or associated liquids the possibility of structural changes near the liquid surface for depths up to several thousand angstroms.[9,10] While this effect does not seem to be important in the liquids studied, it cannot be simply dismissed on the basis of present experimental evidence. Thus, higher resolution experiments are needed for a completely conclusive interpretation of the surface scattering.

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LANDAU LEVELS AND MAGNETO-OPTIC EFFECTS AT SADDLE POINTS

A. Baldereschi
Scuola Normale Superiore, Pisa, Italy

and

F. Bassani
Istituto di Fisica dell'Università di Pisa, Pisa, Italy, and Gruppo Nazionale di Struttura della Materia del Consiglio Nazionale delle Richerche, Rome, Italy

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We give a quantum-mechanical treatment for the eigenstates of electrons near saddle points of the energy bands in the presence of a constant magnetic field. We find that Landau-type levels exist depending on the orientation of the magnetic field. Correspondingly, we find peaks in the interband transition probabilities and discuss selection rules on the Landau quantum numbers. We show the behavior of the optical constants for a chosen direction of the magnetic field, and indicate experimental consequences.

The quantum effects produced by a magnetic field near minima or maxima of energy bands have been studied extensively.[1-3] It has been shown that Landau levels are produced by the magnetic field and singularities in the interband transition probabilities are produced accordingly. This gives rise to magneto-optic effects corresponding to M_0 transitions between maxima of the valence band and minima of the conduction band.[4-6] A general theory of the magnetic quantum states for arbitrary shape of the energy bands has been given by Lifshitz[7] in the semiclassical limit.

We consider nondegenerate bands and expand the energy as follows, taking the origin at the saddle point:

$$E(k)=E_0+\alpha_x\hbar^2k_x^{\,2}+\alpha_y\hbar^2k_y^{\,2}+\alpha_z\hbar^2k_z^{\,2}. \tag{1}$$

We choose the axes in such a way that α_x and α_y have sign opposite to α_z. Following the procedure of Luttinger and Kohn,[8] we obtain the energy values in presence of a magnetic field, by solving the equation

$$\{\alpha_x[p_x-(e/c)A_x]^2+\alpha_y[p_y-(e/c)A_y]^2 +\alpha_z[p_z-(e/c)A_z]^2\}F(\vec{r})=(E-E_0)F(\vec{r}), \tag{2}$$

where $\vec{p}$ is the operator $-i\hbar\nabla$ and $\vec{A}$ is the vector potential. The wave functions are given in zero order by

$$\psi(\vec{r},\vec{H})=F(\vec{r})\psi(\vec{r},\vec{k}_0), \tag{2'}$$

$\psi(\vec{r},\vec{k}_0)$ being the Bloch function at $\vec{k}_0$. For our purposes we choose a gauge where the vector potential is defined as

$$\vec{A} = \tfrac{1}{2}\vec{H}\times\vec{r} + \tfrac{1}{2}\mathrm{grad}[H_y xz + H_z xy - H_x yz]. \tag{3}$$

With the Hamiltonian of Eq. (2) and the vector potential (3), the commuting constants of motion are

$$p_y \tag{4a}$$

and

$$\vec{H}\cdot\vec{p} - (e/c)H_z H_y x = S, \tag{4b}$$

where S indicates the dot product of the momentum and the magnetic field. We make use of the constant of motion (4b) and of expression (3) to perform a canonical transformation which reduces the Hamiltonian (2) to a simple quadratic form. The new canonically conjugate variables are

$$p = p_z - (\alpha_x\alpha_y H_z/\alpha)S \tag{5a}$$

and

$$q = -\frac{c}{eH_y}\left(p_x - \frac{e}{c}H_y z\right) - \frac{c}{e}\frac{\alpha_y H_x H_z}{\beta H_y}\left(p_z - \frac{S}{H_z}\right), \tag{5b}$$

where

$$\alpha = \alpha_x\alpha_y H_z^{\,2} + \alpha_z\alpha_x H_y^{\,2} + \alpha_y\alpha_z H_x^{\,2}, \tag{6$'$}$$

and

$$\beta = \alpha_y H_x^{\,2} + \alpha_x H_y^{\,2}. \tag{6$''$}$$

The Hamiltonian (2) becomes

$$\mathcal{H} = \frac{\alpha}{\beta}p^2 + \frac{e^2}{c^2}\beta q^2 + \frac{\alpha_x\alpha_y\alpha_z}{\alpha}S^2. \tag{7}$$

When $\alpha > 0$, the Hamiltonian (7) is that of a harmonic oscillator and the eigenvalues are

$$E - E_0 = (n + \tfrac{1}{2})\frac{\beta}{|\beta|}\frac{2e\hbar}{c}\alpha^{1/2} + \frac{\alpha_x\alpha_y\alpha_z}{\alpha}S^2. \tag{8}$$

When $\alpha < 0$, the Hamiltonian (7) has continuous eigenvalues.

