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Spin-orbit interaction as a source of spectral and transport properties in quasi-one-dimensional systems

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We present an exact theoretical study of the effect of the spin-orbit (SO) interaction on the band structure and low temperature transport in long quasi-one-dimensional electron systems patterned in two-dimensional electron gases in zero and weak magnetic fields. We reveal the manifestations of the SO interaction which cannot in principle be observed in higher dimensional systems.

It is known that an electron moving in an electric field experiences not only an electrostatic force but also a relativistic influence that is referred to as the spin-orbit (SO) interaction (or spin-orbit coupling[1]). It is caused by Pauli coupling between the spin moment of an electron and a magnetic field which appears in the rest frame of the electron due to its motion in the electric field. The Hamiltonian of the SO interaction has the form:[1]

$$\hat{H}_{SO} = -\frac{\hbar}{(2M_0c)^2}\mathbf{E}(\mathbf{R})\left[\hat{\boldsymbol{\sigma}}\times\left\{\hat{\mathbf{p}}+\frac{e}{c}\mathbf{A}(\mathbf{R})\right\}\right]. \qquad (1)$$

Here M_0 is the free electron mass, $\hat{\mathbf{p}}$ is the canonical momentum operator, $\hat{\boldsymbol{\sigma}}$ is the Pauli matrices, $\mathbf{E}(\mathbf{R})$ is the electric field, $\mathbf{A}(\mathbf{R})$ is a vector potential, and $\mathbf{R}$ is a 3D position vector. Usually the Hamiltonian (1) results in a spin-orientation dependence of the electron energy and/or wave functions. This dependence can become important if electric fields acting on a system of moving electrons are sufficiently strong.

One of the most promising solid-state nanostructures for the observation of SO-interaction effects is the quasi-one-dimensional electron system[2,3] (Q1DES) patterned in two-dimensional electron gases (2DEG). In contrast with higher dimensional structures, Q1DES have *three* independent sources of strong electric fields: (i) crystal-field potential that is present in all dimensionalities owing to the intermolecular forces; (ii) a quantum-well potential[3] that confines electrons to a 2D layer at the surface of the crystal; (iii) a transverse (in-plane) electric potential that is applied to squeeze the 2DEG into a quasi-one-dimensional channel.[2,3] The strength of the in-plane potential determines an effective width of a Q1DES that can be controlled by changing the transverse voltage. In sufficiently narrow channels the transverse electric field can be made comparable with the other two electrostatic contributions.

The study of the SO interaction in Q1DES is interesting from the standpoint of remarkable transport phenomena which they exhibit: ballistic quantization of conductance;[4] the 0.7 conductance structure;[5] magnetic depopulation;[6] and negative magnetoresistance.[7] Since these phenomena depend on the peculiarities of the energy spectrum of electrons, any new mechanism leading to nontrivial changes in the spectrum (especially to those involving the spin) may affect transport properties and thereby help their understanding.

Earlier theoretical[8–11] and experimental[12–17] works on the SO-related effects dealt mainly with 3D and 2D systems and did not touch on aspects of the SO coupling in Q1DES. In this paper we present the results of a theoretical analysis of the effect of the SO interaction on the energy spectrum and low temperature (ballistic) conductance of a long Q1DES. Since the crystal-field contribution to the SO interaction energy can be made negligible in comparison with the quantum-well effect in a variety of systems,[13–17] we take into account two sources of the SO coupling: the quantum-well confinement in the direction perpendicular to the plane of the 2DEG and the confining electric potential transverse to the 2DEG. We show that even if the SO coupling due to the transverse potential is left out, the very presence of this potential changes drastically the SO-interaction effects caused by the quantum-well field in comparison with a purely 2D situation. In addition to this, the contribution of the transverse potential to the SO coupling adds interesting features to the electron energy spectrum and the conductance which cannot be accounted for by simply renormalizing the quantum-well field. Also, we find that relatively weak magnetic fields emphasize the effects of the SO interaction in Q1DES.

