Diffusion and transport of spin pulses in an $n$-type semiconductor quantum well

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We perform a theoretical investigation on the time evolution of spin pulses in an $n$-type GaAs (001) quantum well with and without external electric field at high temperatures by constructing and numerically solving the kinetic spin Bloch equations and the Poisson equation, with the electron-phonon, electron-impurity and electron-electron Coulomb scattering explicitly included. The effect of the Coulomb scattering, especially the effect of the Coulomb drag on the spin diffusion/transport is investigated and it is shown that the spin oscillations and spin polarization reverse along the direction of spin diffusion in the absence of the applied magnetic field, which were originally predicted in the absence of the Coulomb scattering by Weng and Wu [J. Appl. Phys. 93, 410 (2003)], can sustain the Coulomb scattering at high temperatures ($\sim 200$ K). The results obtained are consistent with a recent experiment in bulk GaAs but at a very low temperature (4 K) by Crooker and Smith [Phys. Rev. Lett. 94, 236601 (2005)].

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Semiconductor spintronics, which aims at replacing the charge degrees of freedom with the spin ones in electronic devices, has attracted substantial attention recently. A thorough understanding of transport of spin polarized electrons from one place to another by means of electrical or diffusive current is an important prerequisite for the realization of spintronic devices such as spin transistors and spin valves. Study of the time evolution of a spin pulse provides an ideal platform for this purpose and has been investigated by two of us based on kinetic spin Bloch equations in $n$-type GaAs quantum wells (QW’s). It is pointed out there that for Zinc-blende semiconductors, the spin coherence $\rho_{\sigma\sigma} = \langle c_{\mathbf{k}\sigma}^\dagger c_{-\mathbf{k}\sigma}\rangle$ play an important role in the spin diffusion/transport. It leads to some striking behaviors, such as at high temperatures ($200$ K) the spin polarization can be opposite to the initial one along the spin diffusion even in the absence of an external magnetic field. This spin oscillation along the direction of spin diffusion can not be obtained under the framework of quasi-independent electron model. This behavior has been reproduced later by Monte Carlo simulations by Pershin. Very recently Crooker and Smith have also shown experimentally this feature at very low temperature (4 K) in an $n$-type bulk GaAs with strains which provide a similar effect as the Dresselhaus term in GaAs QW’s in our investigation.

However, it is noted that in our previous spin transport studies as well as the Monte Carlo simulations, the electron-electron Coulomb scattering is not included. Studies of spin kinetics have shown that the Coulomb scattering plays a crucial role in spin dephasing and relaxation. Therefore, it should also strongly affect the spin coherence in spin diffusion and transport. In addition, the diffusion of a pure spin pulse is formed as the spin-up and -down electrons moving in opposite directions. This causes inevitably a Coulomb drag between electrons of opposite spins and therefore may strongly alter the spin diffusion/transport. All these considerations inspire us to investigate how the Coulomb scattering can affect the spin diffusion/transport. Moreover, inclusion of the Coulomb scattering further allows us to investigate the transport properties of high spin polarization. To our knowledge, a theoretical investigation of spin diffusion/transport with the Coulomb scattering explicitly included has never been performed in the literature.

We start our investigation in an $n$-type (001) GaAs QW along the $z$-axis of small well width $a$. The dominant spin dephasing mechanism here is the D’yakonov and Perel’ (DP) mechanism. By taking account of the DP term, the spin kinetic Bloch equations can be written as

$$
\frac{\partial \rho (\mathbf{R}, \mathbf{k}, t)}{\partial t} = \frac{1}{2} \{ \nabla_R \tau (\mathbf{R}, \mathbf{k}, t), \nabla_k \rho (\mathbf{R}, \mathbf{k}, t) \} + \frac{1}{2} \{ \nabla_k \tau (\mathbf{R}, \mathbf{k}, t), \nabla_R \rho (\mathbf{R}, \mathbf{k}, t) \} - \frac{\partial \rho (\mathbf{R}, \mathbf{k}, t)}{\partial t} \bigg|_{\varepsilon_c} \quad (1)
$$

