Magnetocoulomb levels in semiconductors with strongly anisotropic electron dispersion

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The binding energy I between an electron and a charged impurity in a semiconductor with elongated equal-energy surfaces is determined in the presence of a quantizing field. It is shown that $I(B) \sim B^{1/2}$ in a wide range of field intensities, in contrast to the isotropic model for which the $I(B)$ dependence is much weaker. The case of transverse anisotropy is investigated and the optical absorption spectra are analyzed.

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As shown in a number of papers,[1-3] the binding energy of an electron with a Coulomb center can be appreciably increased in the presence of a strong magnetic field. For a hydrogen atom, the required fields are of the order of 10^9 G, and in the case of impurity states or excitons in semiconductors with small effective mass m and large dielectric constant κ, the characteristic fields decrease to values $B \sim (m/m_0\kappa)^2 \times 10^9$ G. The influence of a magnetic field on Coulomb systems in a solid was investigated in[4,5].

In this study we investigate the singularities of the magnetocoulomb levels in crystals with highly anisotropic electron dispersion. We consider the case of strongly elongated equal-energy surfaces, a case realized, e.g., in Ge and Si, and also in the semiconducting $Bi_{1-x}Sb_x$ alloys. In the first section of the article we consider the axially symmetrical case, in the second we show how to take into account the transverse anisotropy of the spectrum, and in the third we estimate certain optical characteristics of the investigated systems. We note that, with the exception of a small number of studies,[6,7] the bulk of the results on magnetocoulomb levels was obtained for a standard isotropic spectrum. A preliminary communication, containing some of the results of the present paper, and also experimental data on $Bi_{1-x}Sb_x$ alloys, was published earlier.[8]

1. We confine ourselves first to the case when the electron dispersion law is described by the formula

$$\varepsilon(\mathbf{k}) = (k_x^2+k_y^2)/2m_\perp + k_z^2/2m_z, \tag{1}$$

and the effective masses satisfy the inequality $m_z \gg m_\perp$. The equal energy surfaces are ellipsoids of revolution that are strongly elongated along the z axis.

Let the magnetic field be parallel to the symmetry axis, and let the potential of the Coulomb field be spherically symmetrical. The Schrödinger equation is written in the form

$$\varepsilon\Psi = \left\{\frac{\hat{k}_x^2+\hat{k}_y^2}{2m_\perp} + \frac{\hat{k}_z^2}{2m_z} - \frac{e^2}{\varkappa r}\right\}\Psi, \tag{2}$$

where

$$\hat{k}_x = -i\frac{\partial}{\partial x} - \frac{e}{c}A_x, \quad \hat{k}_y = -i\frac{\partial}{\partial y} - \frac{e}{c}A_y, \quad k_z = -i\frac{\partial}{\partial z}.$$

It is convenient to choose the vector potential in the form $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$.

The first stage of the procedure for solving (2) is the same as in the isotropic case. The wave function is sought in the factorized form

$$\Psi(\rho, z) = \varphi_{nm}(\rho) f_{nm}(z), \tag{3}$$

where $\varphi_{nm}(\rho)$ is the solution of the purely magnetic problem (see[9]), and the functions $f_{nm}(z)$ satisfy the equation

$$\varepsilon_{nm} f_{nm}(z) = \{\hat{k}_z^2/2m_z + V_{nm}(z)\} f_{nm}(z) \tag{4}$$

with potential energy

$$V_{nm}(z) = -\frac{e^2}{\varkappa}\int \frac{|\varphi_{nm}(\rho)|^2\, d\rho}{(\rho^2+z^2)^{1/2}} \qquad \varepsilon_{nm} = \varepsilon - (2n+m+|m|+1)\frac{eB}{2m_\perp c}.$$

The approximation (3) is valid under the condition that the magnetic length $a = (2c/eB)^{1/2}$ is much smaller than the Bohr radius $a_\perp = \kappa/m_\perp e^2$; this leads to the condition

$$B \gg m_\perp^2 e^3 c/\varkappa^2 \sim (m_\perp/m_0\varkappa)^2 \cdot 10^9 \text{ G}. \tag{5}$$