A unique feature of semiconductor Q1DES is that their properties can be varied significantly at the stage of design (via chemical composition, band engineering, external fields, etc.). In particular, it is possible to create systems with a wide range of carrier concentrations including values where the strength of electron-electron interactions is relatively weak. On the other hand, the strength of the SO coupling can simultaneously be enhanced by, for example, increasing confining electric fields and using materials with larger SO constants (InAs, PbTe, etc.). As a result, experimental situations can be achieved when the SO coupling becomes dominant. In this case it is reasonable to assume that the electron-electron interaction does not remove SO effects in the band structure of Q1DES and they can be studied within the single-particle approximation. As regards the ballistic conductance of a quantum wire, it has been proved not to be renormalized by electron-electron interactions.[18] Based on these arguments, we consider here a free 2DEG within a one-band effective mass approximation.[19] The corresponding Hamiltonian has the form:

$$\hat{H}=\frac{1}{2M}\left(\hat{\mathbf{p}}+\frac{e}{c}\mathbf{A}\right)^2+V(\mathbf{R})+\frac{g}{2}\mu_B(\hat{\boldsymbol{\sigma}}\mathbf{B})+\hat{H}_{SO}. \quad (2)$$

Here M is the effective electron mass, g is the Landé g factor, and μ_B is the Bohr magneton. The vector potential $\mathbf{A}$ is chosen in the Landau gauge $\mathbf{A}(\mathbf{R})=Bx\,\mathbf{y}$ with a magnetic field $\mathbf{B}=\mathrm{curl}\,\mathbf{A}=B\mathbf{z}$ being perpendicular to the 2DEG. In line with Refs. 20–22, the *transverse confining potential* $V(\mathbf{R})$ is approximated by a parabola

$$V(\mathbf{R})\equiv V(x)=(M\omega^2/2)x^2, \quad (3)$$

where ω controls the strength of the confining potential.

We assume that the SO Hamiltonian $\hat{H}_{SO}$ (1) in Eq. (2) is formed by two contributions: $\hat{H}_{SO}=\hat{H}^{\alpha}_{SO}+\hat{H}^{\beta}_{SO}$. The first one, $\hat{H}^{\alpha}_{SO}$, arises from the quantum-well electric field that can reasonably be assumed uniform and directed along the z axis, so that $\hat{H}^{\alpha}_{SO}$ is given by

$$\hat{H}^{\alpha}_{SO}=\frac{\alpha}{\hbar}\left[\hat{\boldsymbol{\sigma}}\times\left(\hat{\mathbf{p}}+\frac{e}{c}\mathbf{A}\right)\right]_z. \quad (4)$$

The SO-coupling constant α takes values 10^{-10}–10^{-9} eV $\times$cm for different systems.[9,14–17] We will refer to this mechanism of the SO coupling as α coupling.

The second contribution $\hat{H}^{\beta}_{SO}$ to $\hat{H}_{SO}$ comes from the in-plane electric field $\mathbf{E}=-\nabla_{\mathbf{R}}V=-M\omega^2\mathbf{x}$ caused by the transverse confining potential (3):

$$\hat{H}^{\beta}_{SO}=\frac{\beta}{\hbar}\frac{x}{l_\omega}\left[\hat{\boldsymbol{\sigma}}\times\left(\hat{\mathbf{p}}+\frac{e}{c}\mathbf{A}\right)\right]_x, \quad l_\omega=\sqrt{\hbar/M\omega}. \quad (5)$$

By comparison with typical quantum-well and transverse electric fields, the SO-coupling constant β in Eq. (5) can be roughly estimated as at least $\beta\sim 0.1\alpha$. Moreover, in square quantum wells where the value of α is considerably diminished,[17] the constant β may well compete with α. We will call the SO interaction arising from the transverse confining potential (3) β coupling.

