^2}{2}\left(\frac{k_1^{\,2}}{m_1}+\frac{k_2^{\,2}}{m_2}-\frac{k_3^{\,2}}{m_3}\right), \tag{1}$$

where ϵ_0 is the value of the energy at the singular point and m_1, m_2, and m_3 are positive quantities (effective masses). The origin of the frame of reference is chosen at the singular point. For $\epsilon=\epsilon_0$ the surface reduces to an elliptical cone with vertex at the singular point. For $\epsilon<\epsilon_0$ the surface exhibits a positive curvature, while for $\epsilon>\epsilon_0$ the curvature of the surface $\epsilon=\text{const}$ is negative (see Fig. 1).

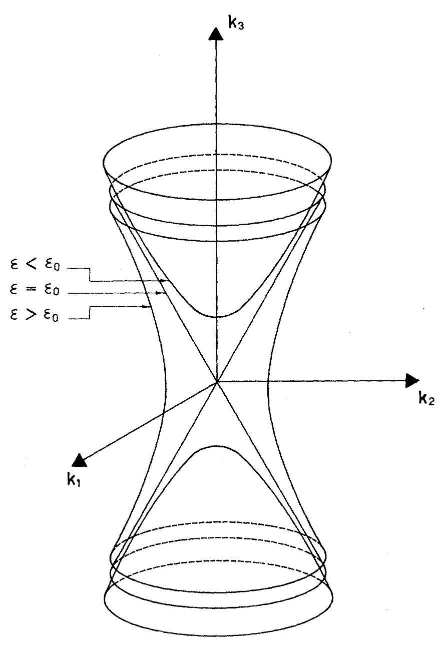

FIG. 1. Dispersion law near the singular point.

Let us now consider the intersection of surface given by Eq. (1) with a general plane π. Without loss of generality, we suppose that the normal $\vec{n}$ at π belongs to the k_2, k_3 plane. We label by k_x, k_y, k_z a new frame of reference having the same origin as k_1, k_2, k_3, but with the k_z axis perpendicular to the plane π.

The intersection between the surface $\epsilon=\text{const}$ and the plane π is a curve parallel to the k_x, k_y plane. Its equation is obtained by writing Eq. (1) in the frame of reference k_x, k_y, k_z and giving to k_z an assigned value ζ.

One obtains the equation

$$\epsilon=\epsilon_0+\alpha\zeta^2+\beta k_x^{\,2}+\gamma k_y^{\,2}+2\delta\zeta k_y, \tag{2}$$

where

$$\alpha=\frac{\hbar^2}{2}\left(\frac{\sin^2\theta}{m_2}+\frac{\cos^2\theta}{m_3}\right),$$

$$\beta=\frac{\hbar^2}{2m_1},$$

$$\gamma=\frac{\hbar^2}{2}\left(\frac{\cos^2\theta}{m_2}-\frac{\sin^2\theta}{m_3}\right),$$

$$\delta=\frac{\hbar^2}{2}\sin\theta\cos\theta\left(\frac{1}{m_2}+\frac{1}{m_3}\right), \tag{3}$$

θ being the angle between k_3 and k_z. Depending on the angle θ, Eq. (2) may describe an ellipse (if $\gamma>0$) or a hyperbola (if $\gamma<0$), which are the orbits of an electron in a magnetic field applied along the k_z direction.

The hyperbolic orbits, however, do not actually exist. The actual orbits must be closed, and only near the saddle point can they be approximated by an arc of hyperbola.

The spacing between Landau levels is $\hbar\omega_c$, ω_c being the cyclotron frequency

$$\omega_c=\frac{2\pi eH}{c\hbar^2}\left[\int\frac{dk_y}{(\partial\epsilon/\partial k_x)}\right]^{-1}, \tag{4}$$

the integral being calculated along the total orbit.

