Diffuse transport and spin accumulation in a Rashba two-dimensional electron gas

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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 asymmetric confinement potential 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 diffusive conductance tensor for a disordered two-dimensional electron gas with spin-orbit interaction and show that the applied bias induces a spin accumulation, but that the electric current is not spin polarized.

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Utilizing the spin degrees of freedom for electronic applications is a declared goal of the research field of magnetoelectronics or spin electronics.[1] Devices made from metallic layered systems displaying the giant[2] and tunnel magnetoresistance[3,4] have been proven useful for read-head sensors and magnetic random access memories. Integration of such devices with semiconductor electronics is desirable but has turned out to be difficult because a large resistivity mismatch between magnetic and normal materials is detrimental to spin injection.[5] Still, this problem can been solved in various ways and spin injection into bulk semiconductors has indeed been reported.[6–11] Electrical spin injection into a high-mobility two-dimensional electron gas (2DEG) and its detection appears to be much more demanding.[12] In this context it would be attractive if application of an electric field alone would suffice to induce a nonequilibrium magnetization or spin accumulation in the presence of the spin-orbit interaction. Such an effect, dubbed the "kinetic magnetoelectric effect," was actually predicted in seminal theoretical work by Levitov *et al.*[13], and is caused by the combined action of the spin-orbit interaction, absence of inversion symmetry, and the time-reversal symmetry breaking by an electric field in disordered systems. In asymmetric heterostructures made from narrow-gap semiconductors the spin-orbit interaction is dominated by the so-called Rashba term,[14] which has a very simple structure, can be quite significant,[15] and is modulated by gate fields.[16] Recent observations of a spin-galvanic effect[17] and spin-orbit scattering-induced localization/antilocalization transition in 2DEGs (Refs. 18 and 19) reflect the interest and importance of the topic.

Edelstein[20] showed that an applied field induces an in-plane magnetization in a Rashba 2DEG. Although he did not make any suggestions in this direction, the interpretation of the spin accumulation being caused by an effective magnetic field has lead subsequently to the misconception that the current is also spin polarized. A microscopic calculation of both spin accumulation and current (or the conductivity tensor) on an equal footing is thus required. Furthermore, the existence of the spin-orbit-induced spin accumulation and the conditions for its observability have recently been a matter of controversy.[21–25]

In this paper we carry out microscopic model calculations of the conductivity tensor and spin accumulation for a disordered Rashba 2DEG in the linear-response regime. This task is complicated by the correction to the electric-field vertex, which does not vanish even for short-range isotropic scatterers. We confirm that a spin accumulation normal to the applied electric-field vector is excited. However, the electric current is not spin polarized, thus solving the controversies mentioned above. We furthermore show that the mobility increases quadratically with the Rashba spin-orbit interaction.

The Rashba Hamiltonian in the momentum representation and Pauli spin space reads

$$H_0=\begin{pmatrix} \dfrac{\hbar^2}{2m}k^2 & i\langle \alpha E_z\rangle k_- \\ -i\langle \alpha E_z\rangle k_+ & \dfrac{\hbar^2}{2m}k^2 \end{pmatrix}, \tag{1}$$

where $k_\pm = k_x \pm i k_y$ with $\mathbf{k}=(k_x,k_y)$ the electron momentum in the 2DEG plane. $\langle \alpha E_z\rangle$ parametrizes the spin-orbit coupling and is experimentally accessible.[15] The eigenfunctions of the Hamiltonian are

$$\phi_{\mathbf{k}s}=\frac{1}{\sqrt{2L^2}}e^{i\mathbf{k}\cdot\mathbf{r}}\begin{pmatrix} is\dfrac{k_-}{k} \\ 1 \end{pmatrix}, \tag{2}$$

with $s=\pm$, $k=\sqrt{k_x^2+k_y^2}$, L^2 the area of the 2DEG, and corresponding eigenvalues are given as $E_{ks}=\hbar^2k^2/2m+s\langle \alpha E_z\rangle k$. The current operator in Pauli spin space is given as

$$j_x = ev_x = e\begin{pmatrix} bk_x & i\lambda \\ -i\lambda & bk_x \end{pmatrix}, \tag{3}$$

$$j_y = ev_y = e\begin{pmatrix} bk_y & \lambda \\ \lambda & bk_y \end{pmatrix}, \tag{4}$$

with $b=\hbar/m$ and $\lambda=\langle \alpha E_z\rangle/\hbar$. In the space of the eigenfunctions of H_0, referred to hereafter as the s space ($s=\pm$), the current operators are transformed as

$$J_{x(y)} = U^\dagger j_{x(y)} U = e\left[bk_{x(y)}\mathbf{1} + \lambda \frac{k_{x(y)}}{k}\,\sigma_z - (+)\lambda\frac{k_{y(x)}}{k}\,\sigma_y\right], \tag{5}$$

by the unitary matrix

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} i\dfrac{k_-}{k} & -i\dfrac{k_-}{k} \\ 1 & 1 \end{pmatrix}. \tag{6}$$