To calculate the energy spectrum of electrons we must find eigenvalues E of the Schrödinger equation $\hat{H}\Psi=E\Psi$, where the wave function $\Psi=\Psi(\mathbf{R})=\{\Psi(\mathbf{R})_\uparrow\Psi(\mathbf{R})_\downarrow\}$ is a two-component spinor. Since the Hamiltonian $\hat{H}$ (2)–(5) is translationally invariant in the y direction, the wave functions $\Psi_{\uparrow\downarrow}(\mathbf{R})$ are plane waves propagating along the y axis, i.e., $\Psi_{\uparrow\downarrow}(\mathbf{R})=\exp(ik_y y)\Phi_{\uparrow\downarrow}(x)$, and the longitudinal energy is given by $E_y=\hbar^2k_y^2/2M$, where k_y is the longitudinal wave number. The equations for $\Phi_{\uparrow\downarrow}(x)$ stem from the Schrödinger equation:

$$\Phi''_{\uparrow\downarrow}+[\varepsilon_x\mp\gamma(l_\omega/l_B)^2-a_{\uparrow\downarrow}t^2-b_{\uparrow\downarrow}t]\Phi_{\uparrow\downarrow}(t)=(l_\omega/l_\alpha)\{\pm\Phi'_{\downarrow\uparrow}+[(l_\omega/l_B)^2t+k_yl_\omega]\Phi_{\downarrow\uparrow}(t)\}, \quad (6)$$

$$a_{\uparrow\downarrow}=1+(l_\omega/l_B)^4\pm(l_\omega/l_B)^2(l_\omega/l_\beta), \quad (7)$$

$$b_{\uparrow\downarrow}=2(k_yl_\omega)[(l_\omega/l_B)^2\pm(1/2)(l_\omega/l_\beta)], \quad (8)$$

where $l_B=\sqrt{c\hbar/eB}$ is the magnetic length and $l_{\alpha(\beta)}=\hbar^2/2M\alpha(\beta)$ are typical spatial scales associated with the α (β) coupling. The quantities $\varepsilon_x\equiv(k_xl_\omega)^2$ and $t=x/l_\omega$ are the dimensionless transverse energy and coordinates, $k_x^2=(2M/\hbar^2)E-k_y^2$, and $\gamma=(M/M_0)g/2$.

As opposed to all the other terms in Eq. (2), the operator $\hat{H}^{\alpha}_{SO}$ (4) is *nondiagonal* in the spin space. Therefore, as long as the α coupling is finite (i.e., if $l_\omega/l_\alpha\neq 0$), the equations (6) are coupled to each other. It is therefore natural that the behavior of the transverse energy ε_x which is determined by Eqs. (6) crucially depends on whether or not the α coupling is present in the system.

For zero α coupling ($l_\omega/l_\alpha=0$), Eqs. (6) decouple and reduce to analytically solvable Hermitian equations. The transverse energy is then given by

$$\varepsilon_x^{\uparrow\downarrow}=(2n+1)a_{\uparrow\downarrow}^{1/2}\pm\gamma(l_\omega/l_B)^2-a_{\uparrow\downarrow}^{-1}[(l_\omega/l_B)^2\mp(1/2)(l_\omega/l_\beta)]^2(k_yl_\omega)^2, \quad (9)$$

$n=0,1,2,\ldots$ and the wave functions $\phi^n_{\uparrow\downarrow}(t)$ form complete sets. The functions $\varepsilon_x^{\uparrow\downarrow}=\varepsilon_x^{\uparrow\downarrow}(k_y)$ resemble well-known magnetoelectric parabolic subbands[23] with the only exception that finite β coupling brings in a spin-orientation dependence of the subband curvature.

