Magnetocoulomb levels in semiconductors with Kane's dispersion law

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An analytic relation between the position of magnetocoulomb levels in semiconductors having Kane's dispersion law and the corresponding levels of the hydrogen atom is found. For a two-level Kane model in strong magnetic fields, the quantity γ^* has an upper limit and the energy of all levels varies as $\sim\sqrt{H}$.

The first calculation of the lower magnetocoulomb levels for n-InSb based on Kane's model was performed by Larsen[1] but a more complete analysis was carried out by Zawadzki and Wlasak.[2] A significant drawback of all existing calculations of this problem[1–4] is that they were performed only for particular values of the parameters in the dispersion law for InSb, so that if the parameters are changed or different compounds are used, then these laborious calculations must be repeated.

In this letter, we propose a new approach to this problem, which makes it possible to analytically determine the position of the magnetocoulomb levels from existing calculations for the hydrogen atom. This approach is based on the fact that a parabolic expansion of the Kane dispersion law can be carried out near the bottom of the corresponding Landau subband. The problem of the magnetocoulomb levels in Kane's model can thus be described by the same Schrödinger equation as in the quadratic case, except that the electron mass depends on the magnetic field.

For simplicity, we shall examine the two-level approximation of Kane's model, which is applicable when the spin-orbit splitting of the valence band, Δ, is larger than the energy of the forbidden band, ϵ_g. In this case, the energy of the electron in a magnetic field, as we know,[5] is described by the expression

$$E^s_N(p_z^2) = \frac{\epsilon_g}{2}\sqrt{1+\frac{4}{\epsilon_g}\left[\left(N+\frac{1}{2}+\frac{sg^*}{4}\right)\hbar\omega_c^0+\frac{p_z^2}{2m^*}\right]}, \qquad (1)$$

where N is the principal quantum number, the number of the Landau subband; $s = \pm 1$ is the spin; m^* is the effective mass at the band bottom; $\omega_c^0 = eH/m^*c$ is the cyclotron frequency; $g^* = \Delta/(\Delta + 2/3\epsilon_g)$ is the effective g factor; and the energy is measured here and everywhere below from the center of the forbidden band with $H = 0$ and $z\|\mathbf{H}$. For $p_z = 0$, expression (1) gives the position of the bottom of the Landau subband with the quantum numbers N and S, E^s_N. The position of the magnetocoulomb levels $E^s_{nm\lambda}$ is determined by the quantum numbers N, M, λ, and s.

We assume that the absolute binding energy $\epsilon^s_{NM\lambda} = E^s_{NM\lambda} - E^s_N$ of an electron in this state is much lower than the corresponding value of E^s_N; i.e., the bound states are shallow. The characteristic values of $p_z^2/2m^*$ for this problem in this case are also

much smaller than the values of E^s_N so that nonparabolic expression (1) can be replaced by its expansion to first order in p_z^2. The Schrödinger equation for this problem can therefore be written in the form

$$\left[\hat{H}(\hat{p}_\perp) + \frac{\hat{p}_z^2}{2m^s_N(H)} + V(\mathbf{r})\right]\Phi^s_{NM\lambda}(\mathbf{r}) = E^s_{NM\lambda}\Phi^s_{NM\lambda}(\mathbf{r}), \tag{2}$$

where $m^s_N(H) = \frac{1}{2}\left[\frac{\partial E^s_N(0)}{\partial p_z^2}\right]^{-1} = \frac{2E^s_N}{\epsilon_g}m^*$, and $H(\hat{p}_\perp)$ is the Hamiltonian which is nonquadratic with respect to $\hat{p}_\perp$ and which describes the purely magnetic two-dimensional ($p_z = 0$) problem for Kane's model. The eigenfunctions $\phi_{NM}(\rho, \phi)$ of $\hat{H}(\hat{p}_\perp)$, as we know,[5] are identical to the corresponding functions for the hydrogen atom. In strong fields, we can use the adiabatic approximation $\Phi^s_{NM\lambda}(\mathbf{r}) = \phi_{NM}(\rho, \phi)f^s_\lambda(z)$ (Ref. 3). As a result, Eq. (2) reduces to the one-dimensional Schrödinger equation

$$\left[\frac{1}{2m^s_N(H)}\frac{d^2}{dz^2} + V_{NM}(z)\right]f^s_\lambda(z) = \epsilon^s_{NM\lambda}f^s_\lambda(z), \tag{3}$$

where

$$V_{NM}(z) = -\frac{e^2}{\kappa}\int\frac{|\phi_{NM}(\rho,\phi)|^2\,\rho\,d\rho\,d\phi}{(\rho^2+z^2)^{1/2}}.$$

This relation is the same as the corresponding equation that is used for finding the magnetocoulomb levels in the parabolic case.[3] The only difference is that the quantity $m^s_N(H)$, which depends on H, is used in this relation, instead of a constant mass m^*. The problem of finding the magnetocoulomb levels for Kane's dispersion law thus reduces to the standard solutions for the hydrogen atom $\epsilon_{NM\lambda}/\mathrm{Ry} = \tilde{f}(\gamma)$, where γ and Ry must be replaced by their renormalized values $\gamma^* = \hbar^3\kappa^2 H|c[m^s_N(H)]^2e^3$ and $\mathrm{Ry}^* = m^s_N(H)e^4/2\hbar^2\kappa^2$. It should be emphasized that this assertion, as will be shown in a more detailed paper, is valid for the complete three-level Kane model for arbitrary magnetic fields, although the dependence $m^s_N(H)$ in this case is different.

The binding energies $\epsilon^s_{NM\lambda}$ for n-InSb obtained by this simple method agree to within 4% with the results of the complicated variational calculations in Ref. 2.

