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The inequality of charge and spin diffusion coefficients

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Since spin and charge are both carried by electrons (or holes) in a solid, it is natural to assume that charge and spin diffusion coefficients will be the same. Drift-diffusion models of spin transport typically assume so. Here, we show analytically that the two diffusion coefficients can be vastly different in quantum wires. Although we do not consider quantum wells or bulk systems, it is likely that the two coefficients will be different in those systems as well. Thus, it is important to distinguish between them in transport models, particularly those applied to quantum wire based devices. © *2008 American Institute of Physics.* [DOI: 10.1063/1.2951448]

In the drift-diffusion model of spin transport, it is customary to assume that the same diffusion coefficient "D" describes charge and spin diffusion. This assumption is commonplace in the literature (see, for example, Refs. 1–5). Reference 6 considers a two-dimensional system with different spin and charge diffusion coefficients but ultimately assumes that the bare spin diffusion coefficient is the same as the charge diffusion coefficient. Reference 7 also examines this issue, and based on an heuristic assumption that spin transport is analogous to bipolar charge transport, reaches the conclusion that the two diffusion coefficients are equal as long as the populations of up-spin and down-spin carriers are equal. In spin polarized transport, the two populations are unequal by definition. Therefore, it is imperative to examine if these two diffusion coefficients are still equal in spin polarized transport, and if not, then how unequal they can be. In this paper, we show that these two diffusion coefficients can be vastly different in quantum wires. Although we do not consider quantum wells and bulk systems, there is no reason to believe *a priori* that even in those systems, the two diffusion coefficients will be equal.

We first consider a narrow semiconductor quantum wire where only the lowest subband is occupied by carriers at all times. All higher subbands are unoccupied. We will assume that there are Rashba[8] and Dresselhaus[9] spin orbit interactions in the wire, but no external magnetic field to cause spin mixing.[10] In that case, we can ignore the Elliott–Yafet spin relaxation mechanism[11] since it will be very weak unless the carrier mobility is extremely poor. Spin relaxation via hyperfine interaction with nuclear spins, or via the Bir–Aronov–Pikus mechanism,[12] is also typically very weak in semiconductor quantum wires with only one kind of carriers (electrons or holes, but not both). Therefore, the only spin relaxation mechanism that is important is the D'yakonov–Perel' relaxation.[13]

In the single channeled quantum wire, we will prove two remarkable results for the D'yakonov-Perel' relaxation: (i)

spin will relax in time (i.e., the spin relaxation time τ_s will be finite), but it will not relax in space (i.e., the spin relaxation length L_s will be infinite), and (ii) if the drift-diffusion model is <u>valid</u> in this system (this model relates L_s and τ_s as $L_s = \sqrt{D_s \tau_s}$), then we must conclude that the spin diffusion coefficient D_s is infinite. However, since there is scattering in the system, the charge diffusion coefficient D_c must be finite. Therefore, the two diffusion coefficients are completely different. This is an extreme case, but even in less extreme cases (multichanneled quantum wires), these two coefficients can be very different. Later, we provide an analytical proof for the single channeled quantum wire case.

Consider an ensemble of electrons injected in a quantum wire at time $t=0$ from the end $x=0$ as shown in Fig. 1. Only the lowest subband is occupied in the wire at all times. There is an electric field E_x driving charge transport, and there is also a transverse electric field E_y breaking structural inversion symmetry, thereby causing a Rashba spin orbit interaction.[8] We will assume that the quantum wire axis is
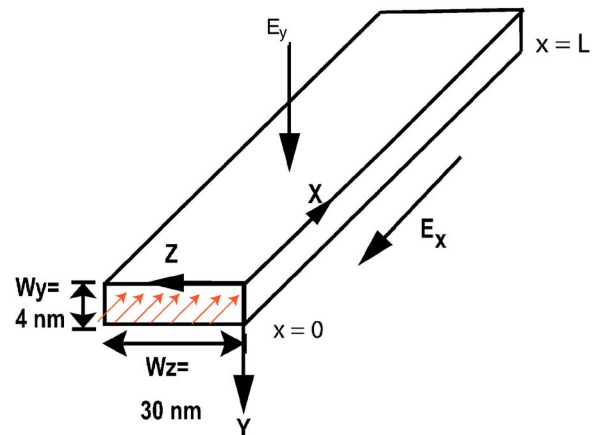