We now consider the case of finite α coupling ($l_\omega/l_\alpha\neq 0$). We do not find that the coupled Eqs. (6) can be solved in an explicitly analytical form. However, a strongly convergent matrix form exists. This is found by expanding *each* unknown wave function $\Phi_\uparrow(t)$ and $\Phi_\downarrow(t)$ in terms of *both* $\phi^n_\uparrow(t)$ and $\phi^n_\downarrow(t)$ and then combining all *four* expansions obtained into a *closed* linear homogeneous system of algebraic equations with respect to the coefficients of one of the expansions. The exact spectrum ε_x has been found numerically as zeros of the corresponding determinant as a function of k_y (see Ref. 25 for more details for the zero-magnetic-field case). The exploitation of the *four* expansions has allowed us to avoid inversions of infinite matrices, while the conveniently chosen bases have made the roots of the determinant rapidly convergent.

Solid lines in Fig. 1(a) present graphs of $\varepsilon_x=\varepsilon_x(k_yl_\omega)$ for zero β coupling ($l_\omega/l_\beta=0$) and zero magnetic field. Here we see two-fold spin degeneracy of all quantum levels at $k_y=0$. Once k_y becomes finite, the SO interaction lifts this degeneracy producing an energy splitting $\Delta\varepsilon_x=\varepsilon_x^\uparrow-\varepsilon_x^\downarrow\neq 0$ between electron states with different spin orientations. For small $k_yl_\omega\lesssim 2$ this splitting is linear in k_y and agrees with results of both theoretical[9,24] and experimental[14–16] research on the SO-interaction effects caused by the quantum-well field in 2D systems. However, in a purely 2D geometry the *linear* splitting $\Delta\varepsilon_x\propto k_y$ is known[9] to be exact for *all* values of k_y, however large. In contrast to this, the Q1DES dispersion curves start to diverge from the linear behavior at $k_yl_\omega\approx 2.5$ and eventually *anticross* with an energy branch corresponding to the next higher (lower) quantum number n. This is a direct consequence of the presence of the transverse confining potential (3). Even though this potential does not contribute to the SO interaction directly (because $l_\omega/l_\beta=0$), it nevertheless strongly affects the other (quantum-well) mechanism of the SO coupling. More specifically, in the presence of the potential (3), the transverse wave functions $\Phi_{\uparrow\downarrow}(x)$ of the unperturbed system (i.e., with $l_\omega/l_\alpha=0$) are no longer simple plane waves $\exp(ik_xx)$ (as it is in a strictly 2D situation) but become parabolic cylinder

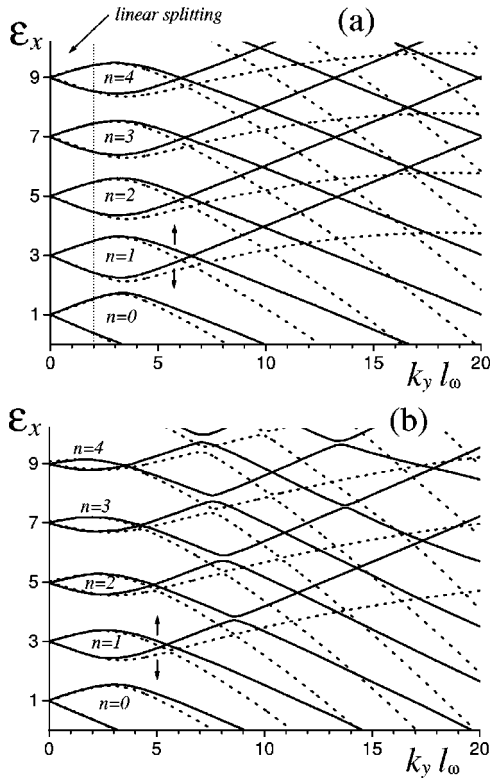

FIG. 1. The transverse energy ε_x vs $k_y l_\omega$ for finite α coupling ($l_\omega/l_\alpha=0.3$): (a) $l_\omega/l_\beta=0$; (b) $l_\omega/l_\beta=0.1$. Solid and dotted lines correspond to zero ($l_\omega/l_B=0$) and finite ($l_\omega/l_B=0.3$) magnetic field respectively.

functions.[1] When the SO perturbation operator [the rhs of Eqs. (6)] acts on these functions, it projects the nth state onto the $(n\pm1)$-st states producing an effective *hybridization* of ''neighboring'' states and therefore the *anticrossing* of the energy branches in Fig. 1(a) and the nonmonotonic dependence $\Delta\varepsilon_x(k_y)$ (see Ref. 25 for more details).

