Theory of spin-dependent transport in ferromagnet-semiconductor heterostructures

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The formalism of spin-dependent transport is used to calculate the conductance of device structures comprised of a two-dimensional electron-gas (2DEG) channel and ferromagnetic source and/or drain for a variety of magnetization configurations. Among the effects predicted by the calculations is spin-dependent current rectification at a 2DEG-ferromagnet interface. [S0163-1829(98)02036-0]

Among the extraordinary properties of high-mobility two-dimensional electron gases (2DEG's), one remarkable characteristic, the spin splitting of the conduction band, is relatively unexploited. It is well known that the high-mobility carriers in the channel of a 2DEG heterostructure [Fig. 1(a)] are confined in a potential well with walls sufficiently steep that momentum states along $\hat{z}$ are quantized, but they can move freely in the x-y plane. The Fermi wave vector $k_F=\sqrt{2\pi n_s}$ is of order 10^6 cm^{-1} for typical carrier densities of order $n_s \sim 10^{12}$ cm^{-2} and the Fermi velocity $v_F \sim 10^7$ cm/sec is weakly relativistic. A perpendicular electric field $\mathbf{E}=E_z\hat{z}$ [Fig. 1(b)] transforms, in the frame of the carrier, as a magnetic field H^* with components in the x-y plane. This ''effective'' field can interact with the spin magnetic moment of the carrier μ_B and split the conduction band into subbands separated by an effective Zeeman energy $\Delta \propto \mu_B H^*$.

Two sources of field E_z are of particular interest. (i) An asymmetry of the confining well has an associated potential gradient $\partial V/\partial z=E_z$. Because this couples the electron spin and orbital terms, Bychkov and Rashba introduced a spin-orbit Hamiltonian[1] $H_{\rm SO}=\alpha(\sigma\times\mathbf{k})\cdot\hat{\nu}$, where σ are the Pauli matricies and $\hat{\nu}$ is a unit vector normal to the plane of the 2DEG. The spin-orbit constant α is proportional to the magnitude of the interfacial field E_z and is therefore material specific. Values of the spin-orbit splitting $\Delta_{\rm SO}\approx 2\alpha k$ ranging from 2 to 5 meV have been measured in $In_xGa_{1-x}As/In_yAl_{1-y}As$ and GaSb/InAs heterostructures by analyzing the beat pattern of Shubnikov–de Haas oscillations.[2–4] (ii) A gate voltage V_g [refer to Fig. 1(a)] results in a variable electric field E_z. Niita *et al.*[3] modulated the zero-field Bychkov-Rashba spin splitting by about 20% by applying gate voltages of order 1 V to their $In_xGa_{1-x}As/In_yAl_{1-y}As$ heterostructures.

For spin splittings $\Delta_{\rm SO}$ of a few meV, the magnitude of the effective field H^*, given by $\Delta=2g\mu_B H^*=[2(g/g_0)\mu_{B0}/(m^*/m_0)]H^*$, is the order of 1 T, where μ_{B0}, g_0, and m_0 are the free-electron values of the Bohr magneton, the g value, and the carrier mass, and typical effective values $g\sim 4g_0$ and $m^*\sim 0.1m_0$ are used. Effective fields of 1 T are substantial and this article investigates several effects on the spins of the carriers.

Referring to the schematic diagram of Fig. 2(a), we consider transport in a high-mobility 2DEG channel between a source and drain. For a heterostructure with electrons as the predominant carriers (with only the first quantized level occupied), the energy dispersion relation is[5]

$$E=E_{c,0}+\frac{\hbar^2}{2m^*}(k_x^2+k_y^2),$$

where $E_{c,0}$ is the energy at the bottom of the band. The density of states (for a valley degeneracy of 1) is given by

$$N(E)=\begin{cases}\dfrac{m^*}{\pi\hbar^2}, & E>E_{c,0}\\ 0, & E<E_{c,0}\end{cases} \tag{1}$$

and the Fermi level lies in the band for most systems of interest.