FIG. 1. (Color online) A quantum wire structure of rectangular cross section. A top gate (not drawn) applies a symmetry breaking electric field E_y to induce Rashba interaction. A battery (not drawn) applies an electric field $-E_x\hat{x}$, $E_x>0$, along the channel. Spin polarized electrons are injected at $x=0$. These electrons travel along $\hat{x}$ and may gradually lose their initial spin polarization. We investigate the spin depolarization of these electrons in time domain as well as in space domain.

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along the [100] crystallographic direction and that there is crystallographic inversion asymmetry along this direction giving rise to Dresselhaus spin-orbit interaction.[9] We choose this system because it is the simplest and includes the two major types of spin orbit interactions found in semiconductor nanostructures, namely the Rashba and the Dresselhaus interactions. Reference 5 has considered this system within the framework of the drift-diffusion model and shown that there is a single time constant describing spin relaxation. In contrast, spin relaxation in a two-dimensional system (quantum well) may be described by more than one time constant.[5]

For illustration purposes, we will assume hypothetically that the spin injection efficiency is 100%, so that at $x=0$, all electrons are spin polarized along some particular, though arbitrary, direction $\hat{\eta}_0$ in space. Their injection velocities are not necessarily the same (in fact, they will be drawn from the Fermi–Dirac distribution in the contact). We are interested in finding out how the net spin polarization of the ensemble $(|\langle \mathbf{S} \rangle|)$ decays in time or space due to the D'yakonov-Perel' process.

In the quantum wire, the electrons experience various momentum relaxing scattering events. Between successive scattering events, they undergo free flight and during this time, their spins precess about a velocity-dependent pseudo-magnetic field $\mathbf{B}_{so}(v_x)$ caused by Rashba and Dresselhaus spin-orbit interactions. This magnetic field can be shown to be spin independent.

The spin precession of every single electron occurs according to the well-known Larmor equation

$$\frac{d\mathbf{S}}{dt} = \mathbf{\Omega}(v_x) \times \mathbf{S}, \tag{1}$$

where $\mathbf{S}$ is the spin polarization vector of the electron and $\mathbf{\Omega}(v_x)$ is a vector whose magnitude is the angular frequency of spin precession. It is related to $\mathbf{B}_{so}(v_x)$ as $\mathbf{\Omega}(v_x) = (g\mu_B/\hbar)\mathbf{B}_{so}(v_x)$, where g is the Lande g factor in the material, and μ_B is the Bohr magneton. Equation (1) is actually the well-known equation for Larmor spin precession and can be derived rigorously from the Ehrenfest theorem of quantum mechanics.

The vector $\mathbf{\Omega}(v_x)$ has two contributions due to Dresselhaus and Rashba interactions

$$\mathbf{\Omega}(v_x) = \mathbf{\Omega}_{\mathrm{D}}(v_x) + \mathbf{\Omega}_{\mathrm{R}}(v_x), \tag{2}$$

where the first term is the Dresselhaus and the second term is the Rashba contribution. In our quantum wire, these two contributions are given by

$$\mathbf{\Omega}_{\mathrm{D}}(v_x) = \frac{2m^* a_{42}}{\hbar^2}\left[\left(\frac{\pi}{W_y}\right)^2 - \left(\frac{\pi}{W_z}\right)^2\right]v_x\hat{x} = \zeta_{D0}v_x\hat{x},$$

$$\mathbf{\Omega}_{\mathrm{R}}(v_x) = \frac{2m^* a_{46}}{\hbar^2}E_y v_x\hat{z} = \zeta_{R0}v_x\hat{z}, \tag{3}$$

where W_z and W_y are the transverse dimensions of the wire, a_{42} and a_{46} are material constants, $\hat{x}$ is the unit vector along the x direction and $\hat{z}$ is the unit vector along the z direction.