We also need the transformed spin matrices, $U^\dagger\sigma_x U$, $U^\dagger \sigma_y U$, and $U^\dagger\sigma_z U$ to evaluate the spin accumulation.

The standard model for disorder consists of randomly distributed, identical point defects, which are neither spin dependent nor flip the spin:

$$V(\mathbf{r}) = V\mathbf{1}\sum_i \delta(\mathbf{r}-\mathbf{R}_i). \tag{7}$$

In the following, we expand the Green function $G=(z\mathbf{1}-H)^{-1}$, where $H=H_0+V(\mathbf{r})$ and $z=\epsilon\pm i\eta$, in terms of the unperturbed Green function, $G_0=[z\mathbf{1}-H_0]^{-1}$, with matrix elements $g_{k\pm}=1/(z-E_{k\pm})$ in s space, and calculate the self-energy Σ in the Born approximation.

After ensemble averaging over the impurity distribution, denoted by $\langle\cdots\rangle_{AV}$, and disregarding a trivial constant term, the self-energy in the Born approximation reads

$$\begin{aligned}\langle\langle \mathbf{k}s|VG_0V|\mathbf{k}''s''\rangle\rangle_{AV} &= \frac{nV^2}{4L^2}\delta_{\mathbf{k}\mathbf{k}''}\sum_{k's'} g_{k's'}\left(1+ss''+ss'\frac{k_+k'_-}{kk'}+s's''\frac{k'_+k_-}{k'k}\right)\\ &= \frac{nV^2}{2L^2}\delta_{\mathbf{k}\mathbf{k}''}\delta_{ss''}\sum_{k's'} g_{k's'} = \Sigma\,\delta_{\mathbf{k}\mathbf{k}''}\delta_{ss''},\end{aligned} \tag{8}$$

where $n\equiv N/L^2$ is the density of impurities per unit area. Equation (8) follows from the odd symmetry of $k_+k'_-$ and k'_+k_- with respect to k'_x or k'_y. The Green function is therefore given as

$$\langle\langle \mathbf{k}s|G|\mathbf{k}''s''\rangle\rangle_{AV} = \frac{1}{g_{ks}^{-1}-\Sigma}\delta_{\mathbf{k}\mathbf{k}''}\delta_{ss''} = \tilde{G}_{ks}. \tag{9}$$

We find both $\tilde{G}$ and Σ to be diagonal in $\mathbf{k}$ and s. By direct inspection it can be seen that $\langle VG_0VG_0VG_0V\rangle$ is diagonal, meaning that the *exact* self-energy must be diagonal as well.

The (longitudinal) conductivity is given by the Kubo formula as

$$\sigma_{xx} = \frac{\hbar}{4\pi L^2}\mathrm{Tr}\langle J_xG^AJ_xG^R + J_xG^RJ_xG^A\rangle_{AV}, \tag{10}$$

where the superscripts A and R denote advanced and retarded, respectively, and will be omitted below for brevity. We evaluate $\langle J_xGJ_xG\rangle_{AV}=J_x\langle GJ_xG\rangle_{AV}\equiv J_xK$ in the ladder approximation, which obeys the Ward relation with the self-energy in the Born approximation:

$$K \sim \tilde{G}J_x\tilde{G} + \tilde{G}\langle VKV\rangle_{AV}\tilde{G}. \tag{11}$$

The matrix elements of $\langle VKV\rangle_{AV}$ are

$$\begin{aligned}\langle\langle ks|VKV|k's'\rangle\rangle_{AV} &= \sum_{k_1s_1}\sum_{k_2s_2}\left(\frac{V}{2L^2}\right)^2\sum_i \langle e^{-i(\mathbf{k}-\mathbf{k}_1)\cdot\mathbf{R}_i}e^{i(\mathbf{k}'-\mathbf{k}_2)\cdot\mathbf{R}_i}\rangle_{AV}\\ &\times\left(1+ss_1\frac{k_+k_{1-}}{kk_1}\right)\left(1+s_2s'\frac{k_{2+}k'_-}{k_2k'}\right)\langle k_1s_1|K|k_2s_2\rangle.\end{aligned} \tag{12}$$

