Cyclotron resonance in multivalley semiconductors with dislocations

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The splitting of Landau levels by dislocations in a multivalley semiconductor is analyzed. At cyclotron resonance in a magnetic field parallel to the dislocations, satellites appear at a distance $\beta\omega_c$ from the fundamental line, where $\beta \sim 1$. The broadening of a satellite line when the magnetic field deviates slightly from the direction of the dislocations is studied.

1. INTRODUCTION

The customary approach in the analysis of interactions between current carriers in an uncharged dislocation is the strain-energy approximation. In a multivalley semiconductor, a dislocation also produces an effective vector potential for the electrons of each valley.[1,2] For example, for a cubic crystal, in which the valley vector **k** lies along an axis of symmetry no lower than twofold, we have

$$A_n{}^d=-w_{jn}k_j+\gamma_1(w_{nj}+w_{jn})k_j+\gamma_2 w_{jj}k_n+\gamma_3 w_{jm}(k_jk_m/k^2)k_n, \quad (1)$$

where $w_{jm} = \partial u_j/\partial x_m$ is the distortion tensor, and $\gamma_i \sim 1$. The first term here is purely geometric, while the three others result from a displacement from the valley vector in **k**-space because of the deformation. In the most common case, $\mathbf{k} = \mathbf{K}/2$ (**K** is a reciprocal-lattice vector), there are no deformation terms, and the dislocation is equivalent to a narrow solenoid with a flux equal to half the quantum. If, on the other hand, we have $\mathbf{k}\neq\mathbf{K}/2$, then the dislocation will produce, in addition to the solenoid field, an effective magnetic field which falls off as $1/r_\perp{}^2$ with distance from the dislocation core.

In the present paper we analyze the splitting of Landau levels by dislocations in a strong magnetic field (we assume $r_c \ll n_d^{-1/2}, \omega_c\tau \gg 1$, where ω_c is the cyclotron frequency, r_c is the Larmor radius, n_d is the density of dislocations, and τ is the relaxation time).

The splitting of Landau levels by a line defect was studied in Refs. 3 and 4, but the interaction of the defect with electrons was described by a scalar potential of small radius. Such a potential would be a small perturbation in the presence of the vector potential (1), since all the wave functions decay in power-law fashion as $r_\perp \to 0$.

In the presence of a dislocation, the Hamiltonian of an electron in a magnetic field is

$$\hat{\mathscr{H}} = \sum_k \left(\frac{1}{2m_\parallel}\left(\hat{p}_\parallel - \frac{e}{c}A_\parallel{}^m - A_\parallel{}^d - k\right)^2 + \frac{1}{2m_\perp}\times\left(\hat{\mathbf{p}}_\perp - \frac{e}{c}\mathbf{A}_\perp{}^m - \mathbf{A}_\perp{}^d\right)^2\right) + U(\mathbf{r}).$$

The subscripts $\parallel$ and $\perp$ specify the components respectively parallel and perpendicular to the vector of the bottom of the valley, $U(\mathbf{r})$ is the strain energy, and $\mathbf{A}^m = (1/2)[\mathbf{r},\mathbf{H}]/2$.

2. SPLITTING OF A CYCLOTRON-RESONANCE LINE IN A MAGNETIC FIELD PARALLEL TO A DISLOCATION

We begin with the very simple case in which there is only a topological interaction between the electron and the dislocation[5–7] (i.e., there is no strain energy, and only the first term is present in the expression for $\mathbf{A}^d$), and the magnetic field is parallel to the dislocation. In this case, the dislocation is equivalent to a solenoid with a flux $\alpha = (\mathbf{kb})/2\pi$, in units of the quantum of flux (**b** is the Burgers vector). We introduce the dimensionless units

$$r_\perp' = \left(\frac{m_\perp}{m_a}\right)^{1/2}\frac{r_\perp}{a_H}, \quad r_\parallel' = \left(\frac{m_\parallel}{m_a}\right)^{1/2}\frac{r_\parallel}{a_H}, \quad \varepsilon = \frac{E}{\hbar\omega_c}.$$