For $\gamma>0$ (elliptical orbit) one obtains, from Eqs. (4) and (2),

$$\omega_c=\frac{eH}{c\hbar^2}2(\beta\gamma)^{1/2}\quad(\gamma>0). \tag{5}$$

Because $\beta\gamma$ is independent of ϵ and ζ, the same holds for ω_c.

When $\gamma<0$, however, following Lifshitz and Kaganoff we may limit our evaluation of the integral of Eq. (6) to the arc of the hyperbola.

Actually, in fact, the largest contribution to the integral is given by the arc of the orbit close to the singular points, in the vicinity of which the electron velocity v becomes smaller and smaller. In such a case, we have

$$\omega_c = \frac{2\pi e H}{c\hbar^2}\left\{\frac{1}{(-\beta\gamma)^{1/2}} \times \ln\left|\frac{-2(\gamma Y+\delta\zeta)+[(\gamma Y+\delta\zeta)^2-\Delta]^{1/2}}{\sqrt{\Delta}}\right|\right\}^{-1}, \quad (6)$$

where $\Delta = \delta^2\zeta^2+\gamma(\epsilon-\epsilon_0-\alpha\zeta^2)$, and Y represents the k_y coordinate of the end point of the arc of the hyperbola. The result diverges logarithmically as the quantity Δ goes to zero. As a consequence, in such a condition ω_c goes to zero and Landau levels no longer exist.

Let us examine briefly the condition of disappearance $\Delta \to 0$.

(1) At the critical energy $\epsilon=\epsilon_0$, and if Δ approaches zero, the quantity $\zeta^2(\delta^2-\alpha\gamma)$ must also approach zero. Because $\delta^2-\alpha\gamma\neq 0$, the disappearance of Landau levels occurs when $\zeta\to 0$, i.e., when the secant plane passes through the singular point.

It is interesting to note, on the other hand, that Landau levels actually exist for the condition $\epsilon=\epsilon_0$, $\zeta=0$, as long as γ is greater than zero (elliptical case). This circumstance may be explained as follows. The condition $\gamma>0$ means that the direction of magnetic field is contained in the elliptical cone $\epsilon=\epsilon_0$. The sections with plane $k_z=\zeta$ are ellipses whose perimeter goes to zero as ζ goes to zero. At the same time, v also goes to zero, i.e., the velocity in k space $|\dot{\vec{k}}| = (e/c)v_\perp H$ vanishes. As a consequence, the period $2\pi/\omega_c$ is left constant. For $\gamma<0$, however, the H direction falls outside the cone $\epsilon=\epsilon_0$ and the sections with plane $k_z=\zeta$ are of nonvanishing length, as $\zeta\to 0$. In such a case, the period becomes infinite as $v\to 0$ and consequently Landau levels disappear.

(2) $\zeta=0$, $\epsilon\neq\epsilon_0$.—Because $\gamma<0$, intersections exist only for $\epsilon<\epsilon_0$.[5] Intersections are again hyperbolas, and Landau levels disappear as $\epsilon\to\epsilon_0$.

(3) $\zeta\neq 0$, $\epsilon\neq\epsilon_0$.—In this case it is to be pointed out that only surfaces $\epsilon_0<\epsilon=\text{const}$ are to be considered. This is because under such conditions $\Delta\to 0$ does not imply the closeness of the orbit to the singular point. Nevertheless, for $\epsilon>\epsilon_0$ (surfaces with negative curvature), there exist saddle points at which $v_\perp$ goes to zero, and therefore the calculation of integral (6) is again correct. For $\epsilon<\epsilon_0$, however, this is not the case. No points exist at which $v_\perp$ goes to zero and Eq. (6) is no longer true.

The condition $\Delta=0$ gives for ζ the values

$$\zeta = \pm\left[\frac{\gamma(\epsilon-\epsilon_0)}{\alpha\gamma-\delta^2}\right]^{1/2}. \quad (7)$$

Substitution of these values into Eq. (2) gives as the intersection two straight lines:

$$k_y = \pm\left(\frac{\beta}{-\gamma}\right)^{1/2} k_x - \left[\frac{(\epsilon-\epsilon_0)\delta^2}{-\alpha\gamma+\delta^2}\right]^{1/2}. \quad (8)$$

This means that the secant plane intersects the surface with negative curvature at a saddle point. Only at this point do Landau levels again disappear.