To evaluate the expression for $\langle VKV\rangle_{AV}$, we first use $\tilde{G}(k_1s_1)\langle k_1s_1|J_x|k_2s_2\rangle\tilde{G}(k_2s_2)$ for $\langle k_1s_1|K|k_2s_2\rangle$. Because J_x is diagonal in k, $\mathbf{k}_1=\mathbf{k}_2$, and the average of the exponential factor leads to $\mathbf{k}=\mathbf{k}'$. Repeating this procedure iteratively, we find that, like $\tilde{G}$, K is diagonal in k. The matrix elements $\langle ks|VKV|ks'\rangle$ may be evaluated iteratively. We call $\langle ks|K|ks'\rangle^{(0)}=\langle ks|\tilde{G}J_x\tilde{G}|ks'\rangle$ and note that $\langle ks|\tilde{G}J_x\tilde{G}|ks'\rangle\propto k_x$ when $s=s'$ and $\propto k_y$ when $s\neq s'$ and keeping terms which are even functions of k_x and k_y in the summation of the equation. Then, by direct inspection,

$$\langle ks|VKV|ks'\rangle_{AV} = \frac{e\lambda'}{k}(k_x\sigma_z - k_y\sigma_y), \tag{13}$$

where

$$\begin{aligned}e\lambda' = \frac{nV^2}{2L^2}\sum_k \frac{1}{k}\big(&k_x\langle k+|\tilde{G}J_x\tilde{G}|k+\rangle - ik_y\langle k+|\tilde{G}J_x\tilde{G}|k-\rangle\\ &+ik_y\langle k-|\tilde{G}J_x\tilde{G}|k+\rangle - k_x\langle k-|\tilde{G}J_x\tilde{G}|k-\rangle\big).\end{aligned} \tag{14}$$

Comparing Eq. (13) with Eq. (11) and the definition of J_x, Eq. (4), we find that $K\equiv\tilde{G}\tilde{J}_x\tilde{G}$ has the same structure as $\tilde{G}J_x\tilde{G}$, where λ in J_x is replaced by $\lambda+\lambda'$ in $\tilde{J}_x$. By replacing $\tilde{G}J_x\tilde{G}$ in Eq. (14) with $K=\tilde{G}\tilde{J}_x\tilde{G}$, we obtain a closed equation for λ':

$$\lambda' = \frac{nV^2}{4L^2}\sum_k \{kbS_1 + (\lambda+\lambda')S_0\}, \tag{15}$$

with $S_1\equiv\Sigma_s s\tilde{G}_{ks}\tilde{G}_{ks}$ and $S_0\equiv\Sigma_{ss'}\tilde{G}_{ks}\tilde{G}_{ks'}$. Here, we have used relations $k_x^2=k_y^2=k^2/2$ in the summation over k.

The conductivity now reads

$$\sigma_{xx}=\frac{\hbar}{2\pi L^2}\mathrm{Tr}\,J_x\tilde{G}\tilde{J}_x\tilde{G}, \tag{16}$$

where the tildes indicate substitution of λ by $\lambda+\lambda'$, and $J_x\tilde{G}\tilde{J}_x\tilde{G}$ is a 2×2 matrix expressed in s space. By carrying out the trace, the conductivity follows as $\sigma_{xx}=\sigma_{xx}^{+}+\sigma_{xx}^{-}$ with

$$\sigma_{xx}^{\pm}=\frac{\hbar e^2}{4\pi L^2}\sum_k \left\{\left(b\pm\frac{\lambda}{k}\right)\left(b\pm\frac{\lambda+\lambda'}{k}\right)k^2\tilde{G}_{k\pm}\tilde{G}_{k\pm} +\lambda(\lambda+\lambda')\tilde{G}_{k\mp}\tilde{G}_{k\pm}\right\}. \tag{17}$$