Here

$$m_a=(m_\perp{}^2 m_\parallel)^{1/3}, \quad \omega_c=eH/cm_c, \quad a_H=(m_c/m_a)\hbar c/eH,$$

$m_c = (\cos^2\theta/m_\perp{}^2 + \sin^2\theta/m_\perp m_\parallel)^{-1/2}$ is the cyclotron mass, and θ is the angle between **k** and **H**. In terms of these units, in the cylindrical gauge, $A_\varphi = \rho/2$, the Schrödinger equation takes the form

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial\psi}{\partial\rho}+\frac{\partial^2\psi}{\partial z^2}+\left(\frac{1}{\rho}\left(\frac{\partial}{\partial\varphi}-i\alpha\right)+\frac{i\rho}{2}\right)^2\psi+2\varepsilon\psi=0.$$

The solution of this equation is

$$\psi_{p_z m n_\rho}(r)=\frac{\exp(ip_z z+im\varphi-\rho^2/4)}{(2\pi L_z)^{1/2}} \times\left(\frac{n_\rho!}{\Gamma(n_\rho+|m-\alpha|+1)}\right)^{1/2}\left(\frac{\rho}{2^{1/2}}\right)^{|m-\alpha|}L_{n_\rho}^{|m-\alpha|}\left(\frac{\rho^2}{2}\right),$$

where $\Gamma(x)$ is the gamma function, and $L_{n_\rho}^{\beta}(x)$ is a generalized Laguerre polynomial. The energy eigenvalues are (in dimensional units)

$$E=\frac{p_z{}^2}{2(m_\parallel\cos^2\theta+m_\perp\sin^2\theta)} + \hbar\omega_c\left[n_\rho+\frac{1}{2}(m-\alpha+|m-\alpha|+1)\right].$$

The dislocation thus gives rise to new energy levels (at $m>0$) $E_\perp = \hbar\omega_c(n-\alpha+1/2)$ (Fig. 1), which are n-fold degenerate. For electrons from the opposite valley we have $E_\perp = \hbar\omega_c(n+\alpha-1/2)$. If the valleys instead lie at the edge of the Brillouin zone, we will have $\alpha = 1/2$, and the new levels appear precisely halfway between Landau levels.

When an alternating electric field is imposed, the resonant transitions between Landau levels may be accompanied

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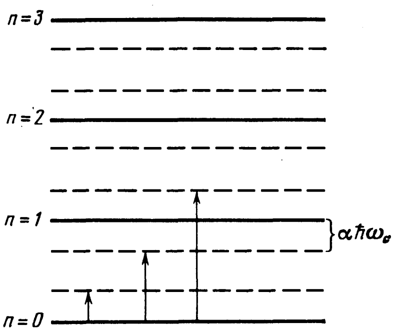

FIG. 1. Splitting of Landau levels by a dislocation in the topological approximation.

by transitions between a Landau level and a splitoff level (Fig. 1). Such transitions can occur between states with $m = 0$ and $m = 1$ (for the valley with $\alpha > 0$) or with $m = -1$ and $m = 0$ (for the opposite valley). Consequently, satellites appear on the cyclotron-resonance curve, in addition to the main peak at the frequency ω_c; these satellites appear at the frequencies $\alpha\omega_c$, $(1-\alpha)\omega_c$, $(1+\alpha)\omega_c$, $(2-\alpha)\omega_c \ldots$. If the valleys lie at the edge of the Brillouin zone, additional transitions arise at the frequencies $\omega_c/2$, $3\omega_c/2, \ldots$. Since there is a single transition at the shifted frequency per dislocation, the ratio of the intensity of the satellite to the intensity of the main peak is on the order of $n_c a_H^2$.

