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Rashba Hamiltonian and electron transport

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The Rashba Hamiltonian describes the splitting of the conduction band as a result of spin-orbit coupling in the presence of an external field and is commonly used to model the electronic structure of confined narrow-gap semiconductors. Due to the mixing of spin states some care has to be exercised in the calculation of transport properties. We derive the velocity operator for the Rashba-split conduction band and demonstrate that the transmission of an interface between a ferromagnet and a Rashba-split semiconductor does not depend on the magnetization direction, in contrast with previous assertions in the literature.

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Narrow-gap semiconductors, most notably InAs, play an important role in the rapidly evolving field of spintronics. As a nonmagnetic element in hybrid devices, these materials are expected to help control the electron spin states, just like the electron charge is controlled in conventional electronic devices. Part of this potential stems from the natural two-dimensional electron gas (2DEG) on clean InAs surfaces, which allows high-quality ohmic contacts to superconductors and ferromagnets. Another reason is the seminal paper of Datta and Das,[1] which describes how the electrical field of an external gate electrode can be used to manipulate the precession of a conduction electron spin. Essential for this mechanism is the field-dependent spin-orbit coupling, which is relatively large and well-established for the 2DEG on InAs. It is now generally accepted that the spin-orbit interaction in narrow-gap 2DEGs is governed by the Rashba Hamiltonian,[2] which increases linearly with the electron wave vector.

The spin-orbit-interaction induced 'spin-splitting' is sometimes confused with an exchange or Zeeman splitting. However, the latter require breaking of the time inversion symmetry and are therefore fundamentally different from the former. It is then not surprising that physical properties like exciton spin splittings or, in the present context, spin-dependent transport properties of narrow-gap hybrid devices are not well understood. In a recent paper, for example, it was argued[3] that the conductance of the interface between a ferromagnet and a spin-orbit spin-split semiconductor should change on a flip of the magnetization direction of the ferromagnet. This obviously cannot be correct because in the absence of an external magnetic field, the spin-quantization axis in the (isotropic) semiconductor can be rotated with the magnetization direction, which should therefore be without physical consequences.[4] The problem with the calculations of Ref. 3 can be traced to an incorrect treatment of the velocity operator, which in the presence of spin-orbit interaction is not simply given by $\hbar\vec{k}/m$, where m is the effective mass of an electron and $\vec{k}$ its wave vector.

It is the purpose of our communication to clarify the issues mentioned above. First, we will discuss the nature of the eigenstates of the Rashba Hamiltonian in some detail and derive the proper velocity operator. For comparison, we give similar expressions for the eigenstates and velocity operator for a Stoner-Wohlfarth ferromagnet. Finally, we calculate explicitly the transmission coefficient between a ferromagnet and a ''Rashba-split'' electron gas and show that the contact conductance is invariant with respect to a magnetization reversal of the ferromagnet.

The Hamiltonian of an otherwise free electron system, but including the Rashba spin-orbit scattering term reads:[2]

$$H=-\frac{\hbar^2\vec{\nabla}^2}{2m}+\alpha(-i\vec{\nabla}\times\vec{E})\cdot\vec{\sigma}, \tag{1}$$

where α is an effective mass parameter and $\vec{\boldsymbol{\sigma}}=(\sigma_x,\sigma_y,\sigma_z)$ is the vector of Pauli spin matrices. For a 2DEG with a confining electric field normal to the interface $\vec{E}=(0,0,E_z)$:

$$H=\begin{pmatrix} E_0-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) & \langle\alpha E_z\rangle\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right) \\ -\langle\alpha E_z\rangle\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right) & E_0-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\end{pmatrix}, \tag{2}$$

where $\langle\alpha E_z\rangle$ is the expectation value over the lowest subband with energy E_0. Experimentally, one typically observes[5,6] values for $\langle\alpha E_z\rangle$ on the order of 10^{-11} eV m. The eigenstates for in-plane motion (identified by their quantum numbers $\vec{k}=(k_x,k_y)$ and $s=\pm1$) are

$$\phi_{\vec{k}s}(\vec{r})=N_{\vec{k}s}e^{i\vec{k}\vec{r}}\begin{pmatrix} is\left(\frac{k_x}{k}-i\frac{k_y}{k}\right) \\ 1\end{pmatrix}, \tag{3}$$

where $N_{\vec{k}s}$ is a normalization factor. From this expression for the eigenstates, it is immediately obvious that the Rashba-split subbands are not spin-polarized.[7] The electron energy dispersion relation $E_{\vec{k}s}$ reads [see Fig. 1(a)]:

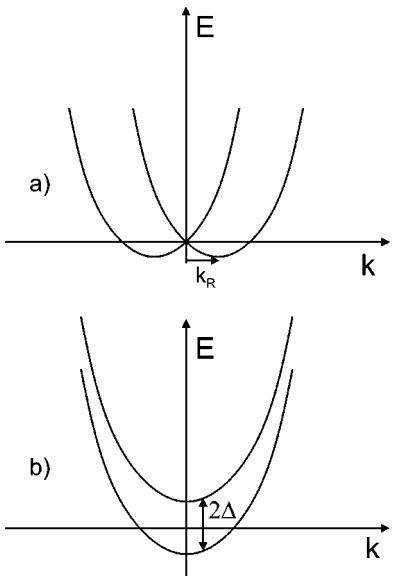

FIG. 1. Schematic representation of the conduction band structure of (a) a semiconductor in which the spin-degeneracy is broken by spin-orbit interaction as described by the Rashba Hamiltonian and (b) a spin-polarized exchange-split band ferromagnet (Stoner-Wohlfarth model).

$$E_{\vec{k}s}=E_0+\frac{\hbar^2}{2m}[(k+sk_R)^2-k_R^2], \tag{4}$$

where $k=\sqrt{k_x^2+k_y^2}$, $k_R=\langle\alpha E_z\rangle m/\hbar^2$.

The normalization factor of the eigenfunctions can be determined in different ways. Normalization of the probability distribution $\int d\vec{r}|\phi_{\vec{k}s}(\vec{r})|^2=1$ gives $N_{\vec{k}s}=1/\sqrt{2S}$ where S is the area of the 2DEG. However, for a calculation of the transport properties it is more convenient to normalize the states such that its currents are unity in the transport, say x, direction. To this end we have to compute the expectation value of the current or velocity operator which, in the presence of the Rashba term, are not simply proportional to the gradient operator anymore. The proper matrix representation in spinor space can be derived via the Hamilton equation of motion:

$$\dot{q}=\frac{\partial H}{\partial p};\quad \dot{p}=-\frac{\partial H}{\partial q};\quad \dot{x}=v_x=\frac{\partial H}{\partial p_x};\quad \dot{p}_x=-\frac{\partial H}{\partial x}. \tag{5}$$

The velocity operator in the x-direction therefore reads:

$$v_x=\frac{1}{\hbar}\begin{pmatrix} -i\frac{\hbar^2}{m}\frac{\partial}{\partial x} & i\langle\alpha E_z\rangle \\ -i\langle\alpha E_z\rangle & -i\frac{\hbar^2}{m}\frac{\partial}{\partial x}\end{pmatrix}. \tag{6}$$

Requiring $\langle\phi_{\vec{k}s}(\vec{r})|v_x|\phi_{\vec{k}s}(\vec{r})\rangle=1$ we find

$$N_{\vec{k}s}=\sqrt{\frac{m}{2\hbar}}\sqrt{\frac{1}{\left|k_x\left(1+s\frac{k_R}{k}\right)\right|}}. \tag{7}$$

This value diverges when the group velocity vanishes, i.e., for $s=-1$ at $k=k_R$.

The above considerations for a 2DEG are only slightly modified for a quantum wire. For the lowest mode:

$$H(x,p_x)=\begin{pmatrix} E_0'+\frac{p_x^2}{2m} & i\frac{\langle\alpha E_z\rangle}{\hbar}p_x \\ -i\frac{\langle\alpha E_z\rangle}{\hbar}p_x & E_0'+\frac{p_x^2}{2m}\end{pmatrix}, \tag{8}$$

$$v_x=\frac{\partial H}{\partial p_x}=\begin{pmatrix} \frac{p_x}{m} & i\frac{\langle\alpha E_z\rangle}{\hbar} \\ -i\frac{\langle\alpha E_z\rangle}{\hbar} & \frac{p_x}{m}\end{pmatrix}. \tag{9}$$

Note that there is no Rashba level splitting in a quantum dot.

