Spin–orbit splitting in cylindrical quantum wires

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The changes caused in the spectrum of quasi-1D electron subbands by the spin–orbit interaction in axisymmetric quantizing potentials are analyzed. The term splitting is found in the case of a parabolic potential. The nonparabolic increments in the dispersion, which are linearized by an external magnetic field, are calculated for degenerate subbands in finite potentials. A weak-field negative magnetoresistance is predicted.

When the spin–orbit coupling is taken into consideration, the energy spectrum in reduced-dimensionality electron systems is modified significantly. In quasi-1D layers, this interaction may lead to an increment in the dispersion law which is linear in the longitudinal momentum.[1–4] In order to derive this correction, however, it is necessary to go beyond the scope of the effective-mass approximation and to consider the region in which the "two-dimensionalizing" potential varies sharply.[4,5] In the present letter we consider a quantum wire in which the motion of an electron is one-dimensionalized by a smooth attractive potential $u(\rho)$, where $\vec{\rho}$ is a 2D radius vector. We show that in this case corrections linear in the spin–orbit constant are found even by the effective-mass approach. These corrections have some interesting and experimentally observable consequences.

Taking this spin–orbit coupling into account, we describe the motion of an electron in the potential $u(\rho)$ by the Hamiltonian

$$\hat{H} = \hat{p}^2/2m + u(\rho) + \tilde{\alpha}[\hat{\vec{\sigma}} \times \vec{\nabla} u]\hat{\mathrm{p}}, \tag{1}$$

where $\hat{\sigma}_i$ are the Pauli matrices, and $\tilde{\alpha}$ is the effective spin–orbit constant. We introduce the dimensionless variables $r = \rho/\alpha$, $E_0 = \hbar^2/2ma^2$, $\alpha = \tilde{\alpha}\hbar/a^2$, and $v(r) = u(\rho)/E_0$, where α is a characteristic radius of the wire. Separating out the longitudinal motion, we find the 2D Schrödinger equation

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\psi}{dr}\right) + v(r)\psi + \frac{\alpha}{r}\frac{dv}{dr}(\hat{\sigma}_z \hat{l} + kr(\sin\theta \cdot \hat{\sigma}_x - \cos\theta \cdot \hat{\sigma}_y))\psi = \epsilon\psi, \tag{2}$$

where $\hbar k/a$ is the longitudinal momentum, $\epsilon = E/E_0 - k^2$, and the operator $\hat{l}$ represents the axial moment. In the case $k = 0$, the quantities l and σ_z are separately good quantum numbers. The effect of the spin–orbit correction thus reduces to an "individual" splitting of those energy levels ϵ_{nl} of the original problem (i.e., of the problem with $\alpha = 0$) which corresponds to the states $|nl\rangle$:

$$(\Delta\epsilon)_{nl} \approx \alpha l < nl \left| \frac{1}{r}\frac{dv}{dr} \right| nl > . \tag{3}$$

For $k \neq 0$, the situation is more complicated. In this case, only the operator representing the resultant angular momentum, $\hat{j} = \hat{l} + \hat{\sigma}_z/2$, commutes with the Hamiltonian of Eq. (2). We thus seek solutions of (2) in the form

$$\psi_{nj}(\vec{\rho}) = \sum_{n'} (c_{n'j\uparrow}|n'l\uparrow> + c_{n'j\downarrow}|n', l+1, \downarrow>), \tag{4}$$

where

$$\hat{\sigma}_z|\uparrow> = |\uparrow>, \quad \hat{\sigma}_z|\downarrow> = -|\downarrow> . \tag{5}$$

We see that in the general case ($\epsilon_{nl} \neq \epsilon_{n,l+1}$) we would find k-dependent spin–orbit increments only in second-order perturbation theory. These increments would be extremely small [$\sim(\alpha k)^2$] and would cause only a minor renormalization of the longitudinal effective mass. However, the mixing of spin states in (4) leads (even in the dipole approximation) to optical intraband transitions with spin flip and to a corresponding increase in the complexity of the optical spectra.