3. LINESHAPE IN THE CASE OF A SMALL ANGLE BETWEEN THE MAGNETIC FIELD AND THE DISLOCATION

The lineshape is sensitive to a deviation of the magnetic field from the direction of the dislocation. Let us assume that the dislocation makes a small angle β' with the direction of the magnetic field and is parallel to the xy plane. In dimensionless coordinates, this angle is related to the real angle β by

$$\cos\beta' = \frac{m_c(\theta)\, m_c(\varphi)}{m_\perp}\left(\frac{\cos\varphi}{m_\parallel} + \left(\frac{1}{m_\perp} - \frac{1}{m_\parallel}\right)\cos\theta\cos\varphi\right)$$

(φ is the angle between the valley vector and the dislocation). We introduce the change of variables $\tilde{x} = x - \varkappa z$ ($\varkappa = \operatorname{tg}\beta'$). In terms of these new variables, the Hamiltonian is

$$\hat{\mathscr{H}} = \frac{1}{2}\left\{\left(p_x - \frac{y}{2} + \frac{\alpha y}{\rho^2}\right)^2 + \left(p_y + \frac{x}{2} - \frac{\alpha y}{\rho^2}\right)^2 + \left[p_z + \varkappa\left(p_x + \frac{y}{2} + \frac{\alpha y}{\rho^2}\right)\right]^2\right\}.$$

A small deviation of the magnetic field from the direction of the dislocation thus gives rise to a perturbation

$$\hat{V} = \frac{1}{2}\left[p_z + \varkappa\left(p_x + \frac{y}{2} + \frac{\alpha y}{\rho^2}\right)\right]^2 - \frac{\hat{p}_z^2}{2}.$$

How does this perturbation affect a transition between the zeroth Landau level ($n_\rho = 0, m < 0$) and a singly degenerate level with an energy $E_\perp = \hbar\omega_c[(3/2) - \alpha]$ ($n_\rho = 0$, $m = 1$)? Since the Hamiltonian does not contain z, the eigenfunctions can be chosen in the form

$$\psi(z, r_\perp) = L_z^{-1/2}\exp(ip_z z)\,\psi(r_\perp).$$

The perturbation lifts the degeneracy at the Landau level for the given p_z. In the absence of a dislocation, in terms of the variables which we have chosen here, the states with $p_z + \varkappa p_x = \text{const}$ have an identical energy; i.e., there is no degeneracy for the given p_z.

We write the eigenfunctions as expansions in the unperturbed states:

$$\psi_\varepsilon(\mathbf{r}_\perp) = \sum_{m=0}^{\infty} C_m^\varepsilon \psi_m(\mathbf{r}_\perp),$$

$$\psi_m(r_\perp) = \frac{e^{-im\varphi}}{(2\pi)^{1/2}}\,\frac{e^{-\rho^2/4}}{[\Gamma(m+\alpha+1)]^{1/2}}\left(\frac{\rho}{2^{1/2}}\right)^{m+\alpha} \qquad (2)$$

The coefficients C_m^ε obey a secular equation of infinite order:

$$\varepsilon C_m^\varepsilon = \sum_{m'} V_{mm'} C_{m'}^\varepsilon. \qquad (3)$$

The intensity of the transition accompanied by the transfer of an energy $1 - \alpha + \varepsilon$ is determined by the square of the matrix element:

$$M^\varepsilon(p_z) = \left|\int d\mathbf{r}_\perp\, \psi_\varepsilon^*(\mathbf{r}_\perp)\, y\, \psi_{10}(\mathbf{r}_\perp)\right|^2,$$

$$\psi_{10} = \frac{e^{i\varphi}}{(2\pi)^{1/2}}\,\frac{e^{-\rho^2/4}}{[\Gamma(2-\alpha)]^{1/2}}\left(\frac{\rho}{2^{1/2}}\right)^{1-\alpha}.$$

Since the matrix element of the dipole-moment operator is nonzero only between the states with $\Delta m = \pm 1$, we can put $M^\varepsilon(p_z)$ in the form

$$M^\varepsilon(p_z) = \frac{\sin\pi\alpha}{2\pi\alpha(1-\alpha)}\,|C_0^\varepsilon|^2.$$