It is instructive to compare the Rashba Hamiltonian with that of a 2D noncollinear ferromagnet with a dispersion as sketched in Fig. 1(b):

$$H_{ncf}=\begin{pmatrix} \frac{p_x^2}{2m}+\frac{p_y^2}{2m} & 0 \\ 0 & \frac{p_x^2}{2m}+\frac{p_y^2}{2m}\end{pmatrix}+\Delta U^+\sigma_z U, \tag{10}$$

where 2Δ is the exchange splitting and

$$U(\theta,\varphi)=\begin{pmatrix} \cos\theta/2 & e^{-i\varphi}\sin\theta/2 \\ e^{i\varphi}\sin\theta/2 & -\cos\theta/2\end{pmatrix} \tag{11}$$

is a unitary rotation matrix corresponding to a magnetization direction of $\vec{m}=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$. For plane wave states with wave vector $\vec{k}$ and $\vec{m}=(0,-1,0)$ the Hamiltonian for the ferromagnet

$$H_{ncf}\left(k,\theta=\frac{\pi}{2},\varphi=-\frac{\pi}{2}\right)=\begin{pmatrix} \frac{\hbar^2}{2m}k^2 & i\Delta \\ -i\Delta & \frac{\hbar^2}{2m}k^2\end{pmatrix} \tag{12}$$

is formally equivalent to that of the Rashba Hamiltonian

$$H_R=\begin{pmatrix} \frac{\hbar^2}{2m}k^2 & i\Delta_R \\ -i\Delta_R^* & \frac{\hbar^2}{2m}k^2\end{pmatrix} \tag{13}$$

with $\Delta_R=\langle\alpha E_z\rangle(k_x-ik_y)$. In the ferromagnet the velocity operator is always diagonal in spin space, however:

$$v_{x,ncf}(k,\theta,\varphi)=\frac{p_x}{m}\begin{pmatrix} 1 & 0 \\ 0 & 1\end{pmatrix}. \tag{14}$$

In order to demonstrate explicitly that transport through a Rashba semiconductor/ferromagnet junction does not depend on the magnetization direction of the ferromagnet, it is sufficient to consider the simple case of a single mode quantum

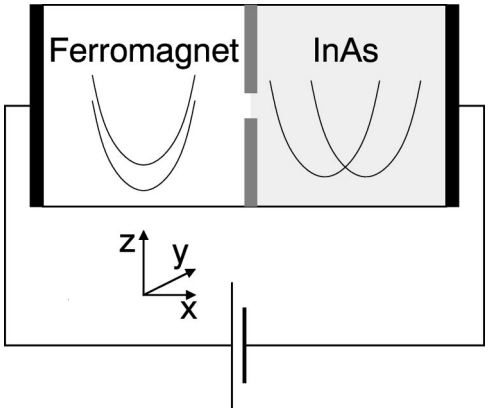

FIG. 2. The system under consideration: we discuss the conductance of a ferromagnet-semiconductor hybrid quantum point contact. The band structures of the two materials are depicted in Fig. 1. The constriction separating the two materials symbolizes the single-channel adiabatic transport we assume in our calculation. The ferromagnet is magnetized in the $-y$-direction and the current flows in the x-direction.

point contact (Fig. 2) without an additional interface potential barrier. A ferromagnet on the left side of the contact (its electronic states will be indicated by superscript $\mathfrak{L}$ in the following) is attached (at $x=0$) to a Rashba semiconductor on the right (superscript $\mathfrak{R}$). In the semiconductor we have eigenstates at the Fermi energy $E_F=(\hbar^2/2m)k_F^2$ at wave vectors $k_s=-sk_R+\sqrt{k_R^2+k_F^2}$ which are taken to be positive in the following. The states at the Fermi energy are right moving:

$$\phi_{k_+}^{\mathfrak{R}}(x)=Ne^{ik_+x}\begin{pmatrix}1\\-i\end{pmatrix};\quad \phi_{k_-}^{\mathfrak{R}}(x)=Ne^{ik_-x}\begin{pmatrix}1\\i\end{pmatrix} \tag{15}$$

and left moving

$$\phi_{-k_+}^{\mathfrak{R}}(x)=Ne^{-ik_+x}\begin{pmatrix}1\\i\end{pmatrix};\quad \phi_{-k_-}^{\mathfrak{R}}(x)=Ne^{-ik_-x}\begin{pmatrix}1\\-i\end{pmatrix} \tag{16}$$

with normalization

$$N=\sqrt{\frac{m}{2\hbar}}\sqrt{\frac{1}{k_s+sk_R}}=\sqrt{\frac{m}{2\hbar}}\sqrt{\frac{1}{\sqrt{k_R^2+k_F^2}}}. \tag{17}$$