We consider electrons injected with momentum $\hbar k_x$, so that the effective field $H^*=H_y^*$ is oriented along the $\hat{y}$ axis. A third of these carriers will have their spins aligned along the $\pm\hat{x}$ axis and a third will have their spins aligned along the $\pm\hat{z}$ axis. The spins will precess about the y axis at the Larmor frequency Ω_L as the electrons move along $\hat{x}$. The remaining third have their spins oriented along the $\pm\hat{y}$ axis. Because their magnetic moments are parallel to the effective field H_y^* they do not precess. However, the one-sixth with spin along $\hat{y}$ have an additional magnetic potential energy $\mu_B H^*$ and the one sixth with spin along $-\hat{y}$ have a magnetic potential energy $-\mu_B H^*$. Thus, for those electrons with momentum k_x the density of states is spin split by $2\mu_B H^*$ in a manner similar to Pauli paramagnetism, even though there is no externally applied field $H_{\rm ext}=0$. This is represented schematically in Fig. 2(b), where Eq. (1) is used for the density of states $N(E)$ and we have assumed $T=0$ for simplicity. The situation is exactly reversed for carriers with momentum $-\hbar k_x$ [Fig. 2(c)]. Here the effective field H^* has the

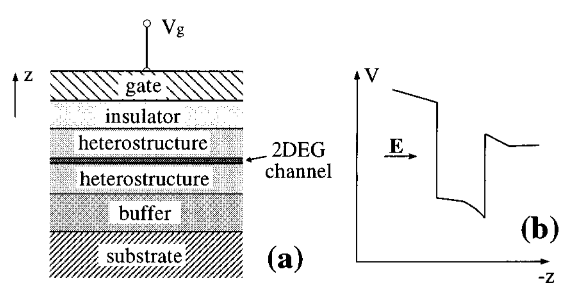

FIG. 1. (a) Layer structure of a typical, gated 2DEG heterostructure. (b) Schematic conduction-band diagram showing the potential well and field E_z.

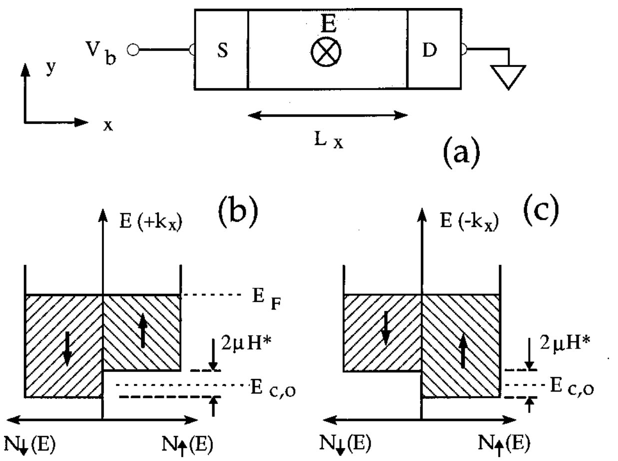

FIG. 2. (a) Top view of the generic device structure. The bias voltage V_b drives a bias current I_b through the source S, into a channel of length L_x, and through the drain D to ground. An intrinsic electric field $\mathbf{E}=E_z\hat{z}$ is perpendicular to the plane of the device. The density of states of the 2DEG channel is spin split by the effective field H^* for (b) electrons with momenta $\hbar k_x$ and (c) electrons with momenta $-\hbar k_x$.

opposite sign $H^*(-\hat{y})$, so that the electrons with spin along $-\hat{y}$ $(\hat{y})$ have an additional magnetic potential energy $\mu_B H^*$ $(-\mu_B H^*)$.

In the transport calculations below, a bias voltage V_b drives a current I_b from source to drain through a 2DEG channel of length L_x [Fig. 2(a)]. The channel conductance g can be calculated within a variety of models. A two-dimensional Landauer form,[6] for example, is

$$g=(e^2/\sqrt{2\pi}\hbar)\ \sqrt{n}t, \tag{2}$$

with t a transmission probability. In general, g is proportional to a positive power of n and the detailed form of g will not be important. Although it is not conventional to define conductance for a Fermi half sphere (or half circle, in two dimensions), we will explore systems where it is useful to introduce definitions of conductance for specific $\hat{k}$ directions as well as for spin-up and spin-down subbands. On a heuristic level, it is clear from Figs. 2(b) and 2(c) that the conductance of up-spin and down-spin carriers differs for each direction of momentum $g_\uparrow(k_x)\neq g_\downarrow(k_x)$ and $g_\uparrow(-k_x)\neq g_\downarrow(-k_x)$ because the densities of carriers differs $n_\uparrow\neq n_\downarrow$. The zero-field spin splitting of the conduction band and differences of spin subband conductance have been inferred from beat patterns in Shubnikov–de Haas oscillations,[2–4] as mentioned above.