The total intensity of the transition accompanied by the transfer of an energy $1 - \alpha + \varepsilon$ is proportional to the expression

$$I^\varepsilon = \int f(p_z)\, M^\varepsilon(p_z)\, \nu(\varepsilon, p_z)\,\frac{dp_z}{2\pi},$$

where $f(p_z)$ is the distribution function of p_z, and $\nu(\varepsilon, p_z) = [2\pi\varkappa(2\varepsilon + p_z^2)^{1/2}]^{-1}$ is the state density.

The secular equation (3) can be solved exactly. We can formally determine the functions $\psi_m(r_\perp)$ from (2) even for $m < 0$. The operator $\hat{p} = -i\partial/\partial x + y/2 + \alpha y/\rho^2$, which is related to the perturbation $\hat{V}$ by $\hat{V} = (1/2)(\hat{p}_z + \varkappa\hat{p})^2 - \hat{p}_z^2/2$, acts on these functions in the following way

$$p\psi_m = -\frac{i}{2^{1/2}}(m+\alpha)^{1/2}\psi_{m-1} + \frac{i}{2^{1/2}}(m+\alpha+1)^{1/2}\psi_{m+1}.$$

Accordingly, if m and m' in Eq. (3) varied from $-\infty$ to ∞, the solution of this equation would be an eigenvector of the operator $\hat{p}$, and we would have $\varepsilon = (1/2)(p_z + \varkappa p)^2 - (1/2)p_z^2$. Since the relation $|m - m'| \leqslant 2$ holds in Eq. (3), we can choose the solution of this equation in the form of a linear combination of eigenvectors of the operator $\hat{p}$ which satisfies the conditions $C^\varepsilon_{-1} = 0$ and $C^\varepsilon_{-2} = 0$. The eigenvectors of the operator $\hat{p}$ can be found from

$$pC_m^p = \frac{i}{2^{1/2}}\left[(m+\alpha)^{1/2}C_{m-1}^p - (m+\alpha+1)^{1/2}C_{m+1}^p\right].$$

This equation has two linearly independent solutions:

$$\varphi_m{}^1(p)=\frac{2^{1/2}}{\pi^{1/4}}[\Gamma(m+\alpha+1)]^{1/2}D_{-m-\alpha-1}(-i\cdot 2^{1/2}p),$$

$$\varphi_m{}^2(p)=\frac{2^{1/2}}{\pi^{1/4}}[\Gamma(m+\alpha+1)]^{1/2}(-1)^m D_{-m-\alpha-1}(i2^{1/2}p);$$

here $D_\nu(x)$ is the parabolic cylinder function.[8] The solution of Eq. (3) can be constructed as a linear combination of the four functions $\varphi^1_m(p^+)$, $\varphi^2_m(p^+)$, $\varphi^1_m(p^-)$, $\varphi^2_m(p^-)$, where $p^\pm=-p_z/\varkappa\pm q$, $q=(2\varepsilon+p_z^2)^{1/2}/\varkappa$. The coefficients in the linear combination are chosen in such a way that conditions $C^\varepsilon_{-1}=0$, $C^\varepsilon_{-2}=0$ hold.

Each eigenvalue ε is thus doubly degenerate. We can choose two orthonormal solutions: C^{I}_m and C^{II}_m.