By using the unitary matrix U, the matrix representation of the conductivity in s-space can be transformed into that in the original Pauli spin space as $\hat{\sigma}_{xx}=\hbar UJ_x\tilde{G}\tilde{J}_x\tilde{G}U^{\dagger}/2\pi L^2$, with $\hat{\sigma}_{xx}^{\uparrow\uparrow},\hat{\sigma}_{xx}^{\uparrow\downarrow}$, etc. By taking the spin trace of $\hat{\sigma}_{xx}$, the relation $\sigma_{xx}^{+}+\sigma_{xx}^{-}=\hat{\sigma}_{xx}^{\uparrow\uparrow}+\hat{\sigma}_{xx}^{\downarrow\downarrow}$ follows naturally. We observe that $\hat{\sigma}_{xx}^{\uparrow\uparrow}=\hat{\sigma}_{xx}^{\downarrow\downarrow}$ and that the nondiagonal elements of the conductance tensor in the original spin space $\hat{\sigma}_{xx}^{\uparrow\downarrow}$ vanish identically by parity. These results prove that the current excited by the electric field is not spin polarized. The expression for σ_{yy} can be derived analogously. We also find that the nondiagonal (Hall) conductivity σ_{xy} vanishes by symmetry.

In calculating the vertex correction and conductivity we encounter integrals over the momentum, which may easily evaluated by an approximation in which the lifetime broadening of the density of states is neglected,

$$\tilde{G}_{ks}^{R}\tilde{G}_{ks}^{A}=\frac{2\pi\tau}{\hbar}\delta(\epsilon-E_{ks}), \tag{18}$$

where the lifetime τ is defined $\Sigma=-i\,\mathrm{sgn}(\eta)\hbar/2\tau$ or $\tau=\hbar/2\pi nV^2D$ with the 2DEG density of states per spin $D=m/2\pi\hbar^2$. We then obtain $\lambda'=-\lambda$, and

$$\sigma_{xx}=\frac{2e^2n_0\tau}{m}+2e^2\tau D\lambda^2, \tag{19}$$

where n_0 is the number of electrons per spin. The conventional Drude conductivity (first term) is increased by the spin-orbit interaction. Since the sign of the coupling constant λ is irrelevant, the enhancement term must be of even order in λ. The result $\lambda'=-\lambda$ shows that the vertex function $\tilde{J}_x$ is diagonal in spin space.[26] In the case of $\lambda=0$, the vertex correction in the ladder approximation vanishes identically due to the isotropic scattering.

It is important to distinguish the spin-polarized currents computed above from the spin accumulation which is excited by the applied field E, which in linear response is given by

$$\langle\mathbf{s}\rangle=\hbar\,\mathrm{Tr}\boldsymbol{\sigma}\langle G^AJ_xG^R+G^RJ_xG^A\rangle_{AV}E. \tag{20}$$

In s space, each component is given as

$$\langle s_i\rangle=\hbar\,\mathrm{Tr}\,U^{\dagger}\sigma_iU\tilde{G}\tilde{J}_x\tilde{G}E. \tag{21}$$

We find $\langle s_z\rangle=\langle s_x\rangle=0$, but

$$\langle s_y\rangle=-\frac{e\hbar}{2L^2}\sum_k\{bkS_1+(\lambda+\lambda')S_0\}E. \tag{22}$$

The expression is simplified as

$$\langle s_y\rangle=e4\pi\tau D\lambda E, \tag{23}$$

by using the approximation (18). The spin accumulation is aligned to the pseudomagnetic field of the spin-orbit interaction and its magnitude is proportional to the applied electric field within the linear-response regime. The magnitude of the spin accumulation may be estimated as

$$|\langle s_y\rangle|/D=2.5\left[\frac{\lambda}{10^{-11}\ \text{eV m}}\right]\left[\frac{eE}{10\ \text{KeV/m}}\right]\times\left[\frac{\mu}{10^5\ \text{cm}^2\ \text{V}^{-1}\ \text{s}^{-1}}\right]\ \text{meV}, \tag{24}$$

with $\lambda=10^{-11}$ eV m.[15] The splitting of the chemical potential thus amounts to a significant 2.5 MeV for typical experimental parameters of the applied field and the mobility μ.

We have thus formulated the conductivity tensor and spin accumulation on an equal footing using linear-response theory. The conductivity is found to be enhanced by the spin-orbit interaction and is isotropic in spin space, i.e., $\hat{\sigma}_{xx}^{\uparrow\uparrow}=\hat{\sigma}_{xx}^{\downarrow\downarrow}$ and $\hat{\sigma}_{xx}^{\uparrow\downarrow}=\hat{\sigma}_{xx}^{\downarrow\uparrow}=0$. We have proven that an electric field has induced a spin-polarized density,[20] but not a spin-polarized current. The recent discovery of the spin-galvanic effect, i.e., that a magnetization along the y direction induces an electric current[17] is reciprocal to the current-induced spin accumulation. We may conclude that his current can also not be spin polarized.