The application of a weak ($l_\omega/l_B\lesssim1$) perpendicular magnetic field bends all the energy curves downwards by an amount $\propto k_y^2$ [cf. solid and dotted lines in Fig. 1(a)]. This behavior is consistent with Eq. (9). We note that a weak magnetic field has only a small effect on the dispersion law to the left of the anticrossing region, i.e., for $k_y l_\omega\lesssim3$. For strong magnetic fields ($l_\omega/l_B\gtrsim10$), when the distance between Landau levels is very large, no anticrossing effects due to the SO interaction can be seen.

From Figs. 1(a) and 1(b) it is seen that switching on the β coupling *enhances* the anticrossing of ''neighboring'' energy branches. Moreover, the strength of the anticrossing now depends on n and grows with n. Interestingly, this effect *reduces* the linear energy splitting $\Delta\varepsilon_x\propto k_y$, in contrast to the expectation that an additional mechanism of the SO interaction should intensify the splitting rather than suppress it. What actually happens is that the β coupling, as well as the α coupling, gives a contribution to the hybridization of neighboring electron states.[25] As a result, the hybridization becomes stronger and leads to the more pronounced anticrossing and effectively to the *suppression* of the energy splitting. This effect indicates the independent nature of β coupling and its irreducibility to the α coupling. Owing to the enhanced interstate hybridization caused by the β coupling, the anticrossing of energy branches in Fig. 1(b) can be seen in a wider region of $k_y l_\omega$ up to $k_y l_\omega\approx13-14$. A weak magnetic field modifies the spectrum in Fig. 1(b) in basically the same way as it does in Fig. 1(a) [cf. solid and dotted lines in Fig. 1(b)].

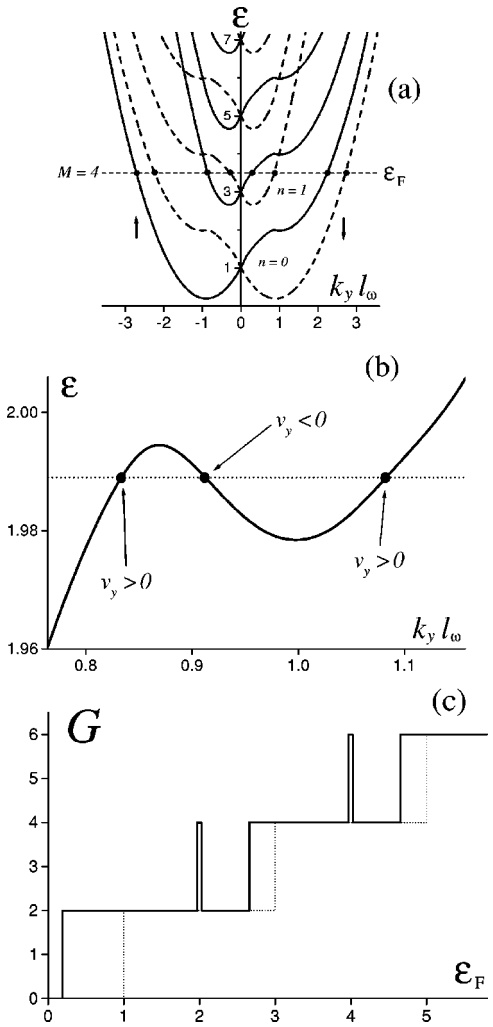

FIG. 2. The dimensionless subband energy ε vs $k_y l_\omega$ (a) and the conductance G vs the Fermi energy ε_F (c) for $l_\omega/l_\alpha=1.8$, $l_\omega/l_\beta=l_\omega/l_B=0$. (b) shows a magnified bump on an $n=0$ energy curve.