The potentials $V_{nm}(z)$ decrease at $|z| \gg a$, if the quantum numbers are not too large, in accord with the Coulomb law, and are cut off near the center at distances on the order of a. The depth of the effective potential well and the behavior of $V_{nm}(z)$ at small z depend on n and m. In particular,

$$V_{00}(z) = \begin{cases} -e^2/\varkappa|z| & \text{if } |z| \gg a \\ -e^2\sqrt{\pi}/\varkappa a + 2e^2|z|/\varkappa a^2 & \text{if } |z| \ll a, \end{cases} \tag{6}$$

$$V_{01}(z) = \begin{cases} -e^2/\varkappa|z| & \text{if } |z| \gg a \\ -e^2\sqrt{\pi}/2\varkappa a + e^2 z^2\sqrt{\pi}/2\varkappa a^3 & \text{if } |z| \ll a. \end{cases} \tag{7}$$

We call attention to the different variations of the energy near the bottom of the potential well. It can be shown that the form of $V_{nm}(z)$ at $m = 0$ and at arbitrary n is analogous to the form (6), and at $m \neq 0$ it is similar to (7).

The distinguishing feature of the anisotropic system becomes manifest in the solution of the one-dimensional Schrödinger equations (4). The point is that in our case, in contrast to the isotropic case, the inequality (5) imposed on the field does not determine the character of the solution uniquely. We have in mind mainly the relation between the scale of the wave function along the z axis and the quantity a. Whereas at $m_z \sim m_\perp$ the condition (5) led automatically to the relation $\bar{z} \gg a$, and the binding energy was much smaller than the depth of the potential well, in the case $m_z \gg m_\perp$, in a certain range of fields, it is possible for the opposite inequality to be satisfied

$$\bar{z} \ll a. \tag{8}$$

This is precisely the situation that is being investigated in this paper.

The binding energy of an electron with center I coin-

cides, if (8) is satisfied, with the depth of the potential well $V_{nm}(z)$, accurate to the "zero-point vibration" energy of the electron near the impurity. For the ground state n = m = 0 we have

$$I=\frac{\sqrt{\pi}}{\varkappa}\frac{e^2}{a}=\left(\frac{\pi eB}{2c}\right)^{1/2}\frac{e^2}{\varkappa}, \tag{9}$$

and for other quantum numbers we have $I_{nm} = \alpha_{nm}(eB/c)^{1/2}e^2/\kappa$ with the constants $\alpha_{nm} \sim 1$. We call attention to the much stronger dependence of I on B than in the isotropic case, where $I \sim \ln^2 B$.[1-3]

The region where (9) is valid is bounded by the condition (8), but to estimate $\bar{z}$ we can use formulas (6) and (7) at $z \ll a$ as well as the uncertainty relation. For n = m = 0 we obtain $\bar{z} \sim (\kappa a^2/m_z e^2)^{1/3}$, and for n = 0 and m = 1 we have $\bar{z} \sim (a^2\kappa/m_z e^2)^{1/4}$, which leads to the following corrections to the binding energy:

$$\delta I_{00}\sim\frac{e^2\bar{z}}{\varkappa a^2}\sim I_{00}\left(\frac{a_z}{a}\right)^{1/2},\quad \delta I_{01}\sim I_{01}\left(\frac{a_z}{a}\right)^{1/2},$$

where

$$a_z=\varkappa/m_z e^2.$$

We see that formula (9) is asymptotically exact in the limit as $m_z \to \infty$, but the small parameter contains m_z raised to small powers, so that for actual systems the accuracy of this formula may not be very high. However, the weakened inequalities $a_z < a < a_\perp$, at which formula (9) is valid at least qualitatively, hold true in a wide range of fields, namely at

$$(m_\perp/m_0\varkappa)^2 10^9\ \text{G} < B < (m_z/m_0\varkappa)^2\cdot 10^9\ \text{G},$$

which yields for Ge, for example, 30 kG < B < 10^8 G, and for the $Bi_{1-x}Sb_x$ alloys an interval 1 G < B < 10^5 G. We note that the experimental data on $Bi_{1-x}Sb_x$ agree with (9).

2. For a fully isotropic electron spectrum, the solution of the problem is much more complicated even in the asymptotic limit as $m_z \to \infty$. The motion of the particle in a plane perpendicular to the magnetic field is described by the two-dimensional Schrödinger equation

$$\varepsilon\Psi(x,y)=\left\{\frac{\hat{k}_x^2}{2m_x}+\frac{\hat{k}_y^2}{2m_y}-\frac{e^2}{\varkappa(x^2+y^2)^{1/2}}\right\}\Psi(x,y), \tag{10}$$

where k_x and k_y are the same as in (2).