The above results indicate that discrete quantum levels exist also at saddle points of the energy bands in solids and are given by formula (8), provided the orientation of the magnetic field with respect to the z axis is within an elliptical cone, as indicated in Fig. 1. The spacing between the quantum levels is given by $(2e\hbar/c)\sqrt{\alpha}$, in agreement with the result of the semiclassical treatment.[7]

The existence of discrete quantum states produces peaks in the magneto-optic constants. The number of such peaks and their sharpness depend on the dipole matrix elements $M_{nk_ys;n'k_y's'}$ for transitions between the state n, k_y, s in the valence band and the state n', k_y', s' in the conduction band. Since the eigenfunctions are given by formula (2$'$), and $F(r)$ is nearly a constant in the unit cell ($\nabla F/F$ can be neglected), we obtain

$$M_{nk_ys;n'k_y's'} = \int d\vec{r}\,\psi_c^*(\vec{k}_0\vec{r})\vec{e}\cdot\nabla\psi_v(\vec{k}_0,\vec{r}) \times \int d\vec{r}\,F_{cn'k_y's'}^*(\vec{r})F_{vnk_ys}(\vec{r}). \tag{10}$$

For allowed transitions at the critical point, the first matrix element in (10) can be taken as a constant, and selection rules are obtained from the second integral. Since p_y and S are the same operators in the valence and the conduction band, the selection rules $k_y = k_y'$ and $s = s'$ are always satisfied, while the selection rule on the magnetic quantum numbers n and n' does not exist in general because the F's are eigenfunctions of different harmonic oscillators, centered at different points. We obtain the usual selection rule $n = n'$ when the Hamiltonian for the valence band is proportional to the analogous Hamiltonian for the conduction band. For a general orientation of the mag-

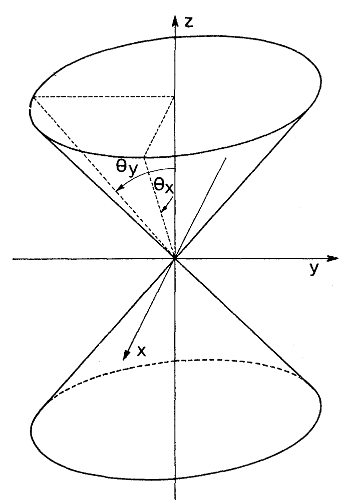

FIG. 1. Orientations of the magnetic field and existence of discrete quantum levels at a saddle point. Discrete quantum magnetic levels exist only if the direction of the magnetic field is inside the elliptical cone, here indicated by the intersections with the planes xz and yz [$\tan\theta_x = (-\alpha_x/\alpha_z)^{1/2}$, $\tan\theta_y + (-\alpha_y/\alpha_z)^{1/2}$].

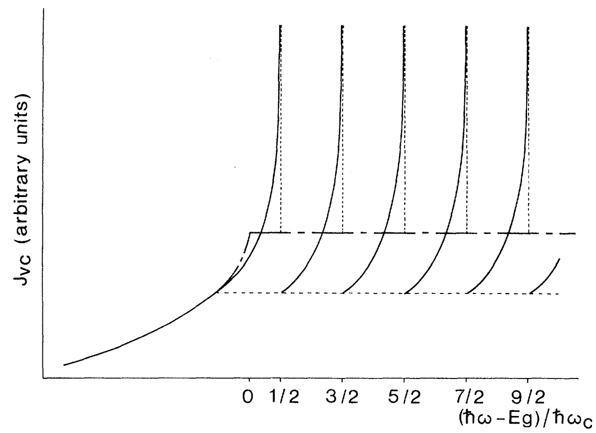

FIG. 2. Joint density of states at a critical point M_1 in the presence of a magnetic field placed in the z direction, where the effective mass is negative. The quantity $\hbar\omega_c$ indicates the cyclotron energy appropriate to the reduced transversal mass $1/m = 1/m_c - 1/m_v$, and E_g is the energy gap at the critical point. The zero-field case is also shown (broken line).

netic field, this implies that the effective masses in the valence band and the conduction band be proportional. When the magnetic field is the z direction and there is rotational symmetry with respect to the z axis, the selection rule $\Delta n = 0$ is satisfied.

When discrete levels exist and the selection rule $\Delta n = 0$ is valid, the divergences in the joint density of states

$$J_{vc} = C\sum_n \int ds\, \sigma(E_{nc}(s) - E_{nv}(s) - \hbar\omega) \qquad (11)$$

give divergences in the optical constants, which result in sharp peaks corresponding to the quantum magnetic levels. If the selection rule on the magnetic quantum number is not valid, the matrix element (10) depends on s and the peaks in the optical constants are broader.

When we consider the removal of the spin degeneracy by the magnetic field we obtain a doubling of all levels, and the usual selection rules for polarized light hold.[3,4]

We present in Fig. 2 the joint density of states computed from Eq. (11) for optical transitions of the type M with rotational symmetry with respect to the z axis, in the presence[1] of a magnetic field in the z direction. It is well known that optical transitions of type M_1 are responsible for strong peaks in the reflectivity of most semiconductors.[9] The results of Fig. 2 indicate that a fine structure due to the quantum levels should be observed by magnetoreflectance experiments. Figure 2 shows that the fine structure appears at the higher energy side of the peak, which is also shifted to higher energy.

We believe that magnetoreflectance experiments of the type suggested should provide even more detailed information on the nature of the critical points than that which can be obtained by electroreflectance experiments.[10] Furthermore, magnetoelectro-optic effects could lead to a measurement of the effective masses at the point M_1 in a similar way to what has been shown for the point M_0.[11]

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