The flux normalization reflects the identical group velocities for the two bands. The normalization is invariant under a unitary transformation which diagonalizes the Hamiltonian. We have seen above that we can interpret the Rashba semiconductor as a pseudoferromagnet in which the magnetization is rotated from the z to the $-y$ direction, and with a k-dependent exchange splitting Δ_R. We simplify the situation by taking the quantization axis of the ferromagnet parallel to the pseudomagnetization of the Rashba Hamiltonian by transforming the Rashba Hamiltonian as follows:

$$U^+\left(\frac{\pi}{2},-\frac{\pi}{2}\right)H_RU\left(\frac{\pi}{2},-\frac{\pi}{2}\right)=\begin{pmatrix}\frac{p_x^2}{2m} & 0\\ 0 & \frac{p_x^2}{2m}\end{pmatrix}\times\langle\alpha E_z\rangle\frac{\partial}{\partial x}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}, \tag{18}$$

yielding the following eigenstates along the quantization $(-y)$ axis of the ferromagnet

$$U\phi_{k_+}^{\mathfrak{R}}(x)=\sqrt{\frac{m}{\hbar\sqrt{k_R^2+k_F^2}}}\begin{pmatrix}1\\0\end{pmatrix}, \tag{19}$$

$$U\phi_{k_-}^{\mathfrak{R}}(x)=\sqrt{\frac{m}{\hbar\sqrt{k_R^2+k_F^2}}}\begin{pmatrix}0\\1\end{pmatrix}. \tag{20}$$

On the left side we assume first a half-metallic ferromagnet, for which the conduction electrons are either all spin up or down with wave vector k_F:

$$\phi_{\uparrow}^{\mathfrak{L}}(x)=\sqrt{\frac{m}{\hbar k_F}}e^{ik_Fx}\begin{pmatrix}1\\0\end{pmatrix}, \tag{21}$$

$$\phi_{\downarrow}^{\mathfrak{L}}(x)=\sqrt{\frac{m}{\hbar k_F}}e^{ik_Fx}\begin{pmatrix}0\\1\end{pmatrix}. \tag{22}$$

Assuming that the spin is up on the left side, we can now write the eigenstates of the ferromagnet in terms of the reflection coefficient $r_\uparrow$:

$$\chi_{\uparrow}^{\mathfrak{L}}(x)=\sqrt{\frac{m}{\hbar k_F}}\left[e^{ik_Fx}\begin{pmatrix}1\\0\end{pmatrix}+r_\uparrow e^{-ik_Fx}\begin{pmatrix}1\\0\end{pmatrix}\right]. \tag{23}$$

On the side of the Rashba-split semiconductor, we have transmission for one spin direction only, which corresponds to a wave vector k_+

$$\chi_{\uparrow}^{\mathfrak{R}}(x)=t_{\uparrow+}\sqrt{\frac{m}{\hbar\sqrt{k_R^2+k_F^2}}}e^{ik_+x}\begin{pmatrix}1\\0\end{pmatrix}, \tag{24}$$

where $t_{\uparrow+}$ is the transmission coefficient. The transport coefficients are determined by the requirement of the continuity of the wave function and its flux (*not simply the derivative*) at the interface $x=0$:

$$\chi_{\uparrow}^{\mathfrak{L}}(0)=\chi_{\uparrow}^{\mathfrak{R}}(0), \tag{25}$$

$$v_x\chi_{\uparrow}^{\mathfrak{L}}(x)|_{x=0}=v_x\chi_{\uparrow}^{\mathfrak{R}}(x)|_{x=0}. \tag{26}$$

The condition for flux continuity can be rewritten as

$$\frac{\hbar}{im}\frac{\partial}{\partial x}\chi_{\uparrow}^{\mathfrak{L}}(x)\Big|_{x=0}=\frac{\hbar}{im}\left(\frac{\partial}{\partial x}+ik_R\right)t_\uparrow\sqrt{\frac{m}{\hbar\sqrt{k_R^2+k_F^2}}}e^{ik_+x}\Big|_{x=0} \tag{27}$$

$$=\frac{\hbar}{m}(k_+ + k_R)=\frac{\hbar}{m}t_\uparrow\sqrt{k_R^2+k_F^2}. \tag{28}$$

