Theory of spin transport in an n-typed GaAs quantum well

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ABSTRACT

We have set up a set of many-body kinetic Bloch equations with spacial inhomogeneity. We reexamined the widely adopted quasi-independent electron model and showed the inadequacy of this model in studying the spin transport. We further pointed out a new decoherence effect based on interference effect along the diffusion in spin transport problem due to the so called inhomogeneous broadening effect in the Bloch equations. We have shown that this inhomogeneous broadening effect can cause the spin decoherence alone even without the scattering and that the resulting decoherence is more important than the dephasing effect due to the D'yakonov-Perel' (DP) term together with the scattering.

Keywords: Spintronics; Spin Diffusion; Dephasing; Many-body Effect; Semiconductors

Study of spintronics has attracted tremendous attention in recent years, both in theoretical and experimental circles [1], thanks to the discovery of the long-lived (sometimes > 100 ns) coherent electron spin states in n-typed semiconductors [2], [3]. Possible applications of spintronics include qubits for quantum computers, quantum memory devices, spin transistors, and spin valves etc. The last two applications involve transporting an electronic spin polarization from a place to another by means of an electrical or diffusive current. Therefore, it is of great importance to study the spin transport. Most theoretical works are based on quasi-independent electron model and focused on the diffusive transport regime [4]–[7], where equations for spin polarized currents can be set up and the longitudinal spin dephasing, generally referred to as spin diffusion length can be achieved. In these theories, the mechanism for the spin relaxation is assumed due to the spin-flipping scatterings. Without the scattering, the spin polarization will not decay in the nonmagnetic sample.

Of particular interest to the spin transport theory in semiconductors has been question as to whether the quasi-independent electron model can adequately account for the experimental results or whether many-body process is important. Flatte *et al.* have concluded that an independent electron approach is quite capable of explaining measurements of spin lifetimes in the diffusive regime [8]. In this paper, we reexamine this issue from a full many-body transport theory and show the inadequacy of the independent electron model in describing the spin transport. We also propose a mechanism that may cause strong longitudinal spin decoherence in addition to the spin dephasing due to the scatterings. The new mechanism results from the interference effect due to the wavevector dependence along the spacial gradients of the spin densities in the spin diffusion. This wavevector dependence can be considered as some sort of "inhomogeneous broadening", which can cause spin decay alone, even without scatterings.

Recently, we presented a many-body kinetic theory to describe the spin precession and dephasing in insulating sample as well as n-doped sample [9]–[11]. In this paper we extend this theory to the spacial inhomogeneous regime and get the many-body transport equations to investigate the spin diffusion in n-typed GaAs system. Here, we only focus on the spin transport inside the semiconductors and avoid the problem of spin injection at the boundary. Based on the two-spin-band model [10] in the conduction bands, we construct the semiconductor Bloch equations by using the nonequilibrium Green function method with gradient expansion as well as generalized Kadanoff-Baym Ansatz [12] as follows:

$$\begin{aligned}&\frac{\partial\rho(\mathbf{R},\mathbf{k},t)}{\partial t}-\frac{1}{2}\{\nabla_{\mathbf{R}}\bar{\varepsilon}(\mathbf{R},\mathbf{k},t),\nabla_{\mathbf{k}}\rho(\mathbf{R},\mathbf{k},t)\}\\&+\frac{1}{2}\{\nabla_{\mathbf{k}}\bar{\varepsilon}(\mathbf{R},\mathbf{k},t),\nabla_{\mathbf{R}}\rho(\mathbf{R},\mathbf{k},t)\}-\left.\frac{\partial\rho(\mathbf{R},\mathbf{k},t)}{\partial t}\right|_c\\&=\left.\frac{\partial\rho(\mathbf{R},\mathbf{k},t)}{\partial t}\right|_s.\end{aligned}\tag{1}$$

