Magnetoelectric subbands and eigenstates in the presence of Rashba and Dresselhaus spin-orbit interactions in a quantum wire

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Abstract

We derive the eigenenergies and eigenstates of electrons in a quantum wire subjected to an external magnetic field. These are calculated in the presence of spin orbit interactions arising from the Rashba (structural inversion asymmetry) and Dresselhaus (bulk inversion asymmetry) effects. We consider three cases: the external magnetic field is oriented (i) along the axis of the wire, (ii) perpendicular to the axis but parallel to the electric field associated with structural inversion asymmetry (Rashba effect), and (iii) perpendicular to the axis as well as the electric field. In all cases, the dispersions of the eigenenergies are non-parabolic and the subbands do not have a fixed spin quantization axis (meaning that the spin polarization of the electron is wavevector dependent). Except in the second case, the dispersion diagrams are also, in general, asymmetric about the energy axis.

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1 Introduction

Consider a semiconductor quantum wire defined by split gates on a two dimensional electron gas confined at a heterointerface. We will derive the eigenstates and the dispersion relations of the eigenenergies in this wire when it is placed in an external magnetic field of flux density \( B \) (Fig. 1).

Referring to Fig. 1, the potential in the y-direction (perpendicular to the heterointerface) is approximately triangular which leads to a structural inversion asymmetry and an associated Rashba spin-orbit interaction [1]. Additionally, if the material has bulk inversion asymmetry (e.g. InAs), then there will be a Dresselhaus interaction [2] which is important at large wavevectors. The potential in the z-direction will be approximately parabolic and hence symmetric about a center under inversion. Thus, there is no significant overall Rashba interaction associated with the z-directed electric field.

We will consider three cases corresponding to the external magnetic field being oriented along three possible coordinate axes – \( x \), \( y \) and \( z \).

2 Magnetic field directed along the wire axis (i.e. x-axis)

When the magnetic field is oriented along the axis of the wire, the effective mass Hamiltonian for the wire, in the Landau gauge \( A = (0, -Bz, 0) \), can be written as

\[
H = \left( p_x^2 + p_y^2 + p_z^2 \right)/(2m^* ) + (eBzp_y)/m^* + (e^2B^2z^2)/(2m^* ) - (g/2)\mu_B Bs_x + V(y) + V(z) + \nu[\sigma_x \kappa_x + \sigma_y \kappa_y + \sigma_z \kappa_z] + \eta[(p_x/\hbar)\sigma_z - (p_z/\hbar)\sigma_x]
\]

where \( g \) is the Landé g-factor, \( \mu_B \) is the Bohr magneton, \( V(y) \) and \( V(z) \) are the confining potentials along the y- and z-directions, \( \sigma \)-s are the Pauli spin matrices, \( \nu \) is the strength of the Dresselhaus spin-orbit interaction and \( \eta \) is the strength of the Rashba spin-orbit interaction.

The quantities \( \kappa \) are defined in ref. [3]. We will assume that the wire is narrow enough and the temperature is low enough that only the lowest magneto-electric subband is occupied. Since the Hamiltonian is invariant in the x-coordinate, the wavevector \( k_x \) is a good quantum number and the eigenstates are plane waves traveling in the x-direction. Accordingly, the spin Hamiltonian (spatial operators are replaced by their expected values) simplifies to

\[
H = \left( \hbar^2 k_x^2 \right)/(2m^*) + E_0 + (\alpha_1 k_x - \beta)\sigma_x + \eta k_x\sigma_z
\]

where \( E_0 \) is the energy of the lowest magneto-electric subband, \( \alpha_1(B) = \nu[< k_y^2 > - < k_z^2 > + (e^2B^2 < z^2 > /\hbar^2 )] \), \( \psi(z) \) is the z-component of the wavefunction, \( \phi(y) \) is the y-component of the wavefunction, \( < k_y^2 > = (1/\hbar^2 ) < \phi(y)| - (\partial^2/\partial y^2)|\phi(y)> \), \( < k_z^2 > = (1/\hbar^2 ) < \psi(z)| - (\partial^2/\partial z^2)|\psi(z)> \), and \( \beta = (g/2)\mu_B B \).

Since the potential \( V(z) \) is parabolic \( (V(z) = (1/2)m^* \omega_0^2 z^2) \), it is easy to show that \( < k_z^2 > = m^* \omega/(2\hbar) \) and \( < z^2 >= \hbar/(2m^* \omega) \) where \( \omega^2 = \omega_0^2 + \omega_c^2 \) and \( \omega_c \) is the cyclotron frequency \( (\omega_c = eB/m^*) \). Furthermore, \( E_0 = (1/2)\hbar \omega + E_\Delta \) where \( E_\Delta \) is the energy of the lowest subband in the triangular well \( V(y) \).