with $\rho (\mathbf{R}, \mathbf{k}, t)$ standing for the 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 vec-
tor $k = (k_x, k_y)$ and spin $\sigma = (\pm 1/2)$ at position $\mathbf{R}$ and time $t$. The off-diagonal elements $\rho_{\sigma\sigma'}(\mathbf{R}, k, t)$ describe the inter-spin-band correlations (coherence) for the spin coherence. $\mathbf{R}(\mathbf{R}, k, t) = \varepsilon_{k} \delta_{\sigma\sigma'} + \mathbf{h}(k) \cdot \sigma_{\sigma\sigma'} / 2 - e\varepsilon(\mathbf{R}, t) + \Sigma_{\sigma\sigma'}(\mathbf{R}, k, t)$. Here $\varepsilon_{k} = k^2 / 2m^{*}$ is the energy spectrum with $m^{*}$ denoting the electron effective mass. $\sigma$ are the Pauli matrices. $\mathbf{h}(k)$ denotes the effective magnetic field from the DP term which contains contributions from both the Dresselhaus term and the Rashba term. For GaAs QW, the leading term is the Dresselhaus term, which can be written as $h_{x}(k) = \gamma k_{x}(k^2 / a^2 - \pi^2 / a^2)$ and $h_{y}(k) = \gamma k_{y}(\pi^2 / a^2 - k^2 / a^2)$ with $\gamma$ standing for the spin-orbit coupling strength. The electric potential $\psi(\mathbf{R}, t)$ satisfies the Poisson equation
\[
\nabla^{2} \psi(\mathbf{R}, t) = e[n(\mathbf{R}, t) - n_{0}(\mathbf{R})] / (\varepsilon\varepsilon_{0}), \tag{2}
\]
in which $n(\mathbf{R}, t) = \sum_{\sigma\mathbf{k}} f_{\mathbf{R}}(\mathbf{R}, \mathbf{k}, t)$ is the electron density at position $\mathbf{R}$ and time $t$ and $n_{0}(\mathbf{R})$ represents the positive background electric charge density. $\Sigma_{\sigma\sigma'}(\mathbf{R}, k, t) = - \sum_{\mathbf{q}} v_{q} \rho_{\sigma\sigma'}(\mathbf{R} - \mathbf{q}, t)$ is the Coulomb Hartree-Fock self-energy. $\partial\rho(\mathbf{R}, k, t) / \partial t_{\mathbf{q}}$ and $\partial\rho(\mathbf{R}, k, t) / \partial t_{\mathbf{q}}$ in Eq. (1) are the coherent and scattering terms respectively. Their expressions are given in detail in Ref. 13. For the scattering, we include the electron-electron Coulomb scattering, the electron-phonon scattering and the electron–non-magnetic-impurity scattering. For electron-phonon scattering, only the electron–longitudinal optical (LO) phonon scattering is considered as we concentrate on the high temperature regime (200 K) where the electron-acoustic phonon scattering is negligible. As we focus on narrow QW’s, the separation of the subband is large enough so that only the lowest subband is needed in our calculation.

We assume that at initial time $t = 0$ there is a pure spin pulse polarized along $z$-axis and centered at $x = 0$. The electrons are locally in Fermi distribution, i.e., $f_{\mathbf{R}}(x, \mathbf{k}, 0) = \exp\{[\varepsilon_{k} - \mu_{\sigma}(x)] / T_{e} + 1\}$, where $\mu_{\sigma}(x)$ stands for the chemical potential of electrons with spin $\sigma$ at position $x$ and is determined by the corresponding electron density: $N_{\sigma}(x, 0) = \sum_{\mathbf{k}} f_{\mathbf{R}}(x, \mathbf{k}, 0)$. The shape of the initial spin pulse is assumed to be Gaussian like
\[
\Delta N_{\sigma}(x, 0) = N_{1/2} - N_{-1/2} = \Delta N_{0} e^{-x^{2}/\delta x^{2}} \tag{3}
\]
with $\Delta N_{0}$ and the $\delta x$ representing the peak and the width of the spin pulse respectively. We further assume that there is no spin coherence at the initial time, $\rho(x, \mathbf{k}, 0) = 0$.

We numerically solve the kinetic Bloch equations (1) together with the Poisson equation (2) following the method developed by two of us in Ref. 4. The tricks of how to deal with the scattering, especially the Coulomb scattering, are laid out in detail in Ref. 13. It is due to these tricks which allow us to include the Coulomb scattering in the spin diffusion/transport computation. By solving the equations, the temporal evolution of the electron distribution functions $f_{\sigma}(\mathbf{R}, \mathbf{k}, t)$ and the spin coherence $\rho(\mathbf{R}, \mathbf{k}, t)$ at different positions $\mathbf{R}$ are obtained self-consistently. From these quantities, all the transport information, such as mobility, particle and spin diffusion lengths as well as spin dephasing and relaxation are obtained explicitly without any fitting parameters and approximations such as the relaxation time approximation widely used in the literature. Moreover, as we include the Coulomb scattering explicitly, we are able to calculate the situation with high spin polarization and the situation with high external electric field in spin transport, where the Coulomb scattering is crucial in the relaxation and thermalization of electrons. It is noted that both cases have been studied in a much simplified case, i.e., pure spin precessions without diffusion/transport (in the absence of the spacial degree of freedom).\textsuperscript{13,22}