To explore the detailed nature of the subband splitting it is necessary to measure the difference $\Delta n=n_\downarrow-n_\uparrow$ or, equivalently, the difference of subband conductance $\Delta g=g_\uparrow(k_x)-g_\downarrow(k_x)$. The approach presented here is to add g in series with the conductance of some element F, which itself has asymmetric spin subband conductance $g_{f,\uparrow}\neq g_{f,\downarrow}$ for two independently controlled cases $g_{f,\uparrow}>g_{f,\downarrow}$ and $g_{f,\uparrow}<g_{f,\downarrow}$. An appropriate element F is a single domain ferromagnetic film.[7] When the magnetization $\mathbf{M}$ of an appropriate ferromagnetic material is up, the conductance of the down-spin subband is typically larger than that of the up-spin subband $g_{f,\downarrow}>g_{f,\uparrow}$, but when the magnetization orientation is reversed, for example, by the application of a small, external

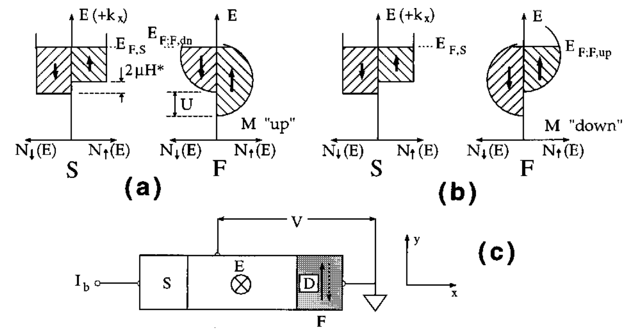

FIG. 3. Density of states diagrams, at $T=0$, for a 2DEG (left) and the exchange split band of a transition metal ferromagnet (right) (a). The magnetization of F is ''up.'' (b) The magnetization is ''down.'' These diagrams are not drawn to scale. The exchange energy U is of order 1 eV and $2\mu H^*$ is of order 1 meV. (c) Top view of a device structure with ferromagnetic drain F, with easy axis of magnetization along $\hat{y}$ so that the magnetization has two orientations $\mathbf{M}=\pm M_s\hat{y}$.

magnetic field $H_{\mathrm{ext},y}$, the inequality reverses, $g_{f,\uparrow}>g_{f,\downarrow}$. Figure 3(c) depicts the device of Fig. 2(a) with a drain composed of a thin ferromagnetic film F.

To develop a notation that includes the spin orientation of charge carriers, we note that the electric current $\mathbf{J}_e$ is a vector and a current of oriented spins is a magnetization current $\overleftrightarrow{J}_M$, a second-rank tensor given by the vector product of the number current $\eta\mathbf{J}_e/e$, where η is the fractional polarization ($\eta=1$ for 100% spin polarization), with the spin magnetic moment $\boldsymbol{\mu}_B$.[7] In the quasi-one-dimensional calculations below, $\mathbf{J}_e=J_{e,x}\hat{x}$ and $J_{e,x}$ is a scalar. For spins polarized along a single axis, e.g., the $\hat{y}$ axis, the magnetization current is $\overleftrightarrow{J}_M=\eta(\mu_B/e)J_e\hat{x}\hat{y}=J_M\hat{x}\hat{y}$ and J_M is also reduced to a scalar: a particle (and charge) current flowing along $\hat{x}$ with spins aligned along $\hat{y}$. More generally, the component $(J_M)_{i,j}$ describes the transport along axis j of the projection of spin magnetization on axis i.

It follows that the electric conductance (along $\hat{x}$) has two orthogonal components defined along $\hat{y}$, $g_\uparrow$ and $g_\downarrow$, and is conveniently considered a vector, $J_e=(g_\uparrow|\uparrow\rangle+g_\downarrow|\downarrow\rangle)V_b$, where $|\uparrow\rangle$ and $|\downarrow\rangle$ are unit vectors for up- and down-spin projections, respectively. Here we are inventing a different notation to stress the fact that $g_\uparrow$ and $g_\downarrow$ do not mix in the absence of spin-flip scattering: The vectors $|\uparrow\rangle$ and $|\downarrow\rangle$ form an orthonormal basis. Any real experiment measures the net conductance

$$J_e=(g_\uparrow+g_\downarrow)V_b=gV_b, \tag{3}$$

so that the vector conductance must be dotted with the basis vectors to find the net, experimentally measured value $g=(\langle\uparrow|+\langle\downarrow|)(g_\uparrow|\uparrow\rangle+g_\downarrow|\downarrow\rangle)=g_\uparrow+g_\downarrow$. The utility of this notation is that the electric current is simply given as the sum of subband conductances [Eq. (3)] and the magnetization current is given by their difference[7]

$$\frac{J_M}{J_e}=\frac{g_\uparrow-g_\downarrow}{g_\uparrow+g_\downarrow}\frac{\mu_B}{e}\equiv\eta\frac{\mu_B}{e}. \tag{4}$$