Diagonalizing this Hamiltonian in a truncated Hilbert space spanning the two spin resolved states in the lowest subband yields the eigenenergies

\[
E^{(1)}_{\pm} = \frac{\hbar^2 k_x^2}{2m^*} + E_0 \pm \sqrt{\left( \eta^2 + \alpha_1^2 \right) \left( k_x - \frac{\alpha_1 \beta}{\eta^2 + \alpha_1^2} \right)^2 + \frac{\eta^2}{\eta^2 + \alpha_1^2} \beta^2}
\]

and the corresponding eigenstates

\[
\Psi^{(1)}_+(B, x) = \begin{bmatrix} \cos(\theta_{k_x}) \\ \sin(\theta_{k_x}) \end{bmatrix} e^{ik_xx} \quad \Psi^{(1)}_-(B, x) = \begin{bmatrix} \sin(\theta_{k_x}) \\ -\cos(\theta_{k_x}) \end{bmatrix} e^{ik_xx}
\]

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Figure 1: A generic semiconductor quantum wire defined by split gates at a heterostructure interface.

where $\theta_k = (1/2)\arctan[(\alpha_1 k_x - \beta)/\eta k_x]$. 

The dispersion relations given by Equation (3) are plotted in Fig. 2 for the case $\eta = \alpha_1$. Note that the dispersions are clearly nonparabolic and asymmetric about the energy axis. More importantly, note that the eigenspinors given in Equation (4) are functions of $k_x$ because $\theta_k$ depends on $k_x$. Therefore, the eigenspinors are not fixed in any subband, but change with $k_x$. In other words, neither subband has a definite spin quantization axis and the orientation of the spin vector of an electron in either subband depends on the wavevector. Consequently, it is always possible to find two states in the two subbands with non-orthogonal spins. Any non-magnetic scatterer (impurity, phonon, etc.) can then couple these two states and cause a spin-relaxing scattering event.

### 2.1 Spin components

The spin components along the $x$, $y$ and $z$ directions are given by

$$ S_m^{(1)\pm} = [\Psi^{(1)\pm}_m][\sigma_m][\Psi^{(1)\pm}_m] \quad m = x, y, z $$

This yields $S_x^{(1)\pm}(k_x) = \pm \sin(2\theta_{k_x})$, $S_y^{(1)\pm} = 0$ and $S_z^{(1)\pm}(k_x) = \pm \cos(2\theta_{k_x})$

It is easy to see that, in general, $S_x^{(1)}(k_x) \neq S_x^{(1)}(-k_x)$ and $S_z^{(1)}(k_x) \neq S_z^{(1)}(-k_x)$. However, if the Dresselhaus interaction vanishes ($\alpha_1 = 0$), then $S_x^{(1)}(k_x) = -S_x^{(1)}(-k_x)$ and $S_z^{(1)}(k_x) = S_z^{(1)}(-k_x)$. This does not always mean that, in the absence of Dresselhaus interaction, oppositely traveling electrons have anti-parallel spin components along the wire axis, and parallel spin components in the $z$-direction. The reason being that the velocity operator is not $p/m^*$ and hence electrons with opposite signs of wavevector $k_x$ need not have opposite signs of velocity.
Figure 2: Energy versus wavevector $k_x$ in a quantum wire where we have assumed $\alpha_1 = \eta = 10^{-11}$ eV-m, the magnetic flux density $= 1$ Tesla, the effective mass $m^*$ is 0.05 times the free electron mass and the Landé g-factor $= 4$. This corresponds to $\beta = 0.115$ meV. The magnetic field is in the x-direction (along the wire).
3 Magnetic field perpendicular to wire axis and along the electric field causing Rashba effect (i.e. along y-axis)

With this orientation of the magnetic field, we will use the Landau gauge $\mathbf{A} = (Bz, 0, 0)$, and the Hamiltonian for the wire can be written as

$$
H = \frac{p_x^2 + p_y^2 + p_z^2}{2m^*} - (eBzp_x)/m^* + \frac{e^2B^2z^2}{2m^*} - \frac{(g/2)\mu_B B}{\eta}(p_x + eBz)\sigma_z - p_z\sigma_z
$$

This yields

$$
4 \text{ Magnetic field perpendicular to wire axis and the electric field causing Rashba effect (i.e. along y-axis)}
$$

Using the definition of the $\kappa$-s, and noting that the expected values $<z> = <p_z> = 0$, the spin Hamiltonian can be simplified to

$$
H = \left(\hbar^2k_z^2/(2m^*) + E_0 + \alpha_2k_x\sigma_y - \beta\sigma_y + \eta k_x\sigma_z \right)
$$

where $\alpha_2(B) = \nu[<k_z^2> - <k_z^2>]$.

