Spin Accumulation in Quantum Wires with Strong Rashba Spin-Orbit Coupling

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We present analytical and numerical results for the effect of Rashba spin-orbit coupling on band structure, transport, and interaction effects in quantum wires when the spin precession length is comparable to the wire width. The situation with only the lowest spin-split subbands occupied is particularly interesting because electrons close to Fermi points of the same chirality can have approximately parallel spins. We discuss consequences for spin-dependent transport and effective Tomonaga-Luttinger descriptions of interactions in the quantum wire.

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Spin-dependent transport phenomena are currently attracting a lot of interest because of their potential for future electronic device applications. Basic design proposals for spin-controlled field-effect switches use the fact that electron waves with opposite spin acquire different phase factors during their propagation in the presence of Rashba spin-orbit coupling (RSOC). The latter arises due to structural inversion asymmetry in quantum heterostructures where two-dimensional (2D) electron systems are realized. The single-electron Hamiltonian is then of the form

\[ H_{2D} = H_0 + H_{so} \]

where

\[ H_0 = \frac{1}{2m} \left( p_x^2 + p_y^2 \right) \]

\[ H_{so} = \frac{\hbar}{m} \sigma_z \left( p_y - \sigma_y p_x \right) \]

with \( m \) denoting the effective electron mass. Possibility to tune the strength of RSOC, measured here in terms of the characteristic wave vector \( k_{so} \), by external gate voltages has been demonstrated experimentally. As a manifestation of broken spin-rotational invariance, eigenstates of \( H_{2D} \) which are labeled by a 2D wave vector \( k \) have their spin pointing in the direction perpendicular to \( \vec{k} \). Hence, no common spin quantization axis can be defined for eigenstates when spin-orbit coupling is present. Confining the 2D electrons further to form a quantum wire, one might naively expect to again be able to define a global spin quantization axis, as the propagation direction of electrons in a one-dimensional (1D) system is fixed. However, this turns out to be incorrect only for a truly 1D electron system with vanishing width. In real quantum wires, such a situation is approximately realized when the spin-precession length \( \pi/k_{so} \) is much larger than wire width. Another way to formulate this condition is to say that the characteristic energy scale \( \Delta_{so} = \hbar^2 k_{so}^2 / 2m \) for RSOC is small compared to the energy spacing of 1D subbands. For a quantum wire defined by a parabolic confining potential, e.g.,

\[ V(x) = \frac{m}{2} \omega^2 x^2 \]

the latter would be \( \hbar \omega \). When spin-orbit coupling is not small (i.e., when \( \Delta_{so} \sim \hbar \omega \) for the case of parabolic confinement), hybridization of 1D subbands for opposite spins becomes important, resulting in the deformation of electronic dispersion relations. The effect of this deformation on transport properties has been the subject of recent investigations, e.g., with respect to implications for the modulation of spin-polarized conductances as a function of RSOC strength which is the principle operation for spin-controlled field-effect devices.

Here we present results for the detailed spin structure of electron states in a quantum wire, defined by the parabolic confining potential \( V(x) \) given in Eq. (2), with strong RSOC present. Contrary to previous assumptions that were uncritically adopted in the recent literature, e.g., we find that electrons with large wave vectors in the lowest spin-split subbands have essentially parallel spin. The spin state that right-moving electrons have their spin pointing in the direction perpendicular to \( \vec{k} \) which are labeled by a 2D wave vector \( \vec{k} \) have their spin pointing in the direction perpendicular to \( \vec{k} \). Hence, no common spin quantization axis can be defined for eigenstates when spin-orbit coupling is present. Confining the 2D electrons further to form a quantum wire, one might naively expect to again be able to define a global spin quantization axis, as the propagation direction of electrons in a one-dimensional (1D) system is fixed. However, this turns out to be incorrect only for a truly 1D electron system with vanishing width. In real quantum wires, such a situation is approximately realized when the spin-precession length \( \pi/k_{so} \) is much larger than wire width. Another way to formulate this condition is to say that the characteristic energy scale \( \Delta_{so} = \hbar^2 k_{so}^2 / 2m \) for RSOC is small compared to the energy spacing of 1D subbands. For a quantum wire defined by a parabolic confining potential, e.g.,

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spin-orbit coupling such that \( \sigma \) induces mixing between the shifted parabolic subbands.