We study the temporal evolution of the spin pulse at $T = 200$ K. The well width and the total electron density are chosen to be 7.5 nm and $4 \times 10^{11}$ cm$^{-2}$ respectively throughout our calculation. The material parameters of GaAs are listed in Ref. 13. The main results of our calculation are summarized in Figs. 1-4.

![FIG. 1: The absolute value of the spin imbalance $|\Delta N_{\sigma}|$ as well as the incoherently summed spin coherence $\rho$ v.s. the position $x$ and the time $t$ for the spin pulse with $\Delta N_{0} = 10^{11}$ cm$^{-2}$ and $\delta x = 0.1 \mu m$. Both the electron-LO phonon scattering and the electron-electron Coulomb scattering are included.](image-url)
\[ \rho(x, t) = \sum_k |\rho_k(x, t)| \] are plotted as functions of position \( x \) along the diffusion direction and the time \( t \) in the absence of the electric field. Both the electron-LO phonon scattering and the electron-electron Coulomb scattering are included in the calculation. From the figure, it can be seen that the spin signal around the center \( x < 0.06 \mu m \) decays very fast due to the diffusion as well as due to the spin dephasing. For the region of 0.06 \( \mu m < x < 0.9 \mu m \), due to the strong diffusion from the center, the spin signal first amplifies then decays resulting from the weakening of the diffusion as well as the dephasing. For the regions further away from the pulse center, i.e., 0.9 \( \mu m < x < 1.02 \mu m \) and 2.9 \( \mu m < x < 2.94 \mu m \), we find that the above counter effects result in the oscillations of the spin polarization with time, which were first discovered in the absence of the electron-electron scattering.\(^4\,5\) Furthermore it is noted that the striking feature that the spin polarization can be opposite to the initial one in the absence of a magnetic field is still retained in the presence of the Coulomb scattering. It is seen from the figure that the spin polarization first reverses at the time about 3 ps and the position around 1.02 \( \mu m \). And for the region 1.02 \( \mu m < x < 2.96 \mu m \), one observes a second peak with its polarization opposite to the initial one. And then after 16 ps, the spin polarization reverses back to the initial one in the region \( x > 2.96 \mu m \).

We next investigate the effect of pulse width on the spin diffusion by comparing two pure spin pulses with different pulse widths (\( \delta x = 0.1 \mu m \) and 1 \( \mu m \)) but the same total spin imbalance (\( \int \Delta N_\sigma(x, t = 0) dx = 1.8 \times 10^{10} \text{ cm}^{-1} \)). The spin polarizations at the center of the spin pulse is 25\% and 2.5\% respectively. The spin diffusions of the two spin pulses are plotted against \( t \) and \( x \) in counter plots in Fig 2. In the calculation we include the electron-electron and electron-LO phonon scattering. It is seen from the figure that the decay at the center of the narrow spin pulse is much faster than that of the wide one and that it is much faster for the narrow spin signal to diffuse out. Also the diffusion of the narrow spin pulse shows stronger spin oscillations along the direction of the diffusion. The reverse of the spin polarization occurs far away from the position of the initial spin pulse. Moreover, the spin polarization reverses back to the initial direction for the narrow spin pulse at positions farther away from the initial pulse. This peak can hardly be seen for the case of the wide pulse. These features are understood as following: The narrower spin pulse leads to larger gradients of the spin densities and hence a larger broadening in the \( k \)-space, and then leads to a faster diffusion. Moreover, a larger momentum \( k \) indicates a stronger effective magnetic field from the DP term, which results in a stronger spin oscillations.

In Fig. 3 we investigate the effect of the Coulomb drag\(^14\,15\) on the spin diffusion by plotting the absolute values of the spin imbalance as functions of \( x \) at \( t = 5, 15, 35 \) and 60 ps, with and without the Coulomb scattering. Contrary to the common impression that the Coulomb scattering conserves the total momentum and should not change the spin diffusion dramatically, one finds that when the Coulomb scattering is included, both the diffusion of the spin pulse and the decay of the spin polarization at the center of the pulse become much slower. Specifically at \( t = 15 \) ps, a third peak with the spin polarization along the initial one has appeared when only the electron-LO phonon scattering is included. This peak is absent when the Coulomb scattering is added. At \( t = 35 \) ps, the third peak also appears in the case with the Coulomb scattering, but with a smaller magnitude. Later at \( t = 60 \) ps, it is interesting to see that the magnitude of the third peak in the case with the coulomb scattering exceeds the one without, which indicates a longer spin diffusion length with the Coulomb scattering.