The result that the conductivity is spin isotropic implies that the spin accumulation in ferromagnet (F)/2DEG hybrids cannot be detected in a two-terminal configuration with one ferromagnetic contact. A single source or drain ferromagnetic contact does not modify the global transport properties in the diffusive regime, because the contacts, which connect the reservoir distribution functions to the semiconductor ones, are not affected by a magnetization reversal.[27] A phenomenological theory[28,29] is at odds with this conclusion. Microscopically, we trace the matrix character of the current operator to be the culprit of this disagreement.[27] Experiments on F/2DEG systems,[21] which were supported by that theory,[28,29] were challenged by Monzon *et al.*[24] and van Wees,[25] who suspected that the measured effects were due to local Hall voltages caused by fringe fields near the ferromagnetic contacts. These[21] and subsequent experiments[22,23] should perhaps be reconsidered in light of the present theoretical results.

The present results are related but different from the spin-Hall effect discussed by Zhang[30] who dealt with a ferromagnetic metal thin film. He suggested to measure the spin accumulation excited by the electric current in a three-terminal configuration, which is also an option for the 2DEG, since we find the spin-accumulation signal to be quite significant.

Spin-polarized transport can be detected in a F/2DEG/F configuration with two ferromagnetic contacts as studied by

Pareek and Bruno.[31] We point out that the spin-dependent conductances $\Gamma_{\uparrow\uparrow}$ and $\Gamma_{\uparrow\downarrow}$ in Ref. 31 must not be confused with the spin-dependent conductivities $\hat{\sigma}_{xx}^{\uparrow\uparrow}$ and $\hat{\sigma}_{xx}^{\uparrow\downarrow}$ defined above. The former conductances are defined as $\Gamma_{\uparrow\uparrow(\downarrow)} = (e^2/h)\mathrm{Tr}\mathbf{t}_{\uparrow\uparrow(\downarrow)}\mathbf{t}^{\dagger}_{\uparrow(\downarrow)\uparrow}$, where $\mathbf{t}$ is a transmittance matrix, whereas $\hat{\sigma}_{xx}^{\uparrow\downarrow}=0$ as shown above, is in general $\Gamma_{\uparrow\downarrow}\neq 0$. It is possible to decompose the conductivity $\hat{\sigma}_{xx}^{\uparrow\uparrow}$ by "cutting lines" in the conductivity diagram such that $\hat{\sigma}_{xx}^{\uparrow\uparrow}=\hat{\sigma}_{xx}^{\uparrow\uparrow\uparrow\uparrow}+\hat{\sigma}_{xx}^{\uparrow\downarrow\downarrow\uparrow}$, which is simplified by the spin-diagonal vertex function in the ladder approximation. The two components are then given as

$$\hat{\sigma}_{xx}^{\uparrow\uparrow\uparrow\uparrow}=\frac{\hbar e^2}{16\pi L^2}\sum_{k,s}(b^2k^2+sb\lambda k)\tilde{G}_s(\tilde{G}_+ + \tilde{G}_-), \quad (25)$$

$$\hat{\sigma}_{xx}^{\uparrow\downarrow\downarrow\uparrow}=\frac{\hbar e^2}{16\pi L^2}\sum_{k,s}s(b^2k^2+sb\lambda k)\tilde{G}_s(\tilde{G}_+ - \tilde{G}_-). \quad (26)$$

We did not find as simple a relation as Eq. (19) but in general $\hat{\sigma}_{xx}^{\uparrow\downarrow\downarrow\uparrow}\neq\hat{\sigma}_{xx}^{\uparrow\uparrow\uparrow\uparrow}$, because in the limit $\lambda=0$, $\hat{\sigma}_{xx}^{\uparrow\downarrow\downarrow\uparrow}=0$, whereas $\hat{\sigma}_{xx}^{\uparrow\uparrow\uparrow\uparrow}$ tends to the Drude conductivity. This conclusion appears to be at odds with the numerical findings of Pareek and Bruno in the limit of long samples $\Gamma_{\uparrow\uparrow}\sim\Gamma_{\uparrow\downarrow}$.

In summary, we derived explicit expressions for the conductivity tensors and spin accumulation of a Rashba 2DEG with isotropic scattering centers, taking into account the vertex correction in the ladder approximation. The diffusive conductivity limited by nonmagnetic impurity scattering is not spin dependent, although the applied bias does excite a spin accumulation.

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