Note that the vector $\mathbf{\Omega}$ lies in the $x-z$ plane and subtends an angle θ with the $\pm x$ axis (quantum wire axis) given by

$$\theta = \arctan\left[\frac{\zeta_{R0}}{\zeta_{D0}}\right] = \arctan\left[\frac{a_{46}E_y}{a_{42}\left\{\left(\frac{\pi}{W_y}\right)^2 - \left(\frac{\pi}{W_z}\right)^2\right\}}\right]. \tag{4}$$

Note also that since θ is independent of v_x, the axis (but not the magnitude) of both $\mathbf{\Omega}$ and $\mathbf{B}_{so}$ is independent of electron velocity. Therefore, every electron, regardless of its velocity, precesses about the same axis, as long as only one subband is occupied. The direction of precession (clockwise or counterclockwise) depends on the sign of the velocity and therefore can change if the velocity changes sign, but the precession axis remains unchanged. However, the precession frequency depends on the velocity and is therefore different for different electrons as long as there is a spread in their velocities caused by varying injection conditions or random scattering. As a result, at any given instant of time $t=t_0$, the spins of different electrons will be pointing in different directions because they have precessed by different angles since the initial injection. Consequently, when we ensemble average over all electrons, the quantity $|\langle \mathbf{S} \rangle|$ decays in time, leading to spin relaxation in time.

To show this more clearly, we start from Eq. (1) describing the spin precession of any one arbitrary electron

$$\frac{d\mathbf{S}}{dt} = \hat{x}\frac{dS_x}{dt} + \hat{y}\frac{dS_y}{dt} + \hat{z}\frac{dS_z}{dt} = \mathbf{\Omega}(v_x) \times \mathbf{S}$$

$$= \det\begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ \Omega_D(v_x) & 0 & \Omega_R(v_x) \\ S_x & S_y & S_z \end{bmatrix}$$

$$= -\hat{x}[\Omega_R(v_x)S_y] - \hat{y}[\Omega_D(v_x)S_z - \Omega_R(v_x)S_x]$$

$$+ \hat{z}[\Omega_D(v_x)S_y], \tag{5}$$

where S_n is the spin component along the n axis of that arbitrary electron.

Equating each Cartesian component separately, we get

$$\frac{dS_x}{dt} = -\zeta_{R0}v_x S_y,$$

$$\frac{dS_y}{dt} = \zeta_{R0}v_x S_x - \zeta_{D0}v_x S_z, \tag{6}$$

$$\frac{dS_z}{dt} = \zeta_{D0}v_x S_y.$$

If every electron in an ensemble had the same v_x at every instant of time (no dispersion in velocity), then the last equation tells us that every electron would have the exact same spin components S_x, S_y, and S_z at any instant of time as long as they were all injected at time $t=0$ with the same spin polarization. In that case, we could replace S_n in the last equation by the ensemble averaged value $\langle S_n \rangle$ over the entire ensemble, so that

$$\frac{d|\langle S\rangle|^2}{dt} = \frac{d\langle S_x\rangle^2}{dt} + \frac{d\langle S_y\rangle^2}{dt} + \frac{d\langle S_z\rangle^2}{dt}$$

$$= 2\langle S_x\rangle\frac{d\langle S_x\rangle}{dt} + 2\langle S_y\rangle\frac{d\langle S_y\rangle}{dt} + 2\langle S_z\rangle\frac{d\langle S_z\rangle}{dt}$$

$$= -2\zeta_{R0}v_x\langle S_y\rangle\langle S_x\rangle + 2\zeta_{R0}v_x\langle S_x\rangle\langle S_y\rangle - 2\zeta_{D0}v_x\langle S_z\rangle\langle S_y\rangle$$

$$+ 2\zeta_{D0}v_x\langle S_y\rangle\langle S_z\rangle = 0. \tag{7}$$

In that case, $|\langle S\rangle|$ will not decay in time and there will be no D'yakonov-Perel' spin relaxation in time. However, if v_x is different for different electrons either due to different injection conditions, or because of scattering, then we cannot replace S_n with $\langle S_n\rangle$ in Eq. (6). As a result, Eq. (7) will not hold, so that $d|\langle S\rangle|/dt \neq 0$, and there will be a D'yakonov–Perel' relaxation in time. As a result, the spin relaxation time τ_s will be finite.