Here $\rho(\mathbf{R},\mathbf{k},t)$ represents a single particle density matrix. The diagonal elements describe the electron distribution functions $\rho_{\sigma\sigma}(\mathbf{R},\mathbf{k},t)=f_\sigma(\mathbf{R},\mathbf{k},t)$ of wave vector $\mathbf{k}$ and spin $\sigma(=\pm 1/2)$ at position $\mathbf{R}$ and time t. The off-diagonal elements $\rho_{\sigma-\sigma}(\mathbf{R},\mathbf{k},t)$ describe the inter-spin-band polarization components (coherences) for the spin coherence. The quasi-particle energy $\bar{\varepsilon}_{\sigma\sigma'}(\mathbf{R},\mathbf{k},t)$, in the presence of a moderate magnetic field $\mathbf{B}$ and with the DP mechanism [13] included, can be written as

$$\bar{\varepsilon}_{\sigma\sigma'}(\mathbf{R},\mathbf{k},t) \;=\; \varepsilon_k\delta_{\sigma\sigma'}+\left[g\mu_B\mathbf{B}+\mathbf{h}(\mathbf{k})\right]\cdot\frac{\sigma_{\sigma\sigma'}}{2}$$

$$- e\psi(\mathbf{R},t) + \Sigma_{\sigma\sigma'}(\mathbf{R},\mathbf{k},t) \ . \quad (2)$$

Here $\varepsilon_k = k^2/2m^*$ is the energy spectrum with m^* denoting electron effective mass, σ are the Pauli matrices and $\mathbf{h}(\mathbf{k})$ originate from the DP mechanism which contains both the Dresselhaus [14] and the Rashba terms [15]. In this paper, we only consider the first one. For [001] quantum well, it can be written as [16] $h_x(\mathbf{k}) = \gamma k_x(k_y^2 - \kappa_z^2)$, $h_y(\mathbf{k}) = \gamma k_y(\kappa_z^2 - k_x^2)$, with κ_z^2 denoting the average of the operator $-(\partial/\partial z)^2$ over the electronic state of the lowest subband. $\gamma = 4m^*\eta/(3m_{cv}\sqrt{2m^{*3}E_g}\sqrt{1-\eta/3})$ and $\eta = \Delta/(E_g+\Delta)$. Here E_g denotes the band gap, Δ represents the spin-orbit splitting of the valence band, and m_{cv} is a constant close in magnitude to free electron mass m_0 [17]. The electric potential $\psi(\mathbf{R},t)$ satisfies Poisson equation

$$\nabla^2_{\mathbf{R}}\psi(\mathbf{R},t) = -e\big[n(\mathbf{R},t) - n_0(\mathbf{R})\big]/\epsilon \ , \quad (3)$$

where $n(\mathbf{R},t) = \sum_{\sigma\mathbf{k}} f_\sigma(\mathbf{R},\mathbf{k},t)$ is the electron density at position $\mathbf{R}$ and time t, and $n_0(\mathbf{R})$ is the background positive electric charge density. $\Sigma_{\sigma\sigma'}(\mathbf{R},\mathbf{k},t) = -\sum_{\mathbf{q}} V_{\mathbf{q}}\rho_{\sigma\sigma'}(\mathbf{R},\mathbf{k}-\mathbf{q},t)$ is the Hartree-Fock self-energy, with $V_{\mathbf{q}}$ denoting the Coulomb matrix element. In 2D case, $V_{\mathbf{q}}$ is given by $V_{\mathbf{q}} = \sum_{q_z} \frac{4\pi e^2}{\epsilon_0(\mathbf{q}^2+q_z^2+\kappa^2)}|I(iq_z)|^2$, in which $\kappa = 2e^2m^*/\epsilon_0\sum_\sigma f_\sigma(K=0)$ is the inverse screening length. ε_0 represents the static dielectric constant. The form factor $|I(iq_z)|^2 = \pi^2\sin^2 y/[y^2(y^2-\pi^2)^2]$ with $y = q_z a/2$. It is noted that when one takes only the diagonal elements $\rho_{\sigma\sigma}$ of Eq. (1) and neglects all off-diagonal ones $\rho_{\sigma-\sigma}$, the first three terms on the left hand side of the equation correspond to the drift terms in the classical Boltzmann equation, modified with the DP terms and self energy from Coulomb Hartree term. $\frac{\partial\rho(\mathbf{R},\mathbf{k},t)}{\partial t}\Big|_c$ and $\frac{\partial\rho(\mathbf{R},\mathbf{k},t)}{\partial t}\Big|_s$ in Eq. (1)represent the coherent part and the scattering part of the Bloch equation and are given in detail in Ref. [11].