Evidently, this approximation gives reasonable results for the lowest spin-split subband, even in the present case of a rather large spin-orbit coupling strength.

and \( H_{\text{mix}} = -\hbar k_{so} \sigma_y p_x / m \). Straightforward calculation yields eigenstates of \( H_{pb} \) which are also eigenstates of \( \sigma_x \) with eigenvalue \( \sigma = \pm 1 \) and have energies \( E^{(pb)}_{n\sigma}(k_y) = \frac{\hbar^2}{2m}(2n + 1 + \frac{k^2}{2m}(k_y + \sigma k_{so})^2) - \Delta_{so}. \) The term \( H_{\text{mix}} \) induces mixing between the shifted parabolic subbands \( E^{(pb)}_{n\sigma}(k_y) \). To lowest order in perturbation theory, it results in a uniform shift of eigenenergies by \( -\Delta_{so} \) and a small deviation of spin quantization in \( x \) direction [17]. Hence, for \( \Delta_{so} \ll \hbar \omega \), eigenstates of \( H_{1D} \) have energies \( E^{(pb)}_{n\sigma}(k_y) - \Delta_{so} \) and are, to a good approximation, eigenstates of \( \sigma_x \). When \( \Delta_{so} \) becomes comparable to the subband splitting, anticrossings occur between neighboring subbands with opposite spin index \( \sigma \). As a result, no common spin-quantization axis can be defined anymore for eigenstates within any subband. Far enough from anticrossings, eigenstates of \( H_{so} \) will essentially be eigenstates of \( H_{pb} \). In particular, their spins will be approximately aligned in \( x \) direction. In the lowest two subbands, right-movers with wave vectors larger than that of the anticrossing point can then have approximately parallel spin. The same is true for left-movers whose asymptotic spin direction is opposite to that of right-movers.

In Fig. 1, we show as thick lines numerically calculated spectra of \( H_{1D} \) for a large value of spin-orbit coupling. Deviation from parabolicity is clearly visible. Interestingly, it is possible to obtain a good quantitative description of the lowest spin-split subband by diagonalizing \( H_{1D} \) in a truncated Hilbert space which is spanned by the lowest and first-excited spin-degenerate parabolic subbands of the Hamiltonian \( H_0 + V(x) \). We call this the two-band model and find an approximate expression for the dispersion of the lowest spin-split subband,

\[
\frac{2E^{(2b)}_{n\sigma}}{\hbar \omega} = 2 + (k_y l_\omega)^2 - \sqrt{(1 - \gamma k_{so} k_y l_\omega^2)^2 + 2(k_{so} l_\omega)^2},
\]  

where \( l_\omega = \sqrt{\hbar / m \omega} \) is the oscillator length of the parabolic confinement, and \( \gamma = \pm 1 \) a subband index that does not have the meaning of a spin quantization number. We show Eq. (4) and the corresponding result for the first excited subband as thin lines in Fig. 1. It is seen that the two-band model is quite adequate for the lowest subbands, even for rather strong spin-orbit coupling.

Results shown in Fig. 2 confirm conclusions reached in our previous discussion of the spin structure of electron eigenstates with RSOC present. Panel a) shows the expectation value of spin component in \( x \) direction for eigenstates of \( H_{1D} \) in the lowest and first excited spin-
split subbands for the same value of $k_{so}$ used in Fig. 1. Data in Figs. 1 and 2 for the same subband are indicated by the same line type. For the lowest subbands, we also give, as thin lines, results obtained analytically within the two-band model. It is clearly seen that spins of eigenstates with large absolute value of wave number are approximately quantized in $x$ direction, with spin direction of left-movers being opposite to that of right-movers. This fact is underscored by the properties of the energy spectrum in a finite magnetic field $B$ in $x$ direction which is shown in panel b). Clearly, Zeeman shift of states at large positive wave number is opposite to that for states with large negative wave number. Shown as thin lines in the main figure of panel a) are curves obtained analytically within the two-band model which yields again reliable results for the lowest subbands. We therefore use it to calculate the variation of spin density $\tilde{s}(x) = \Phi^\dagger(x) \tilde{\sigma} \Phi(x)$ across the wire. [The spinor $\Phi(x)$ denotes the transverse part of an eigenfunction of $H_{1D}$ which, in the presence of spin-orbit coupling, depends on wave vector.] It turns out that the density $s_y(x)$ of spin component parallel to the wire vanishes identically. Hence, only the $x$ and $z$ components of spin density are shown in Fig. 3, displaying an interesting texture-like variation with coordinate $x$ whose structure reflects the mixing between subbands due to $H_{mix}$. Note that the expectation value for the $z$ component of spin vanishes for eigenstates of $H_{1D}$.