Finding the net conductance of a system of n structural components in series is now straightforward. A conductance is calculated for each spin subband of each component. Using the boundary condition that there is no spin-flip scattering at the interface between any two components, the net conductance of each spin subband is calculated for the entire structure and then the overall conductance of the structure is the sum of the contributions from both spin subbands,

$$g_{N,\uparrow}^{-1}=\sum_{i=1}^{n} g_{i,\uparrow}^{-1}, \quad g_{N,\downarrow}^{-1}=\sum_{i=1}^{n} g_{i,\downarrow}^{-1}, \quad G\equiv g_{\rm net}=g_{N,\uparrow}+g_{N,\downarrow}.$$

This formalism is first applied to calculate the conductance of a two-component, semiconducting 2DEG-ferromagnet (2DEG-F) system for two magnetization orientations. The calculation can be intuitively followed with simple density of states diagrams [Figs. 3(a) and 3(b)]. The diagrams on the right are appropriate for the $3d$ (or hybridized $3d$-$4s$) band of a three-dimensional transition metal ferromagnetic film F exchange split by an energy U of order 1 eV. We use the convention that F in Fig. 3(a) has up magnetization [along $\hat{y}$ in Fig. 3(c)] and down magnetization in Fig. 3(b). Referring to Fig. 3(a), charge transport in the ferromagnet involves only those carriers near the Fermi level, $g\propto N(E_F)$, and the minority spin subband conductance is larger than that of the majority spin subband $g_{\min,F}>g_{\mathrm{maj},F}$. The conductance $G_{F;\mathrm{up}}$ of F with magnetization up is[8] $G_{F;\mathrm{up}}=g_{\mathrm{maj},F}|\uparrow\rangle+g_{\min,F}|\downarrow\rangle$. Similarly, the conductance $G_{F;\mathrm{down}}$ [Fig. 3(b)] is $G_{F;\mathrm{down}}=g_{\min,F}|\uparrow\rangle+g_{\mathrm{maj},F}|\downarrow\rangle$.

On the left-hand side of Figs. 3(a) and 3(b), the density of states of a 2DEG heterostructure with Fermi energy in the band is depicted and the chemical potentials of F and S are aligned (voltage drops at the interface, or along the channel and drain, are ignored). Consistent with Fig. 3(c), for a current bias source I_b that drives electrons from source to drain, the density of states diagrams are drawn for electrons with momentum $\hbar k_x$, with a splitting of $2\mu_B H^*$. The down-spin subband conductance of the 2DEG is larger than that of the up-spin subband because $n_\downarrow > n_\uparrow$; we can denote the former as the majority spin subband and the latter as the minority spin subband and the conductance G_S of the semiconducting 2DEG channel can be written as $G_S=g_{\min,S}|\uparrow\rangle+g_{\mathrm{maj},S}|\downarrow\rangle$.

We take the vector sum of subband conductances and compare the net conductance for the cases with the magnetization of F up and down:

$$\frac{1}{G_1}=\frac{1}{G_S}+\frac{1}{G_{F;\mathrm{up}}}, \quad \frac{1}{G_2}=\frac{1}{G_S}+\frac{1}{G_{F;\mathrm{down}}}.$$

The algebra is straightforward with the result

$$\frac{G_1-G_2}{G_1+G_2}=\frac{\Delta G}{2G_{\mathrm{av}}}=\frac{\Delta R}{2R_{\mathrm{av}}}=\frac{(g_{\mathrm{maj},S}-g_{\min,S})(g_{\min,F}-g_{\mathrm{maj},F})}{(g_{\mathrm{maj},S}+g_{\min,S})(g_{\min,F}+g_{\mathrm{maj},F})}$$
$$=\eta_F P, \tag{5}$$

where

$$\eta_F=(g_{\min,F}-g_{\mathrm{maj},F})/(g_{\min,F}+g_{\mathrm{maj},F}), \tag{6}$$