Let us examine in greater detail the two-level approximation of Kane's model. From the dependence $m^s_N(H) = 2E^s_N m^*/\epsilon_g$ it follows that in strong magnetic fields, such that $\hbar\omega^0_c \gg \epsilon_g$, the quantity γ^* approaches the limit

$$\gamma^*_\infty = \frac{1}{\alpha^2}\frac{1}{3(N+\frac{1}{2}+\frac{s}{4}g^*)}, \tag{4}$$

where $\alpha = e^2/\kappa\hbar K$ is the Born parameter, and K is the matrix element in Kane's model.

Thus, in semiconductors in which a two-level Kane dispersion law applies, the model-based parameter γ^* of the magnetocoulomb problem is bounded. Furthermore, the value $\gamma_\infty{}^*$ does not depend on ϵ_g. This nontrivial result leads to several interesting consequences.

First, the binding energy *for all* magnetocoulomb levels satisfying the condition $E_N^s \ll \Delta$ varies as $\sqrt{H}$ in a strong magnetic field

$$\epsilon_{NM\lambda}^s = \frac{e^2}{2\kappa\lambda}\frac{1}{\sqrt{\gamma_\infty^*}}\tilde{f}_{NM\lambda}(\gamma_\infty^*)\,, \tag{5}$$

where $\lambda = \sqrt{c\hbar/eH}$ is the magnetic length.

Second, the anisotropy of the wave function of the bound state is bounded, and the characteristic length of the exponential decay of $\Phi^s_{NM\lambda}(\mathbf{r})$ longitudinally in a strong magnetic field is described by

$$(a_\parallel^*)_\infty = \lambda\sqrt{\gamma_\infty^*}\, w_{NM\lambda}(\gamma_\infty^*)\,, \tag{6}$$

where $w_{NM\lambda}(\gamma)$ relates $a_\parallel$ for the corresponding wave function $\Phi_{NM\lambda}(\mathbf{r})$ of the hydrogen atom to the Bohr radius a_B: $a_\parallel = a_B w_{NM\lambda}(\gamma)$.

The basic assumption of our analysis that the bound states are shallow is satisfied for singly charged centers in a strong magnetic field when the following parameter is small:

$$\beta = \left(\frac{|\epsilon^s_{NM\lambda}|}{E_N^s}\right)_\infty = \frac{3}{4}\alpha^2\tilde{f}_{NM\lambda}(\gamma_\infty^*)\,. \tag{7}$$

The most convenient objects for checking the experimental results are alloys of

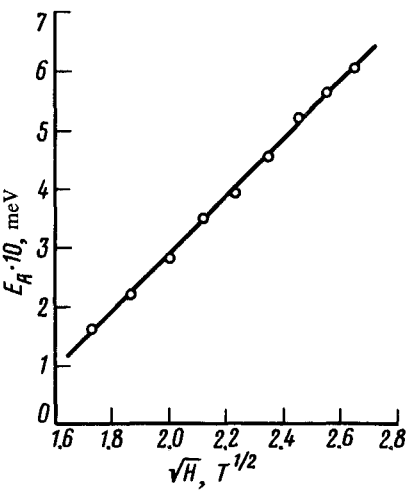

FIG. 1. The activation energy E_A of the temperature dependence of the resistance in the region of impurity conductivity for $Hg_{0.8}Cd_{0.2}Te$ as a function of $H^{1/2}$.[8]

$A^{II}B^{IV}$ compounds in the region of the direct spectrum near the gapless state, in particular, the alloys $Hg_{1-x}Cd_xTe$ with $0.16 \leqslant x \leqslant 0.2$, for which experimental data are currently available.

Using the characteristic values $\hbar K = 8.4 \times 10^{-8}$ eV·cm (Ref. 6) and $\kappa = 18$, (Ref. 7), we find that for $Hg_{1-x}Cd_xTe$ the parameter $\beta \leqslant 6 \times 10^{-2}$ for any values of N, M, and s. For the ground state, we then obtain $\gamma_\infty^* = 150$, while $(a_\parallel^*/a_\perp^*)_\infty = 3.6$. The condition $\hbar\omega_c^0 = \epsilon_g$ with $x = 0.18$ is satisfied for $H = 8$ kOe.

Figure 1 shows the measured values of the activation energies E_A, obtained from the temperature dependences of the resistance in the region of impurity conductivity for $Hg_{0.8}Cd_{0.2}Te$, (Ref. 8) as a function of $H^{1/2}$. In accordance with expression (5), these data are described well by a straight line.

The metal–insulator transition in strong magnetic fields in n-InSb was studied in detail in Ref. 9 and it was established that the critical donor concentration N_d is related to the values of $a_\parallel^*$ and $a_\perp^*$ for the ground state by a relation analogous to Mott's relation $N_d^{1/3}(a_\perp^{*2}a_\parallel^*)^{1/3} = 0.26$. An unusual criterion for such a transition was proposed for $Hg_{1-x}Cd_xTe$ ($0.13 \leqslant z \leqslant 0.19$) in Ref. 10: $N_c^{1/3} \times 2\lambda = 0.37$, where N_c is the electron density in the conduction band. A remarkable property of this relation is that it is satisfied for samples with different values of x and, therefore ϵ_g. The apparent discrepancy between the results of Refs. 9 and 10 is eliminated in our analysis, since, according to expression (6), $(a_\parallel^*)_\infty \sim \lambda$ and since it does not depend on ϵ_g. If the known parameters of $Hg_{1-x}Cd_xTe$ are used, then the expression $N_d \times 2\lambda = 0.34$ can be obtained in a strong magnetic field from the relation in Ref. 9, obtained with $\hbar\omega_c^0 \ll \epsilon_g$.

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