The Bloch equations (1) can be reduced to the equations in the independent electron approach as follows. By discarding the spin coherence $\rho_{\sigma-\sigma}(\mathbf{R},\mathbf{k},t)$ as well as the DP terms, and carrying out the summation over $\mathbf{k}$, one gets the equation of continuity for electrons of spin σ,

$$\frac{\partial n_\sigma(\mathbf{R},t)}{\partial t} - \frac{1}{e}\nabla_{\mathbf{R}}\cdot\mathbf{J}_\sigma(\mathbf{R},t) = -\frac{n_\sigma(\mathbf{R},t) - n_0(\mathbf{R},t)}{\tau_s} \ , \quad (4)$$

in which $-e$ is the electron charge and $n_0(\mathbf{R},t)$ $\{= [n_\sigma(\mathbf{R},t)+n_{-\sigma}(\mathbf{R},t)]/2\}$ is the total electron number at $\mathbf{R}$. It is noted that in writing out the above equation, we have adopted relaxation time approximation to describe the longitudinal spin dephasing due to the DP term and the scattering. In the equation $\mathbf{J}_\sigma(\mathbf{R},t) = \sum_{\mathbf{k}}(-e)\mathbf{v}_{\sigma\mathbf{k}}f_\sigma(\mathbf{R},\mathbf{k},t)$ is the electric current of spin σ. The spin dependent velocity is $\mathbf{v}_{\sigma\mathbf{k}} = \nabla_{\mathbf{k}}\bar{\varepsilon}_{\sigma\sigma}(\mathbf{R},\mathbf{k},t)$ where $\bar{\varepsilon}_{\sigma\sigma}(\mathbf{R},\mathbf{k},t)$ is given by Eq. (2) but without the DP term $\mathbf{h}(\mathbf{k})$. In the steady state, $\mathbf{J}_\sigma(\mathbf{R},t)$ can be written out by multiplying $\mathbf{v}_{\sigma\mathbf{k}}$ to the above mentioned simplified Bloch equations Eq. (1) (*i.e.*, without the DP terms and the off-diagonal elements $\rho_{\sigma-\sigma}$ and with the relaxation time approximation), and then carrying out the summation over $\mathbf{k}$:

$$\mathbf{J}_\sigma(\mathbf{R},t) = n_\sigma(\mathbf{R},t)e\mu\mathbf{E}(\mathbf{R},t) + eD\nabla_{\mathbf{R}}n_\sigma(\mathbf{R},t), \quad (5)$$

where μ and D represent the electron mobility and diffusion constant respectively. Equations (4) and (5) are the diffusion equations in the independent electron approach [4]–[7]. One can see from the derivation of above diffusion equations that, by summing over $\mathbf{k}$, the $\mathbf{k}$ dependence of the coefficients of $\nabla_{\mathbf{R}}\rho(\mathbf{R},\mathbf{k},t)$ in the Bloch equation (1) is removed. This will not cause any problem when there is no spin precession in the diffusion. However, when the electron spin precesses along the diffusion in the presence of a magnetic field or an effective one (*i.e.* the DP term), this kind of $\mathbf{k}$ dependence may cause additional decoherence along the spin diffusion.