These features are understood as following: The interchange of the momentums between the oppositely moving spin-up and -down electrons due to the Coulomb scattering induces an effective friction, which is known as the Coulomb drag.\(^14\,15\) This drag weakens the diffusion of the spin pulse dramatically as shown in Fig. 3. In addition to the Coulomb drag, the Coulomb scattering also markedly affects the spin dephasing.\(^12\) It drives electrons
the spin signals do not diffuse symmetrically around the center any more, but transport against the direction of the electric field. Moreover, the features of the transport/diffusion of the spin polarization in the side against the external electric field become much richer than the side parallel to the field. All these results are consistent with what observed in the experiment.\textsuperscript{8} From the figure, one can further see the effect of the Coulomb scattering by comparing the curves with (solid curve) and without (dashed curve) the Coulomb scattering. It is found that similar to the field free case, the spin signal is more difficult to diffuse/transport out due to the Coulomb drag. Moreover as the Coulomb scattering impedes the spin dephasing, combined with the drag effect, it leads to the slower decay of the spin signal at the center. When the impurity with impurity density \( N_i = 0.5N_e \) is added to the system, it further slows the spin transport and the decay of the center of the spin signal as the impurity scattering impedes both the mobility and the spin dephasing.

Finally we investigate the transport of the spin pulse under an external electric field \( E = 500 \text{ V/cm} \) along the \(-x\)-direction. The hot-electron effect is not important under this field.\textsuperscript{13} Figure 4 shows the differences of the spin-up and -down electron densities versus the diffusion length \( x \) at \( t = 6, 12, 16 \) and \( 24 \) ps in different cases such as with/without the Coulomb and impurity scattering. From the figure, one finds that due to the electric field, to a more homogeneous states in the \( k \)-space, suppresses the anisotropy caused by the DP term, and reduces the spin dephasing.\textsuperscript{12} Both effects slow down the decay of the spin signal at the center of the pulse. Moreover, the spin diffusion length is determined by the above two counter effects: On one hand, the Coulomb drag shortens the spin diffusion length; On the other hand, the increase of the spin dephasing time by the Coulomb scattering leads to a longer spin diffusion length. And our results indicate that for the case of our study, the later effect is more important in the long run, which gives rise to a longer spin diffusion length.

We further explore the effect of impurities on spin diffusion in the presence of the Coulomb scattering. The result is also plotted in Fig. 3. From the figure one can see that as expected, the spin diffusion becomes much slower due to the decrease of the mobility. This effect, together with the well known fact that the spin dephasing time is increased by the electron-impurity scattering,\textsuperscript{17,23} make the decay of the spin polarization at the center of the pulse much slower.

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In conclusion, we have performed a study on the time evolution of spin pulses at a high temperature (200 K) through self-consistently solving the kinetic spin Bloch equations with the electron-LO phonon, electron-impurity and electron-electron Coulomb scattering explicitly included. The effect of the Coulomb scattering on the spin diffusion/transport is clearly demonstrated: The Coulomb scattering on one hand prolongs the spin dephasing time, which helps to sustain the spin signal. On the other hand, it causes the Coulomb drag which weakens the diffusion of the spin signal. In the case of our study, the Coulomb scattering leads to a slower spin diffusion speed but a longer spin diffusion length.

It is also shown that the Coulomb scattering does not kill the striking feature of the spin oscillation and the spin reverse along the spin diffusion direction, which were originally predicted where only the electron-LO phonon scattering is considered. In addition, when an external electric field is applied, the spin signal tends to transport against the direction of the electric field. All these phenomena have been observed in a recent experiment in bulk GaAs at very low temperature. Our study shows that one may observe these features at much higher temperature in QW’s with small well width. Experiments are suggested to verify these effects.

Moreover we also study the effects of the pulse width and the impurity on the spin diffusion. The results indicate that the wider the pulse width is, the weaker the spin diffusion and the fewer the times of the reverse of the spin polarization along the diffusion. Also the impurity affects the spin diffusion in two competing directions, i.e. impeding the spin diffusion and reducing the spin dephasing.

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