Next, let us consider D'yakonov–Perel' spin relaxation in space. From Eq. (6), we obtain (using the chain rule of differentiation)

$$\frac{dS_x}{dx}\frac{dx}{dt} = \frac{dS_x}{dx}v_x = -\zeta_{R0}v_xS_y,$$

$$\frac{dS_y}{dx}\frac{dx}{dt} = \frac{dS_y}{dx}v_x = \zeta_{R0}v_xS_x - \zeta_{D0}v_xS_z, \tag{8}$$

$$\frac{dS_z}{dx}\frac{dx}{dt} = \frac{dS_z}{dx}v_x = \zeta_{D0}v_xS_y.$$

The earlier equation shows that the spatial rates dS_n/dx are independent of velocity. This is a remarkable result with remarkable consequence. It tells us that even if different electrons have different velocities, as long as they were all injected with the same spin polarization at $x=0$, they will all have the exact same spin polarization at any arbitrary location $x=X_0$! That is, every electron's spin at $x=X_0$ is pointing in exactly the same direction. Therefore, we can always replace S_n in the earlier equation by its ensemble averaged value $\langle S_n\rangle$ whether or not there is scattering causing a spread in the electron velocity between different members of the ensemble. Consequently,

$$\frac{d|\langle S\rangle|^2}{dx} = \frac{d\langle S_x\rangle^2}{dx} + \frac{d\langle S_y\rangle^2}{dx} + \frac{d\langle S_z\rangle^2}{dx}$$

$$= 2\langle S_x\rangle\frac{d\langle S_x\rangle}{dx} + 2\langle S_y\rangle\frac{d\langle S_y\rangle}{dx} + 2\langle S_z\rangle\frac{d\langle S_z\rangle}{dx}$$

$$= -2\zeta_{R0}\langle S_y\rangle\langle S_x\rangle + 2\zeta_{R0}\langle S_x\rangle\langle S_y\rangle - 2\zeta_{D0}\langle S_z\rangle\langle S_y\rangle$$

$$+ 2\zeta_{D0}\langle S_y\rangle\langle S_z\rangle = 0. \tag{9}$$

Thus, there is never any D'yakonov–Perel relaxation in space as long as a single subband is occupied. Therefore, the spin relaxation length L_s is infinite. This is true whether or not there is scattering.

The earlier result has been confirmed independently with a many-particle Monte Carlo simulation of spin transport in a single channeled quantum wire.[14] Here, we have provided an analytical proof.

The foregoing analysis also shows that in a quantum wire with single subband occupancy and D'yakonov–Perel' as the only spin relaxation mechanism, there is a fundamental difference between spin relaxation in time and spin relaxation in space. Spin can relax in time while not relaxing in space. The physical origin of this difference is explained later.

From Eq. (3), we see that the precession frequency for any arbitrary electron is given by

$$\frac{d\phi(t)}{dt} = |\mathbf{\Omega}|(t) = \sqrt{\zeta_{D0}^2 + \zeta_{R0}^2}\,v_x(t) = \zeta_0 v_x(t), \tag{10}$$

where $\phi(t)$ is the angle by which the electron's spin precesses in time t.

If all electrons are injected with the same spin polarization at time $t=0$, then the angle by which any given electron's spin has precessed at time $t=t_0$ is

$$\phi(t_0) = \zeta_0\int_0^{t_0} v_x(t)dt = \zeta_0[x(t_0) - x(0)] = \zeta d_0, \tag{11}$$

where d_0 is the distance between the location of the electron at time t_0 and the point of injection. Obviously d_0 is history dependent because different electrons with different injection velocities and/or scattering histories would traverse different distances in time t_0. Consequently, if we denote the angle by which the nth electron's spin has precessed in time t_0 as $\phi_n(t_0)$, then $\phi_1(t_0) \neq \phi_2(t_0) \neq , \ldots, \phi_m(t_0)$. As a result, if we take a snapshot at t_0, we will find that the spin polarization vectors of different electrons are pointing in different directions. Therefore, ensemble averaged spin at t_0 is less than what it was at time $t=0$. Consequently, spin depolarizes with time leading to temporal D'yakonov–Perel' relaxation.