To reveal this effect , we apply the above kinetic equation to study the stationary state in the plane of n-doped GaAs quantum wall (QW), with its growth direction along the z-axis. The width of the QW is assumed to be small enough so that only the lowest subband is important. We assume one side of the sample ($x=0$) is connected with an Ohmic contact which gives constant spin polarized injection. In this study, we assume the electric field $E=0$. The diffusion is along the x direction. The electron distribution functions at the interface are assumed to be Fermi distributions

$$f_\sigma(0,\mathbf{k},t) \equiv f^0_\sigma(\mathbf{k}) = \{\exp[(\varepsilon_k - \mu_\sigma)/T] + 1\}^{-1} \ , \quad (6)$$

with T, the temperature and μ_σ, the electron chemical potential of spin σ. The spin coherence at the interface is assumed to be zero

$$\rho_{\sigma-\sigma}(0,\mathbf{k},t) \equiv 0 \ . \quad (7)$$

We first consider a much simplified case by neglecting the DP terms $\mathbf{h}(\mathbf{k})$, the self energies as well as the scattering terms in the Bloch equations (1). The simplified equations are therefore as follows

$$\frac{k_x}{m^*}\partial_x f_\sigma(x,\mathbf{k}) - g\mu_B B\,\mathrm{Im}\big[\rho_{-\sigma,\sigma}(x,\mathbf{k})\big] = 0, \quad (8)$$
$$\frac{k_x}{m^*}\partial_x\rho_{\sigma-\sigma}(x,\mathbf{k}) - i\frac{g\mu_B B}{2}\Delta f_\sigma(x,\mathbf{k}) = 0. \quad (9)$$

Here we take the magnetic field $\mathbf{B}$ along the x-axis. $\Delta f_\sigma(x,\mathbf{k}) = f_\sigma(x,\mathbf{k}) - f_{-\sigma}(x,\mathbf{k})$. The solution for this simplified equations with the boundary conditions (6) and (7) can be written out directly

$$\Delta f_\sigma(x,\mathbf{k}) = \Delta f^0(\mathbf{k})\cos\frac{g\mu_B Bm^*x}{k_x} \ , \quad (10)$$
$$\rho_{\sigma-\sigma}(x,\mathbf{k}) = \frac{i}{2}\Delta f^0(\mathbf{k})\sin\frac{g\mu_B Bm^*x}{k_x} \ . \quad (11)$$

Equations (10) and (11) clearly show the effect of the k-dependence to the spin precession along the diffusion direction. For each fixed k_x, the spin precesses along the diffusion direction with fixed period without any decay. Nevertheless, for different k_x the period is different. The total difference of the electron densities with different spin is the summation of all wavenumbers $\Delta N = \sum_{\mathbf{k}} \Delta f_\sigma(x, \mathbf{k})$. It is noted that the phase at the contact $x = 0$ for different k_x is all the same. However, the speed of the phase of spin precession is different for different k_x. Consequently, when x is large enough, spins with different phases may cancel each other. This can further be seen from Fig. 1 where the electron densities $N_\sigma = \sum_{\mathbf{k}} f_\sigma(x, \mathbf{k})$ for up and down spin are plotted as functions of position x. The boundary electron densities at $x = 0$ are $N_{1/2}(0) = 2.05 \times 10^{11}$ cm^{-2} and $N_{-1/2}(0) = 1.95 \times 10^{11}$ cm^{-2}. $B = 1$ T and $T = 200$ K. In order to show the transverse spin dephasing, we plot in the same figure incoherently summed spin coherence $\rho(t) = \sum_{\mathbf{k}} |\rho_{\frac{1}{2}-\frac{1}{2}}(x, \mathbf{k})|$. It is understood that both true dissipation and the interference among the $\mathbf{k}$ states may contribute to the decay. The incoherent summation is therefore used to isolate the irreversible decay from the decay caused by interference [10]. From the figure, one can see clearly the longitudinal decoherence caused by the interference effect. It is also noted from the figure that ρ does not decay with the distance. This is consistent with the fact that there is no scatterings in Eqs. (10) and (11) and the decay comes from the interference effect.