$$P=(g_{\mathrm{maj},S}-g_{\min,S})/(g_{\mathrm{maj},S}+g_{\min,S}). \tag{7}$$

Changing the polarity of bias current has the same effect as reversing the magnetization orientation of F and Eq. (5) predicts that the 2DEG-F interface should rectify alternating current, as long as F is uniformly magnetized along the $\hat{y}$ axis. This is an effect that is unrelated to the p-n junction behavior and derives entirely from interfacial spin-dependent transport. Equation (6) is analagous to Eq. (4); it defines η_F as the fractional spin polarization of current inside a ferromagnet. For transition-metal ferromagnets, η can be as large as 0.9.[9] Similarly, Eq. (7) defines P as the fractional polarization of current in the channel, which will depend on the 2DEG heterostructure. It is likely to have the largest values for narrow gap materials, with $P\approx 10\%$.[4] The observation of a sizable effect, with magnitude of order $\Delta R \sim 0.1 R_{\mathrm{av}}$ for quasi-one-dimensional structures, is expected, but would require Ohmic contact at the 2DEG-F interface to eliminate rectification caused by a Schottky contact.

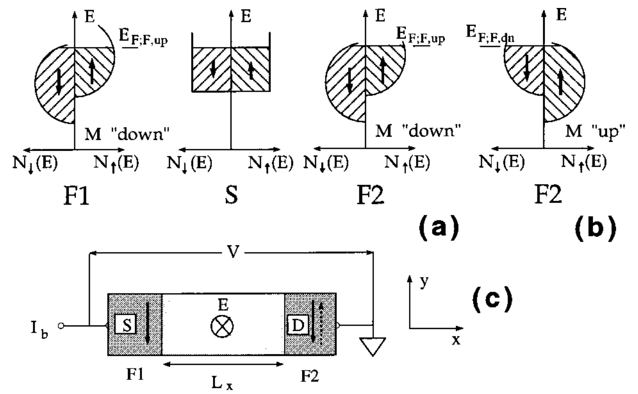

FIG. 4. Density of states diagrams for transport in a $F1$-2DEG-$F2$ structure. The magnetization of $F2$ is (a) down, aligned parallel to that of $F1$, or (b) up, aligned antiparallel to that of $F1$. (c) Top view of the device structure with ferromagnetic source $F1$ and drain $F2$. The magnetization of $F1$ is assumed to remain fixed along $-\hat{y}$.

We next apply this formalism to calculate the conductance of a ferromagnet-semiconducting–2 DEG-ferromagnet (F-2DEG-F) system, for the case of a semiconducting 2DEG with negligible spin-orbit coupling and therefore zero spin subband splitting. The structure depicted in Fig. 4(c) is similar to that introduced in the seminal work by Datta and Das,[10] but we consider two different magnetization orientations along $\hat{y}$. A ferromagnetic source $F1$ with magnetization fixed in the down orientation [along $-\hat{y}$ in Fig. 4(c)] delivers spin-polarized carriers to a high-mobility 2DEG channel. The device conductance will be larger when the magnetization of the ferromagnetic drain $F2$ is also down [parallel to that of $F1$, Fig. 4(a)] and smaller when the magnetization orientation is up [antiparallel, Fig. 4(b)]. In an ideal device, L_x is comparable to the carrier mean free path l so that transport is ballistic, or quasiballistic, and the channel is sufficiently narrow that trajectories with momentum components along $\hat{y}$ are suppressed. However, as discussed in Ref. 10, spin-dependent transport may not be diminished in multimode devices if the subbands are sufficiently far apart. In this case, elevated temperatures and relatively large bias could be used.

By defining g as an interfacial conductance,[7] where ‘‘interface’’ is defined to be a region with thickness equal to a mean free path on either side of the interface itself, the device conductance $G=I_b/V$ can be calculated as a two-step process characterized by the series sum of the interfacial conductance from $F1$ to S and from S to $F2$. The vector conductance from $F1$ to S is

$$G_{F1\to S}=g_{\min}|\uparrow\rangle+g_{\mathrm{maj}}|\downarrow\rangle.$$

The conductance from S to $F2$ for parallel magnetization alignment is

$$G_{\mathrm{par};S\to F2}=g_{\min}|\uparrow\rangle+g_{\mathrm{maj}}|\downarrow\rangle.$$

The conductance from $F1$ to S to $F2$ is the series combination $G^{-1}_{F1\to F2}=G^{-1}_{F1\to S}+G^{-1}_{S\to F2}$,

$$\frac{1}{G_1}\equiv\frac{1}{G_{\mathrm{par}}}=\frac{2}{g_{\min}|\uparrow\rangle+g_{\mathrm{maj}}|\downarrow\rangle}.$$