The spatial rate of precession, on the other hand, is obtained as

$$\frac{d\phi(t)}{dt} = \frac{d\phi(x)}{dx}\frac{dx}{dt} = \frac{d\phi(x)}{dx}v_x(t) = \zeta_0 v_x(t),$$

$$\frac{d\phi(x)}{dx} = \zeta_0. \tag{12}$$

Therefore, the angle by which any given electron's spin has precessed when it arrives at a location $x=X_0$ is

$$\phi(X_0) = \int_0^{X_0}\frac{d\phi(x)}{dx}dx = \zeta_0\int_0^{X_0}dx = \zeta_0 X_0. \tag{13}$$

This angle is obviously history independent since it depends only on the coordinate X_0 which is the same for all electrons at location X_0, regardless of how and when they arrived at that location. In fact, an electron may have visited the location X_0 earlier, gone past it, and then scattered back to X_0. Or it may have arrived at X_0 for the first time. It does not matter. The angle by which an electron's spin has precessed when it is located at X_0 is a constant independent of past history. Therefore, if all electrons were injected with their spins exactly parallel to each other at $x=0$, then every single electron at $x=X_0$ has its spin polarization vector pointing in the same direction as every other electron, and the ensemble averaged

magnitude of spin at $x=X_0$ is the same as that at $x=0$. Consequently, spin does not depolarize in space and there is no D'yakonov–Perel spin relaxation in space, unlike time.

Since spin relaxes in time but not in space, the relaxation time (τ_s) is finite whereas the relaxation length (L_s) is infinite. According to the drift-diffusion model, these two quantities are always related in steady state as[4]

$$L_s = \sqrt{D_s \tau_s}, \tag{14}$$

where D_s is the spin diffusion coefficient. Note that the quantities L_s, D_s, and τ_s are spin transport constants. As such, they are independent of both space and time.

Since L_s is infinite while τ_s is finite, the only way the earlier equation can be satisfied is if the steady-state spin diffusion coefficient D_s is infinite. But the steady state diffusion coefficient D_c associated with charge transport is certainly finite since we have frequent momentum relaxing scattering in our system. Therefore, there must be two very different diffusion coefficients D_s and D_c associated with spin and charge diffusion. This completes our analytical proof that $D_c \neq D_s$.

Two final questions remain regarding the generality of the earlier result. First, is it only valid for the extreme case of a quantum wire with single subband occupancy (single channeled transport) and second, is it only true for D'yakonov–Perel' relaxation? We cannot treat the case of multichanneled transport analytically, but we have examined that case numerically using Monte Carlo simulation in both space[15] and time.[16] We studied spin transport in a GaAs quantum wire of cross section 30 nm $\times$ 4 nm, where multiple subbands are occupied and D'yakonov–Perel' relaxation does occur in both time and space. At a lattice temperature of 77 K and a driving electric field $E_x = 2$ kV/cm, the value of L_s extracted from that study is ~ 10 μm while the value of $\tau_s \sim 1$ ns. This yields $D_s \sim 10^3$ cm^2/s [from Eq. (14)] which is still several orders of magnitude higher than the charge diffusion coefficient D_c in the same quantum wire calculated under the same conditions.[17,18] Thus $D_s \neq D_c$, even in multichanneled transport, and the two quantities can be vastly different.

Finally, what if we include other modes of spin relaxation, such as Elliott–Yafet?[11] If Elliott–Yafet is the domi-nant mode, then spin relaxation is intimately connected with momentum relaxation. In that case, the charge diffusion constant, determined by momentum relaxing scattering, and spin diffusion constant may not be as unequal. Nonetheless, there is no reason to assume *a priori* that the two diffusion coefficients are exactly equal even in this case. A rigorous Monte Carlo simulation (based on random walk model) recently carried out by us has shown that the two diffusion coefficients, in general, are vastly different. How different they are depends on the details of the scattering processes that relax momentum and spin.[19]

In conclusion, we have shown that in quantum wires the spin and charge diffusion coefficients can be vastly different. Although we have not examined quantum wells and bulk systems in this study, there is no reason to presuppose that the charge and spin diffusion coefficients will be equal in these systems either. Thus, it is important to distinguish between these two diffusion coefficients in solid state systems.

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