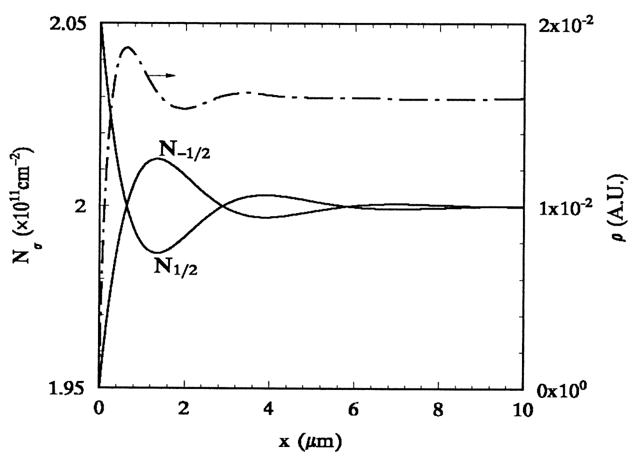

Figure 1: Electron densities of up spin and down spin (solid curves) and incoherently summed spin coherence ρ (dashed curve) versus the diffusion length x. $B = 1$ T. Note the scale of the spin coherence is on the right side of the figure.

Facilitated with above understanding, we turn to the spin diffusion problem with the DP terms, self energies and scatterings included. $\mathbf{B} = \mathbf{E} = 0$. Specifically, in the evolution equation of $\rho_{\sigma\sigma'}(\mathbf{R}, \mathbf{k}, t)$, the coefficients of $\partial_x \rho_{\sigma\sigma'}$, $\partial_x \rho_{\sigma-\sigma'}$ and $\partial_x \rho_{-\sigma\sigma'}$ are $\frac{k_x}{m^*} + \frac{1}{2}\partial_{k_x}[\Sigma_{\sigma\sigma}(\mathbf{R}, \mathbf{k}, t) + \Sigma_{\sigma'\sigma'}(\mathbf{R}, \mathbf{k}, t)]$, $\frac{1}{2}\partial_{k_x}[h_x(\mathbf{k}) + i\sigma h_y(\mathbf{k}) + \Sigma_{\sigma-\sigma}(\mathbf{R}, \mathbf{k}, t)]$, and $\frac{1}{2}\partial_{k_x}[h_x(\mathbf{k}) - i\sigma' h_y(\mathbf{k}) + \Sigma_{-\sigma'\sigma'}(\mathbf{R}, \mathbf{k}, t)]$ respectively. They are all k-dependent. The kinetic equations (1) and the Poisson equation (3), together with the boundary conditions (6) and (7) can be solved numerically in the iterative manner to achieve the stationary solution. The numerical results for a typical QW with width $a = 7.5$ nm, boundary spin polarization $N_{1/2}(0) = 2.05 \times 10^{11}$ cm^{-2} and $N_{-1/2}(0) = 1.95 \times 10^{11}$ cm^{-2} at temperature $T = 200$K is plotted in Fig. 2. In this computation, we only take the scattering due to LO-phonon into account. It is seen from the figure that the surplus of the spin up electrons decreases rapidly along the diffusion, similar to the simplified model shown above.

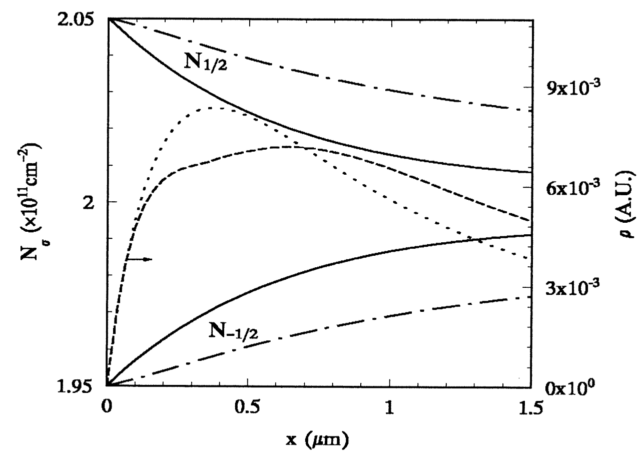

Figure 2: Electron densities of up spin and down spin and incoherently summed spin coherence versus the diffusion length x. Solid curves and dashed curve: N_σ and ρ from the full Bloch equations; Dash-dotted curves and dotted curve: N_σ and ρ from the equations without the interference effect. Note the scale of the spin coherence is on the right side of the figure.