To illustrate these arguments, we consider a parabolic quantum wire with $u(\rho) = m\omega^2\rho^2/2$. In this case we have $\alpha = \sqrt{\hbar/m\omega}$, and the unperturbed energy values are $\epsilon_{nl} = 2n + |l| + 1$. Since we have $r^{-1}(dv/dr) = 1$, the matrix elements of the spin–orbit perturbation are extremely simple in the $|nl\rangle$ basis. The only nonzero matrix elements are

$$< nl \left| \frac{1}{r}\frac{dv}{dr} \right| n'l > = \delta_{nn'} , \tag{6}$$

$$< n, l+1 \left| \frac{dv}{dr} \right| n', l > = \sqrt{n + |l| + 1}\,\delta_{nn'} + \sqrt{n}\,\delta_{n-1,n'} .$$

The matrix of the system of equations for the coefficients $c_{nj\sigma}$ is thus tridiagonal. One can therefore derive expressions for ϵ_{nj} (and for $c_{nj\sigma}$) in the form of chain fractions.[6] Since α is small, we restrict the discussion to the first terms of the power-law expansion. These first terms give the energy splitting of the original $|nl\rangle$ state in the form of noninteracting terms:

$$\epsilon_{nj}^{(1)} = 2n + |j - 1/2|(1+\alpha) + 1 - (k\alpha)^2(|j - 1/2| + 1 + \alpha(2n + |j - 1/2| + 1)) ,$$

$$\epsilon_{n,j-\mathrm{sgn}j}^{(2)} = 2n + |j - 1/2|(1-\alpha) + 1 + (k\alpha)^2(|j - 1/2| + \alpha(2n + |j - 1/2|)). \tag{7}$$

[According to (6), these values are exact in the case $k = 0$]. Since the matrix elements of optical transitions are determined by the same expression, (6), in the dipole approximation, we can immediately write the absorption spectrum of this system (for the case in which the polarization is perpendicular to the wire). In the leading approximation, this spectrum is a double line at the frequency $\omega = 1$, with a spacing of 2α between the components. When the k-dependent terms are taken into account, equidistant satellites appear on each side of this main doublet (again with a spacing of 2α). The intensity and number of these satellites increase with the temperature (and with the Fermi energy).

A more interesting case is that of an initial degeneracy, in which the transversely quantized spectrum, with $\alpha = 0$, has values of n, n', and l such that the approximate equality $\epsilon_{nl} \approx \epsilon_{n',l+1}$ holds (within an error $\sim\alpha$). A situation of this sort is possible, for example, for decreasing $|v(r)|$ with a sufficiently "thin" tail or for two-scale potentials with an additional dip near $r = 0$. Introducing

$$B = < n', l+1 \left| \frac{dv}{dr} \right| nl >; \quad B_{nl} = < nl \left| \frac{1}{r}\frac{dv}{dr} \right| nl >, \tag{8}$$

we find, for this case,

$$\epsilon_{nj}^{(1,2)} = \frac{1}{2}(\epsilon_{nl} + \epsilon_{n',l+1} + \alpha(B_{nl}|j-1/2| - B_{n',l+1}(|j-1/2|+1))$$
$$\pm\sqrt{(\epsilon_{nl} - \epsilon_{n',l+1} - \alpha(B_{nl}|j-1/2| + B_{n',l+1}(|j-1/2|+1)))^2 + (k\alpha B)^2}. \tag{9}$$

The lifting of degeneracy thus leads (as usual) to a significant deviation of the spectrum from a nonparabolic shape. The spectrum may also become linear in k if the expression inside parentheses in the radical vanishes. This effective "linearization" can be achieved with the help of a weak external longitudinal magnetic field. Specifically, in the natural gauge of the vector potential $\vec{A} = [\mathscr{H} \times \vec{\rho}]/2$, we find, in the linear approximation,

$$\hat{H}(\mathcal{H}) = \hat{H}(0) + \gamma\hat{l} + g\gamma\hat{\sigma}_z/2, \tag{10}$$

where $\gamma = \hbar e\mathscr{H}/2mcE_0$. The corresponding increments in the equations for $c_{nj\sigma}$ lead to a case in which a term of $2\gamma j$ is added to the parenthetical expression outside the radical in expression (9), while a term $\gamma(g-1)$ is added to the parenthetical expression inside the radical. Accordingly, the latter expression can be completely "eliminated" through the appropriate choice of the sign and magnitude of the weak ($\gamma\sim\alpha$) magnetic field. Such a radical change in the spectrum should lead to observable effects, an obvious one being the possible presence of a weak-field region of a negative longitudinal magnetoresistance.

We conclude with an estimate of the magnitude of the effects we are talking about here. Some attractively large values of the effective spin–orbit constant can be reached in (for example) narrow–gap semiconductors. If we take the width of the gap to be $\sim$0.4 eV, and if we take the electron mass to be $\sim 0.02m_0$ (these property values correspond to InAs), then for a quantum wire 100 Å in diameter we find the dimensionless value $\alpha \sim 5 \times 10^{-2}$. The fine structure in the absorption spectra which we described above would be characterized by a splitting ~ 1 meV. Finally, the strength of the linearizing magnetic field would be $\sim 10^3$ G. These effects could thus be seen easily, and it is quite clear that fabricating quantum wires of this sort is feasible, in view of recent advances in the fabrication of nanostructures.

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