In the case of antiparallel alignment, with the magnetization orientation of $F2$ reversed, the conductance from S to $F2$ is

$$G_{\mathrm{anti};S\to F2}=g_{\mathrm{maj}}|\uparrow\rangle+g_{\min}|\downarrow\rangle. \qquad (8)$$

The series combination of conductances is

$$\frac{1}{G_2}=\frac{1}{G_{\mathrm{anti}}}=\frac{1}{g_{\min}|\uparrow\rangle+g_{\mathrm{maj}}|\downarrow\rangle}+\frac{1}{g_{\mathrm{maj}|\uparrow\rangle}+g_{\min}|\downarrow\rangle}.$$

After straightforward algebra, the variation of conductance is found to be

$$(\Delta G/G_{\mathrm{av}})=(\Delta R/R_{\mathrm{av}})=2\,\eta^2. \qquad (9)$$

Here η is the fractional spin polarization of current crossing the F-2DEG interface (or the 2DEG-F interface) and may differ from the polarization of currents inside F.[7]

The calculation is not substantially changed if transport is diffusive rather than quasiballistic, i.e., $L_x \geqslant l$. In particular, an allowance for spin-flip scattering in S can be made. If the mean path length over which spin orientation becomes random is Λ_s, the calculation proceeds as above with the result

$$\Delta R/R_{\mathrm{av}}=2e^{-L_x/\Lambda_s}\eta^2. \qquad (10)$$

Extension of the formalism to the case where the 2DEG is a material with substantial spin-orbit coupling and significant spin splitting of the conduction band is straightforward. The polarization P' of the carriers in S is enhanced by spin injection from $F1$:

$$P'=\frac{g_{\min,S}(1+\eta)-g_{\mathrm{maj},S}(1-\eta)}{g_{\min,S}(1+\eta)+g_{\mathrm{maj},S}(1-\eta)}=\frac{(g_{\min,S}-g_{\mathrm{maj},S})+\eta(g_{\min,S}+g_{\mathrm{maj},S})}{(g_{\min,S}+g_{\mathrm{maj},S})+\eta(g_{\min,S}-g_{\mathrm{maj},S})}=\frac{P+\eta}{1+\eta P}. \qquad (11)$$

The relative change of conductance is given, as before in Eq. (5), by

$$(\Delta G/2G_{\mathrm{av}})=(\Delta R/2R_{\mathrm{av}})=\eta P'. \qquad (12)$$

Since η is the order of tens of percent, the enhancement of P may be substantial.

The transport pictures developed above can be used to address questions about the nature of spin-flip scattering in a quasi-one-dimensional semiconducting 2DEG. We compare the densities of states sketches of Figs. 2(b) and 2(c) and consider an electron moving in one dimension in a state $|k_x,\downarrow\rangle$ [Fig. 2(b)] that reverses its direction in an elastic scattering event to a state $|-k_x,\downarrow\rangle$ [Fig. 2(c)]. Formally, the transition rate Γ for a scattering event could be derived with a golden rule calculation $\Gamma\propto|M^2|N_i(E)N_f(E)$, where $|M^2|$ is a matrix element, $N_i(E)$ is an initial density of filled states, and $N_f(E)$ is a final density of available (empty) states. However, $N_f(E)$ is zero for some of the electrons in initial states $|k_x,\downarrow\rangle$ and the transition rate for electrons in these states to elastically scatter *without* flipping their spin is therefore zero. For example, a down-spin electron with energy $E_{C,0}-\mu_B H^* < E < E_{C,0}+\mu_B H^*$ has no available phase space for momentum $-\hbar k_x$ and a scattering event from $+k_x$ to $-k_x$ is either forbidden or must include a spin flip. Physically, spin-flip scattering is associated with the application of a magnetic torque over a finite time interval. The interesting case arises in a 2DEG that there may be no torque on the spin and no apparent mechanism for a spin flip, but the carrier spin may be required to flip by phase-space considerations. The alternative is equally interesting: Scattering is suppressed because no phase space is available for the spin.

By the arguments above, scattering events in which the spin state is conserved are suppressed for a significant fraction of the carriers, but scattering events accompanied by a spin flip are not suppressed. Thus spin randomization is expected to be rapid and the phenomenon of spin accumulation[11] should be inhibited in a 2DEG. Generalization from quasi-one-dimension to two dimensions does not promote spin accumulation since spin relaxation has been shown to be rapid in the latter case.[12]

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