Again, diagonalizing this Hamiltonian in a truncated Hilbert space spanning the two spin-resolved states in the lowest subband yields the eigenenergies

$$
E^{(2)}_\pm = \frac{\hbar^2k_z^2}{2m^*} + E_0 \pm \sqrt{(\eta^2 + \alpha^2_2)k_z^2 + \beta^2}
$$

and the corresponding eigenstates

$$
\Psi^{(2)}_\pm(B, x) = \begin{bmatrix} \cos(\theta'_{k_z}) \\ \sin(\theta'_{k_z})e^{-i\phi_{k_z}} \end{bmatrix} e^{ik_xx}, \quad \Psi^{(2)}_\mp(B, x) = \begin{bmatrix} \sin(\theta'_{k_z}) \\ -\cos(\theta'_{k_z})e^{-i\phi_{k_z}} \end{bmatrix} e^{ik_xx}
$$

where $\theta'_k = (1/2)\arctan[\sqrt{(\alpha_2k_z^2 + \beta^2)/\eta k_z}]$ and $\phi_{k_z} = \arctan[\beta/\alpha_2k_z]$.

In Fig. 3, we plot the dispersion relations for the case $\eta = \alpha_2$. Note that the dispersions are again clearly nonparabolic, but this time they are symmetric about the energy axis. The eigenspinors are functions of $k_x$ because $\theta'_k$ and $\phi_k$ depend on $k_x$. Therefore, the eigenspinors are again not fixed in any subband, but change with $k_x$. Neither subband has a definite spin quantization axis and the spin of an electron in either subband depends on the wavevector. Consequently, it is always possible to find two states in the two subbands having non-orthogonal spins and a non-magnetic scatterer can couple these two states causing a spin-relaxing scattering event.

3.1 Spin components

The spin components along the $x, y$ and $z$ directions are given by

$$
S^{(2)}_{m\pm} = [\Psi^{(2)}_\pm]d[\sigma_m][\Psi^{(2)}_\pm] \quad m = x, y, z
$$

This yields $S^{(2)}_x(k_x) = \pm\sin(2\theta'_{k_z})\cos(\phi_{k_z})$, $S^{(2)}_y(k_x) = 0$ and $S^{(2)}_z(k_x) = \pm\cos(2\theta'_{k_z})$.

Again, $S^{(2)}_x(k_x) \neq S^{(2)}_x(-k_x)$ and $S^{(2)}_y(k_x) \neq S^{(2)}_y(-k_x)$. However, if the Dresselhaus interaction vanishes ($\alpha_2 = 0$), then $S^{(2)}_x(k_x) = -S^{(2)}_x(-k_x)$ and $S^{(2)}_y(k_x) = S^{(2)}_y(-k_x)$.

4 Magnetic field perpendicular to wire axis and the electric field causing Rashba effect (i.e. along z-axis)

In this case, using the Landau gauge $\mathbf{A} = (-B(y - y_0), 0, 0)$, the Hamiltonian for the wire can be written as

$$
H = \frac{p_x^2 + p_y^2 + p_z^2}{2m^*} + (eByp_x)/m^* + \frac{e^2B^2y^2}{2m^*} - \frac{(g/2)\mu_B B}{\eta}(p_x + eBy)\sigma_z - p_z\sigma_z
$$

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Figure 3: Energy versus wavevector $k_x$ in a quantum wire where the magnetic flux density is along the y-direction. We have assumed $\alpha_2 = \eta = 10^{-11}$ eV-m. All other parameters are the same as in Fig. 2.
where $y_0$ is a gauge constant.

Using the definition of the $\kappa$-s, the spin Hamiltonian can be simplified to

$$H = \left(\frac{\hbar^2 k_x^2}{2m^*}\right) + (\alpha_3 k_x + \Delta) \sigma_x - \beta \sigma_z + \eta (k_x + eB(y - y_0))/\hbar \sigma_z$$

(12)

where $E'_0$ is the energy of the lowest magneto-electric subband, $\alpha_3 = \nu [< k_y^2 > - < k_z^2 > ]$, and $\Delta = (\nu eB/\hbar) I(B)$ where $I(B) = \int_0^\infty (y - y_0) (\partial \zeta(y, B)/\partial y)^2 dy$, $\zeta(y, B)$ is the y-component of the wavefunction and $< y > = \int_0^\infty |\zeta(y, B)|^2 y dy$. We choose the gauge constant $y_0$ such that $< y > = y_0$. This simplifies the Hamiltonian to

$$H = \left(\frac{\hbar^2 k_x^2}{2m^*}\right) + E'_0 + (\alpha_3 k_x + \Delta) \sigma_x - \beta \sigma_z + \eta k_x \sigma_z$$