The fast decay above is understood mainly from the decoherence from the interference effect due to the inhomogeneous broadenings. Other dephasing effects such as those caused by the DP terms in the coherent part of the Bloch equation as well as spin conserving LO phonon scattering also contribute to the decay. Besides, we pointed out that the inhomogeneous broadening effect combined with spin-conserving scattering can also cause spin dephasing [10]. Therefore, above mentioned inhomogeneous broadening may also cause spin dephasing in the presence of LO phonon scattering. To compare the decoherence due to interference and the dephasing due to the DP term together with the scatterings, we remove the interference effect in the transport equations by replacing k in the coefficients of $\partial_x \rho_{\sigma\sigma'}$, $\partial_x \rho_{\sigma-\sigma'}$ and $\partial_x \rho_{-\sigma\sigma'}$ with $k = k_F$. Here k_F represents the Fermi wavevector. Therefore, if there is any decay of spin polarization along the diffusion, it comes from the spin dephasing. The numerical result is plotted in Fig. 2. It is shown clearly that the decay of spin polarization due to the dephasing effect alone (dash-dotted curves) is much slower than that due to the decoherence (interference) effect. In the figure we also plot the corresponding incoherently summed spin coherences ρ. One can see from the figure that both coherences ρ decay slowly and their decay rates are comparable when $x > 1\ \mu$m. This further justifies what mentioned above that the fast decay of the spin polarization is mainly due to the interference effect.

We further study the spin diffusion/transport from the full many-body theory with the DP terms (The spin dephasing mechanism for n-typed GaAs QW at high temperature is the DP mechanism.) and the scattering included. By numerically solving the kinetic Bloch equations, together with the Poisson equation, we are able to investigate the spin diffusion in the steady state under the constant spin injection. We have shown the spin diffusion in the absence/presence of an applied electric field along the diffusion direction as well as with/without impurities. By applying an electric field along the diffusion direction, one gets much longer spin diffusion length as the electrons are driven by the electric field and get a net drift velocity. Also in the presence of the electric field, the spin diffusion length is reduced if one introduces impurities into the sample. However, when there is no applied electric field, the spin diffusion length is *enlarged* by adding impurities into the sample. This is contrary to what is predicted by the QIEM. The reason of this qualitative difference is also discussed. We also study the effects of the magnetic field in the Voigt configuration and the applied electric fields along the QW growth direction to the spin diffusion. In the present of the magnetic field, the spin polarization exhibits oscillation along the direction of diffusion and the decay due to the interference is much more effective than that of the dephasing and therefore the spin diffusion length is greatly reduced. We also investigate the spin diffusion at different temperatures. We find that as the temperature increases, the interference effect reduces as the electron distribution near $k_x = 0$, which is main contributor to the inhomogeneous broadening, becomes smaller. As a result, the spin diffusion length increases with the temperature. We show that the applied electric field along the growth direction makes the Rashba term more pronounced and hence both the decoherence and the dephasing get enlarged. Consequently the diffusion length is reduced. We have also demonstrated the time evolution of the diffusion of a spin package. The spin signals near the center of the package always decay with time due to the diffusion as well as the dephasing. Whereas the spin signals away from the center first increase then drop. For positions beyond the regime of the initial spin package, the spin polarization can be opposite to the initial one due to the spin flipping by the relatively large local effective magnetic field originated from the DP term together with the spin coherence $\rho_{\sigma-\sigma}$, with the later coming from both the diffusion and the spin precession. We also predict the spin oscillations with time at some positions. These features cannot be obtained from the QIEM. The detail of these results can be found in our recent paper [18].

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