From the above it has become clear that, in general, spin quantum number is not an appropriate way to characterize electron states in a quantum wire with strong RSOC. Only states with wave number $k_y$ far enough from anticrossing points will asymptotically have their spin quantized in $x$ direction. From considering Figs. 1 and 2, the following special situation can be envisioned which has rather counterintuitive consequences. At low enough electron density such that only states in the lowest spin-split subbands are occupied, states near the Fermi energy $E_F$ will be localized near four Fermi points. When electron density is not too low, their spins are approximately quantized in $x$ direction. As pointed out above, spins of states near Fermi points for right-movers are approximately spin-down, opposite to the spin direction of left-moving states near $E_F$. Assuming it to be possible to selectively raise (lower) the electrochemical potential of right-movers (left-movers), a spin-polarized current could be generated. Usually, creating a population of left-movers and right-movers with different electrochemical potentials is achieved by coupling the quantum wire adiabatically to ideal contacts. However, the underlying assumption that excess electrons injected from the right (left) reservoir will only be spin-up (spin-down) is not realistic because, typically, RSOC will be absent in the contacts. The different nature of electron states in the wire and the leads will result in strong scattering at wire-lead interfaces. Similar to the approach taken in Ref. [2], we model this situation by attaching semi-infinite leads with $k_{so} = 0$ to the wire where $k_{so} \neq 0$. The transmission problem can be solved exactly by matching appropriate ansätze for wave functions in the wire and the leads. The usual condition for ensuring current conservation has to be modified because the group velocity for electrons in the quantum wire with RSOC reads

$$v_y = \hbar(k_y + k_{so}\sigma_z)/m.$$  

Despite the unusual spin structure at the four Fermi points which is asymmetric with respect to right-movers and left-movers, no spin-polarized current is generated in the leads. However, as is shown in Fig. 4 a process of current conversion occurs close to the interfaces in the wire that results in a finite spin polarization of current in the wire. We have therefore found a unique type of spin accumulation that is not, as in the usual case, induced by ferromagnetic contacts. Our analysis shows that current conversion is enabled by scattering into evanescent modes of the wire because of the peculiar form of the velocity operator. A four–terminal measurement with ferromagnetic contacts as weakly coupled voltage probes should enable experimental verification of spin accumulation in the wire.

Finally, we briefly remark on the effective low-energy description of an interacting quantum wire with strong RSOC. In the spirit of Tomonaga-Luttinger models for interacting 1D systems, we linearize...
Fermi points are far enough away from anticrossings, a magnetic field \( B \) applied in \( x \) direction will shift right-movers (left-movers) to higher (lower) energies. [See Fig. 2(b).] The Zeeman term in bosonized form reads then \( H_Z = -\frac{\Delta B}{\sqrt{2}} \int x \Psi \), where \( \Psi \) is canonically conjugate to the phase field \( \theta \), which is related, within the usual phase-field formalism, to the total electron density \( \rho_{\text{tot}} = \sum_{\alpha=A,B} \rho_{\alpha} \). Approximate orthogonality of transverse parts of electron wave functions enables spin-flip processes, in the long-wave-length limit, only between left-moving and right-moving branches of the same type (A or B). In general, any spin-flip process incurs a large momentum transfer.

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[26] Band nonparabolicity typically plays no rôle in the low-density quantum wires considered here.
[27] This result contradicts the spin labeling of subbands adopted in Refs. 23, 24.