The electron eigenstates that were discussed above can be proven to obey the fundamental *current-conservation identity*[25,26] so that a current can travel adiabatically in any of these states without scattering into any other. This property allows the low temperature (ballistic) conductance G of a Q1DES to be calculated directly from the energy spectrum by relating it to the number M of forward propagating electron modes at a given Fermi energy ε_F via simple Landauer formula:[27] $G=(e^2/h)M(\varepsilon_F)$.

The most interesting effects on G are obtained for strong α coupling when $l_\omega/l_\alpha\gtrsim1.4$. Here the anticrossing (nonmonotonic) portion of curves $\varepsilon_x(k_y)$ in Fig. 1(a) comes so close to the y axis that the longitudinal term $(k_y l_\omega)^2$ in the total subband energy $\varepsilon=\varepsilon_x+(k_y l_\omega)^2$ does not disguise completely the original nonmonotonicity of $\varepsilon_x(k_y)$. As a result, we see a small *nonmonotonic* portion (''bump'') on all the energy curves $\varepsilon(k_y)$ in Fig. 2(a) [see a magnified bump for the lowest level $n=0$ in Fig. 2(b)]. Remarkably, these bumps

give rise to *three* propagating electron modes as opposed to just one created by any monotonic interval of the spectrum. Furthermore, two of these modes [the two leftmost black circles in Fig. 2(b)] ''mirror'' each other in the sense that they have nearly the same spatial wave functions but oppositely directed longitudinal group velocities $v_y = \hbar^{-1}(\partial\varepsilon/\partial k_y)$. It is therefore likely that weak elastic scattering between the forward and backward propagating modes may cause directed localization[28] and the twin modes will not contribute to the net current. However, in a sufficiently clean system, the existence of such unusual modes could give rise to sharp ($\sim$0.1 meV wide) periodic peaks in the dependence $G(\varepsilon_F)$ [Fig. 2(c)].

A second manifestation of the α coupling in Fig. 2(c) is a shift of the conductance quantization steps to lower energies in comparison with the case of zero SO interaction (cf. solid and dotted lines). This effect is caused by energy branches that go downwards in the region of the linear energy splitting [see Fig. 1(a)] and therefore lower the energy of a band edge.

In Fig. 1(b) we saw that switching on the β coupling reduces the energy splitting created by the α coupling. As applied to the subband energy $\varepsilon(k_y)$ this means suppression of the nonmonotonic bumps and eventually quenching the peaklike structure in $G(\varepsilon_F)$. For example, for $l_\omega/l_\beta = 0.2$ only one (the lowest) bump in Fig. 2(a) survives and hence only the first peak in $G(\varepsilon_F)$ can potentially be observed. The existence of the single peak (or just a few peaks) could be a clear experimental indication of the presence of the β coupling in the system.

In contrast to β coupling, a weak perpendicular magnetic field emphasizes the conductance features caused by the α coupling. Indeed, a *negative* effective potential $\propto k_y^2$ due to a magnetic field [see Eq. (9) and Figs. 1(a) and 1(b)] compensates partially to the contribution of the longitudinal energy $(k_y l_\omega)^2$ to the total subband energy $\varepsilon = \varepsilon_x + (k_y l_\omega)^2$. Hence the nonmonotonic portions of the transverse energy spectrum ε_x in Figs. 1(a) and 1(b) are now more important in forming ε than they were in the zero magnetic field. As a result, the amplitude (height) of the bumps in Fig. 2(a) will increase and the conductance peaks in Fig. 2(c) become wider (2–3 times). As regards the peaks destroyed by the β coupling, they reappear one by one starting from the lowest as the magnetic field is being increased.

In conclusion, we have revealed features of the energy spectrum of electrons and low temperature conductance arising from the specifics of the spin-orbit interaction in quasi-one-dimensional electron systems: nonmonotonic wave vector dependence of subband energies, anticrossings between subbands, additional subband minima, and sharp peaks in the ballistic conductance.

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