The possible existence of Landau quantization for H outside the θ cone is related to the finiteness of the orbits, while their disappearance is related to the vanishing of $v_\perp$. However, in the Baldareschi and Bassani treatment the disappearance of quantization seems to be related to the infinite length of electron orbit that holds for H outside the θ cone, if the expansion for the function $\epsilon=\epsilon(k)$ is assumed valid in the entire k space.

In conclusion we have the following picture: When the plane orthogonal to H becomes tangent to the surfaces $\epsilon=\text{const}$ at a point of positive curvature, Landau levels exist. If the plane becomes tangent at a point of negative curvature, Landau levels do not exist. At a singular point, levels do or do not exist depending on the orientation of the magnetic field.

The magnetoacoustic effect offers the possibility for checking the results listed above. In fact, it is possible to change continuously the value of ζ, maintaining fixed the H direction, outside the θ cone. Therefore, the oscillations of the acoustic absorption coefficient would disappear only when ζ takes the value given by Eq. (7). Such measurements have been performed in our laboratory, and are still in progress.[6] The experimental results confirm our point of view: In fact, we observe the Landau quantization for every H direction and its disappearance, for particular directions of H, only with a particular value of ζ.

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POSITRON ANNIHILATION IN COPPER SINGLE CRYSTALS AND ITS RELEVANCE TO THE FERMI SURFACE*

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Positron annihilation studies with a collinear point detector geometry have been carried out on a copper single crystal and reveal an angular dependence consistent with the shape of the Fermi surface superimposed upon an anisotropic contribution from the filled Brillouin zones.

The first attempt to relate the results of positron annihilation in copper single crystals to the shape of the copper Fermi surface was made by Berko and Plaskett.[1] Their results revealed little anisotropy since their detector geometry was arranged in the standard manner known as the "wide-slit" geometry. In this geometry the specimen is placed with respect to two parallel detector slits so that coincidences are detected only between annihilation γ rays corresponding to a well-defined z component of the center-of-mass momentum of the electron-positron pair. No restriction is placed upon the size of the other momentum components. The results obtained revealed that a considerable fraction of the annihilation occurred at momenta larger than the Fermi momentum, and it was suggested that the results could be treated as a superposition of the momentum distribution of the $3d$ and $4s$ electrons.

Fujiwara and collaborators[2] have since improved the resolution by restricting the length of the two slits so as to limit a second component of the momentum to a value less than the Fermi momentum. This substantially reduces the fraction of the coincidences due to high-momentum states while retaining those due to states within the Fermi surface. The results reveal considerable structure which may be correlated with the known Fermi surface of copper[3]; in particular, the necks forming contact with the Brillouin-zone boundary may be detected. In a preliminary experiment[4] using a rather different detection geometry which we shall call a collinear point geometry, our group independently observed the necks in the copper Fermi surface. The present Letter reports an experiment carried out with improved resolution.

The specimens used were copper single crystals which were neutron irradiated at Chalk River to produce positron-active Cu^{64} (half-life 12.7 h) and then flown to Vancouver. The initial positron activity of the samples of approximately 200 mCi allowed useful measurements to be taken for two days. Each detector presented a small circular aperature of 6 mm diam to the γ rays, and the detectors and sample were arranged collinearly so that coincidences were detected only between γ-ray pairs having an angular correlation of 180° to within the resolution of the apparatus. The detectors were 25 ft distant from the specimen and the experimental resolution function was calculated to be closely a Gaussian of half-width 1 mrad with cylindrical symmetry about the axis of the apparatus.

Neglecting the small effect of the positron momentum, the coincidences observed correspond, in the limit of infinitely narrow resolution, to those electrons whose momenta are in the direction of the γ-ray detectors. Were