In the case $m_x \neq m_y$, the variables in (10) cannot be separated, and calculation by perturbation theory is made difficult by the high degree of degeneracy of the states in the magnetic field. To trace qualitatively the dependence of the particle binding energy on the relation between m_x and m_y, we use the quasiclassical approximation in Eq. (10), assuming, just as in Sec. 1, the Coulomb field to be weak.

The equation of the classical trajectory of a particle with different masses is written in the form

$$x=(m_x\omega)^{-1/2}\sin\omega t,\quad y=(m_y\omega)^{-1/2}\cos\omega t, \tag{11}$$

where $\omega = eB/(m_x m_y)^{1/2}c$, and the amplitudes of the oscillations correspond to the free-state energy $\epsilon = \omega/2$. We then calculate with the aid of (11) the mean value of the Coulomb energy, which coincides, apart from the sign, with the binding energy I. We have

$$I=\frac{e^2}{\varkappa T}\int_0^T\frac{dt}{[x^2(t)+y^2(t)]^{1/2}}$$

$$=\frac{e^2\omega}{2\pi\varkappa}\int_0^{2\pi/\omega}dt\left(\frac{1}{m_x\omega}\sin^2\omega t+\frac{1}{m_y\omega}\cos^2\omega t\right)^{-1/2}$$

$$=\frac{e^2\sqrt{\omega}}{2\pi\varkappa}\int_0^{2\pi}d\varphi\left(\frac{\sin^2\varphi}{m_x}+\frac{\cos^2\varphi}{m_y}\right)^{-1/2}. \tag{12}$$

For $m_x = m_y$ we obtain from (12) $I = (eB/c)^{1/2}e^2/\kappa$, which differs insignificantly from the exact formula (9). In the case of large transverse anisotropy ($m_x \ll m_y$), Eq. (12) goes over into

$$I=\frac{e^2(m_x\omega)^{1/2}}{\pi\varkappa}\ln\frac{m_y}{m_x}=\left[\frac{1}{\pi}\left(\frac{m_x}{m_y}\right)^{1/2}\ln\frac{m_y}{m_x}\right]\frac{e^2}{\varkappa}\left(\frac{eB}{c}\right)^{1/2}.$$

We see that the particle binding energy decreases quite slowly as the ratio m_x/m_y tends to zero. We note, in concluding this section, that the results of the quasiclassical treatment of the problem agree very well with computer calculations. In particular, a noticeable decrease of I was obtained only at $m_x/m_y \sim 0.05$.

3. Let us dwell briefly on the singularities of the optical characteristics of the considered systems. We have in mind the spectra of electron absorption by impurity centers, so that problems of exciton absorption will not be considered here specially. For simplicity we deal mainly with the axially-symmetrical case.

We consider first the absorption of a wave whose electric vector is parallel to the magnetic field. In the principal approximation in the parameter $a/a_\perp$, formula (3) is valid, so that transitions can take place between states with identical n and m, i.e., between levels of a definite one-dimensional well. When the inequality (8) is satisfied for the ground state, a certain number of levels will also have a region of localization smaller than a, and the energy of these levels can be estimated with the aid of the quasiclassical quantization rules. For m = 0 this leads to a dependence on the number l of the level in the form $\epsilon_l \sim I(a_z/a)^{1/3}l^{2/3}$, and for $m \neq 0$ it leads to a dependence $\epsilon_l \sim I(a_z/a)^{1/2}l$. In the former case, for the most intense transitions, we have essentially a nonequidistant spectrum, and in the latter case the spectrum is equidistant. With increasing excitation energy, naturally, the condition $\bar{z}_l \ll a$ will no longer hold and will give way ultimately to the opposite inequality $\bar{z}_l \gg a$. The energy of these levels is given by the Balmer formula[1-3].

An appreciable difference between the absorption spectra of the isotropic and anisotropic systems appears in the case when the light is polarized perpendicular to the magnetic field. The selection rules cause the transition to take place with a change of m by ±1, particularly from the ground state with n = 0 and m = 0 to states with n = 0 and m = ±1. If we turn to formulas (6) and (7), we readily understand that the different behavior of the potential energy in the region $z < a$, and the unlike character of the dependence of the wave functions on z and on the magnetic field make the transitions between arbitrary states of the two groups sufficiently intense. The absorption spectrum will consist of a large number of lines of commensurate intensity.

To the contrary, in the isotropic model the wave functions have a scale $z \gg a$, the systems of levels with different n and m differ little, and the overlap integrals of functions with different numbers l are small. The absorption spectrum will therefore contain an intense line corresponding to the transition between the

corresponding states of different one-dimensional wells, and much weaker lines of other transitions.

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