(13)

Finally, diagonalizing this Hamiltonian in the truncated Hilbert space spanning the two spin resolved states in the lowest subband yields the eigenenergies

$$E_\pm^{(3)} = \frac{\hbar^2 k_x^2}{2m^*} + E'_0 \pm \sqrt{(\eta^2 + \alpha_3^2) k_x^2 + 2(\alpha_3 \Delta - \eta \beta) k_x + \Delta^2 + \beta^2}$$

(14)

and the corresponding eigenstates

$$\Psi^{(3)}_+(B, x) = \begin{bmatrix} \cos(\theta_{k_x}^u) \\ \sin(\theta_{k_x}^u) \end{bmatrix} e^{ik_x x} \quad \Psi^{(3)}_-(B, x) = \begin{bmatrix} \sin(\theta_{k_x}^u) \\ -\cos(\theta_{k_x}^u) \end{bmatrix} e^{ik_x x}$$

(15)

where $\theta_{k_x}^u = (1/2) \arctan[(\alpha_3 k_x + \Delta)/(\eta k_x - \beta)]$.

In Fig. 4, we plot the dispersion relations for the case $\eta = \alpha_3$ and $\Delta = \beta$. As before, the dispersions are clearly non-parabolic and unless $\alpha_3 \Delta = \eta \beta$, they are asymmetric about the energy axis. The eigenspinors are functions of $k_x$ because $\theta_{k_x}^u$ depends on $k_x$. Therefore, the eigenspinors are again not fixed in any subband, but change with $k_x$. Neither subband has a definite spin quantization axis and the spin of an electron in either subband depends on the wavevector. Consequently, it is again always possible to find two states in the two subbands having non-orthogonal spins and a non-magnetic scatterer can couple these two states causing a spin-relaxing scattering event.

4.1 Spin components

The spin components along the $x$, $y$ and $z$ directions are given by

$$S_m^{(3)\pm} = [\Psi^{(3)}_{\pm}] [\sigma_m] [\Psi^{(3)}_{\pm}] \quad m = x, y, z$$

(16)

This yields $S_x^{(3)\pm}(k_x) = \pm \sin(2\theta_{k_x}^u)$, $S_y^{(3)\pm} = 0$ and $S_z^{(3)\pm}(k_x) = \pm \cos(2\theta_{k_x}^u)$.

In this case, $S_x^{(3)}(k_x) \neq S_x^{(3)}(-k_x)$ and $S_z^{(3)}(k_x) \neq S_z^{(3)}(-k_x)$ unless the Dresselhaus interaction vanishes so that $\alpha_3 = \Delta = 0$. In the latter case, $S_x^{(3)}(k_x) = -S_x^{(3)}(-k_x)$ and $S_z^{(3)}(k_x) = S_z^{(3)}(-k_x)$.

5 Conclusion

We have shown here that the dispersion relations of the lowest eigenstates in a quantum wire placed in a magnetic field are always non-parabolic and the subbands do not have fixed spin quantization axes since the eigenspinor in any subband changes with the wavevector. As a result, a non-magnetic scatterer can always couple two states in two subbands and flip spin. However, if the magnetic field is absent, then the eigenspinors become wavevector-independent since then $\theta = \theta' = \theta'' = (1/2) \arctan[\alpha_m/\eta]$ ($m = 1, 2, 3$). In that case, each subband has a definite spin quantization axes.
Figure 4: Energy versus wavevector $k_x$ in a quantum wire where the magnetic flux density is along the $z$-direction. We have assumed $\Delta = \beta = 0.115$ meV and $\alpha_3 = \eta = 10^{-11}$ eV-m. All other parameters are the same as in Fig. 2. This dispersion is symmetric about the energy axis only because the parameters were so chosen that $\alpha_3 \Delta = \eta \beta$; otherwise, it would have been asymmetric.
and the eigenspinors in two subbands are orthogonal. Consequently, a non-magnetic scatter cannot couple the two subbands and flip spin. Spin transport can then be ballistic, particularly because the Elliot-Yafet spin flip mechanism [4] will also be suppressed since the eigenspinors are wavevector independent. This effect, whereby a magnetic field can cause a crossover from ballistic to non-ballistic spin transport, can have applications in magnetic field sensors [5].

References

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