The lineshape is determined by the combination $|C^{\mathrm{I}}_0|^2+|C^{\mathrm{II}}_0|^2$, for which the following expression can be derived:

$$|C_0{}^{\mathrm{I}}|^2+|C_0{}^{\mathrm{II}}|^2=\frac{16\pi^{1/2}q^2[|D_{-\alpha}(i\cdot 2^{1/2}p^+)|^2+|D_{-\alpha}(i\cdot 2^{1/2}p^-)|^2]}{\Gamma(1+\alpha)\,|D_{-\alpha}(-i\cdot 2^{1/2}p^+)D_{1-\alpha}(i\cdot 2^{1/2}p^-)+D_{-\alpha}(i\cdot 2^{1/2}p^-)D_{1-\alpha}(-i\cdot 2^{1/2}p^+)|^2}$$

In the limiting case $\varkappa\ll p_z$, the expression for $M^\varepsilon(p_z)$ simplifies:

$$M^\varepsilon(p_z)=\frac{\sin\pi\alpha}{\pi^{1/2}\alpha(1-\alpha)}\frac{1}{\Gamma(1+\alpha)\,|D_{-\alpha}(i\,2^{1/2}\varepsilon/\varkappa p_z)|^2}. \qquad (4)$$

In this case the line remains symmetric with respect to the frequency $(1-\alpha)\omega_c$ and has a width on the order of $\varkappa p_z a_H\omega_c$ (in dimensional units).

If only the zeroth Landau level is filled in the ground state, the inequality $p_z<1$ holds for all the important p_z. In this case there is a region of values of parameter $\varkappa$ ($p_z\ll\varkappa\ll 1$) in which the lineshape is not given by expression (4), but the line is nevertheless narrow. In this region, with $\varepsilon>p_z^2$, we can derive the expression

$$M^\varepsilon(p_z)=\frac{2\sin\pi\alpha}{\pi^{1/2}\alpha(1-\alpha)}\frac{\varepsilon}{\Gamma(1+\alpha)\,|D_{1-\alpha}(2i\varepsilon/\varkappa^{1/2})|^2}. \qquad (5)$$

The linewidth is on the order of $\varkappa^2$, so that in this case it is also necessary to consider the correction to the energy of a nondegenerate level, $\Delta\varepsilon=\varkappa^2/4$; the effect is a shift of the line. The line is highly asymmetric: The linewidth to the left of the central point is on the order of $(p_z a_H)^2\omega_c$, while that to the right is on the order of $\varkappa^2\omega_c$.

4. CONCLUSION

This study of the splitting of cyclotron-resonance line on the basis of a "topological" interaction is exact [i.e., it holds for a vector **A** in the general form (1)] for a screw dislocation, with the vector **k** parallel to the dislocation, if we make the substitution $\alpha\to(1-\gamma_1)\alpha$. In germanium, where the bottom of the valley is at the boundary of the Brillouin zone, the results derived here will be accurate to first order in the deviation of the momentum of the excitations from the bottom of the valley, when the entire interaction essentially reduces to a topological interaction.

If the Burgers vector of a dislocation has a component perpendicular to the dislocation, deep levels will generally appear in the energy gap because of the presence of broken bonds, and dislocations will become charged as they capture carriers. The result will be a Coulomb repulsion of free carriers from the dislocation, so that there will actually be no splitting. In this case the effect can be observed under nonequilibrium conditions such that electrons are excited from deep levels. The deep levels disappear if reconstruction occurs in the dislocation core[9] and also when the semiconductor is saturated with hydrogen.[10]

In addition to the vector potential **A** given in (1), the strain field near a dislocation results in the appearance of a scalar potential $U(r)=gP(\varphi)/p$, where $P(\varphi)$ is some function of the angle φ, and the constant g is determined by the Burgers vector and the elastic constants. The condition of a weak strain energy, $g/a_H<\hbar\omega_c$, leads to a restriction on the magnetic field: $H>cg^2m_c^2/e\hbar^3$. An estimate puts the critical field on the order of 100 kG.

In the general case in which the valley does not lie at the edge of the Brillouin zone, and **k** is not parallel to the dislocation, there is a strain contribution to (1). The cyclotron line is split again in this case; the satellites lie at a distance $\beta\omega_c$, where the value of $\beta<1$ depends on the phenomenological parameters γ_i.

In summary, we have shown that when a multivalley semiconductor contains uncharged dislocations the cyclotron-resonance line should acquire satellites at distances of order $\beta\omega_c$, with an intensity $n_d a_H^2$.

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