We can now calculate the conductance via the Landauer formula:

$$G_\uparrow=\frac{e^2}{h}|t_\uparrow|^2=\frac{e^2}{h}\frac{4\sqrt{1+(k_R/k_F)^2}}{(1+\sqrt{1+(k_R/k_F)^2})^2}. \tag{29}$$

To calculate $G_\downarrow$, we flip the magnetization of the ferromagnet on the left side, yielding as incoming state

$$\chi_\downarrow^{\mathfrak{L}}(x)=\sqrt{\frac{m}{\hbar k_F}}\left[e^{ik_F x}\begin{pmatrix}0\\1\end{pmatrix}+r_\downarrow e^{-ik_F x}\begin{pmatrix}0\\1\end{pmatrix}\right] \tag{30}$$

while transmission occurs only into

$$\chi_\downarrow^{\mathfrak{R}}(x)=t_\downarrow\sqrt{\frac{m}{\hbar\sqrt{k_R^2+k_F^2}}}e^{ik_- x}\begin{pmatrix}0\\1\end{pmatrix}. \tag{31}$$

Flux continuity gives

$$v_x\chi_\downarrow^{\mathfrak{L}}(x)|_{x=0}=\frac{\hbar}{im}\frac{\partial}{\partial x}\chi_\downarrow^{\mathfrak{L}}(x)|_{x=0}=v_x\chi_\downarrow^{\mathfrak{R}}(x)|_{x=0} \tag{32}$$

$$=t_\downarrow\frac{\hbar}{m}(k_- - k_R)=\frac{\hbar}{m}t_\downarrow\sqrt{k_R^2+k_F^2} \tag{33}$$

and, comparing this expression with Eq. (28), we see that the transmission coefficient is identical for up and down spins. This is in contrast with the counterintuitive results of Ref. 3 where, we believe, an incorrect velocity operator has been applied.

Since the effective-mass Rashba Hamiltonian of Eq. (1) is isotropic, the interface conductance is invariant under arbitrary rotations of the magnetization direction. In addition, the above calculations may be generalized to transmission from a weak ferromagnet with both spins occupied up to Fermi numbers $k_{\uparrow/\downarrow}$ with

$$G=\frac{e^2}{h}\sum_{\sigma=\uparrow,\downarrow}\frac{4\sqrt{k_R^2+k_F^2}}{(1+\sqrt{(k_R^2+k_F^2)/k_\sigma^2})^2}. \tag{34}$$

The interface conductance should therefore not affect anisotropies due to interference effects in the Datta transistor.[1]

We hope that this paper will help to dispel the confusion concerning the transport properties of semiconductors with spin-orbit interactions. We compared eigenstates and velocity operators for two systems, a nonmagnetic 2DEG in the presence of the Rashba Hamiltonian and a noncollinear Stoner-Wohlfarth model ferromagnet. As expected, the transmission coefficient of an interface between a ferromagnet and a Rashba-split semiconductor is found independent on the magnetization direction of the ferromagnet.

Note that the independence of the total conductance of a single ferromagnetic/normal metal interface on the magnetization direction is quite general, but does not mean that the interface is not spin-selective. Indeed, a ferromagnet does—in the absence of a significant conductivity mismatch—inject a net spin into the nonmagnetic material, with efficiencies that depend on the specific electronic band structures.[8,9] Small modulations of a single interface conductance could be achieved in principle by forcing the magnetization vector of the ferromagnet into directions which deviate from the crystal symmetry axes. However, in order to detect a strongly spin-polarized interface transmission by a transport experiment, an analyzing ferromagnet is essential. This is employed, of course, in the giant magnetoresistance effect. In semiconductors, the spin-polarized current can also be detected by the circular optical polarization of the electroluminescence of a light emitting diode.[10]

Note added: After submission of this manuscript, we received a preprint by Zülicke and Schroll with similar results. Bruno and Pareek, cond-mat/0105506, report numerical calculations for the same system. In contrast to what we report here, the latter authors find a small anisotropy in the transport as a function of the magnetization angle. These anisotropies are allowed by (Casimir-Onsager) symmetry, but they vanish for the effective mass Hamiltonian (1), which does not contain any ''warping'' corrections which reflect the reduced symmetry of the crystalline lattice.

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