Electron Spin Dynamics in Impure Quantum Wells for Arbitrary Spin-Orbit Coupling

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Strong interest has arisen recently on low-dimensional systems with strong spin-orbit interaction due to their enhanced efficiency in some spintronic applications. Here, the time evolution of the electron spin polarization of a disordered two-dimensional electron gas is calculated exactly within the Boltzmann formalism for arbitrary couplings to a Rashba spin-orbit field. It is shown that the classical Dyakonov-Perel mechanism of spin relaxation gets modified for sufficiently strong Rashba fields, in which case new regimes of spin decay are identified. These results suggest that spin manipulation can be greatly improved in strong spin-orbit interaction materials.

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The physics of transport of electron spins in low-dimensional systems has become a popular theme of research due to the possible impact in future electronic applications. Key subjects of studies concern the problem of controlling the electron spin polarization through the tailoring of the spin-orbit (SO) interaction, and of clarifying to which extent the classical Dyakonov-Perel mechanism of spin relaxation gets deeply modified for sufficiently strong Rashba fields, in which case new regimes of spin decay are identified. These results suggest that spin polarization can be greatly improved in strong spin-orbit interaction materials.

In this letter, a generalized kinetic equation for $S$ is formulated for arbitrary strengths of the SO interaction and in the presence of spin-conserving coupling with impurities. For the case of a two-dimensional electron gas confined in the $x-y$ plane subjected to the Rashba interaction, the kinetic equation for the $z$-component of $S$ is solved explicitly for any value of $\Delta_{so}/\epsilon_F$. It is found that for a sufficiently strong Rashba interaction the DP relaxation mechanism gets modified, with the spin polarization displaying a slow (power law) decay with time. Furthermore, in the extreme $\Delta_{so}/\epsilon_F \gg 1$ limit, a fast exponential decay is obtained with $\tau_s \propto \frac{\pi^2 k_F^2}{\Delta_{so}} \propto \frac{1}{\epsilon_F}$, i.e., spin relaxation is enhanced by disorder. These findings suggest that tailoring of spin memory through $\Delta_{so}/\epsilon_F$ can be much more effective than previously thought.

Let us consider an electron gas whose non-interacting hamiltonian $H_0$ is:

$$H_0 = \sum_{k, s} \epsilon_k c_k^d c_k + \frac{\hbar}{2} \sum_{k, s, s'} \Omega_k \cdot \hat{\sigma}_{s's} c_k^d c_{ks'},$$

where $c_k^d$ ($c_k$) is the creation (annihilation) operator for an electron with momentum $k$ and spin index $s = \uparrow, \downarrow$, $\hat{\sigma}$ is the spin-vector operator with components $(\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z)$ given by the Pauli matrices, and $\Omega_k$ is a $k$ dependent SO pseudopotential vector whose explicit form is not essential for the moment. In the above expression, $\epsilon_k$ is the electron dispersion in the absence of SO coupling. Let us consider as momentum-relaxation mechanism a coupling $V_{kk'}$ to spin-conserving impurities located at random positions $R_i$. Additional interaction channels as those provided by phonons or electron-electron couplings can be treated as well by following the same steps described below. Assuming that $V_{kk'}$ is switched on at time $t = t_0$, the time evolution of $S(t)$ for $t > t_0$ can be obtained from the equation of motion of the density matrix $\rho(t)$:

$$\frac{d\rho_{kk'}(t)}{dt} = -i \hbar [\bar{E}_k \rho_{kk'}(t) - \rho_{kk'}(t) \bar{E}_k] - \frac{i}{\hbar} \Gamma_{kk'}(t),$$

where $\rho_{kk'}(t)$ is a $2 \times 2$ matrix with elements $\rho_{ks', k's}(t) = \ldots$
\[\langle ks|\rho(t)|k's\rangle, \hat{E}_k = \epsilon_k - \mu + \frac{i}{2}|\Omega_k| - \hat{\sigma}, \text{and} \]
\[
\hat{\Gamma}_{kk'}(t) = \sum_{pi} \left[ V_{kp} e^{i\hat{R}_k(p-k')\rho_{kp}(t)} - V_{pk} e^{i\hat{R}_p(p-k')\rho_{kp}(t)} \right]. \tag{3}
\]
Equation (2) can be formally integrated and, after the usual adiabatic (\(t_0 \to -\infty\)) and Markov approximations \([20,21], \hat{\rho}_{kk'}(t)\) can be expressed as:
\[
\hat{\rho}_{kk'}(t) \approx -i \int_0^\infty dt' e^{-i\hat{E}_k t'/\hbar} \hat{\Gamma}_{kk'}(t)e^{i\hat{E}_k t'/\hbar}, \tag{4}
\]
where the limit \(\delta \to 0^+\) must be taken after the integration. By using the anticommutation property of the Pauli matrices, \(\hat{\sigma}_j \hat{\sigma}_i + \hat{\sigma}_i \hat{\sigma}_j = \hat{1} \delta_{ij}\), the exponential operators in Eq. (4) can be put in a form more suitable for integration over \(t'\):
\[
e^{\pm i\hat{E}_k t'/\hbar} = \frac{1}{2} \sum_\alpha e^{\pm iE_{\alpha} t'/\hbar}(1 + \alpha \hat{\Omega}_k \cdot \hat{\sigma}), \tag{5}
\]
where \(\alpha = \pm 1, \hat{\Omega}_k = \Omega_k/|\Omega_k|, \text{and } E_{\alpha} = \epsilon_k \pm \frac{\hbar}{2} |\Omega_k|\) are the eigenvalues of \(H_0 [\text{Eq. (1)}]\). At this point, averaging over the impurity positions \(\mathbf{R}_i\) restores the translational invariance: \((\hat{\rho}_{kk'}(t))_{\text{imp}} = \delta_{k,k'}\hat{\rho}_{kk'}(t)\), and, finally, the equation of motion of electron spins for a given wave vector \(k\), \(\hat{S}_k = \frac{1}{2} \text{Tr}[\sigma \hat{\rho}_{kk'}]\), is obtained by integrating over \(t'\). By retaining only the scattering contributions (Boltzmann approximation) \([19]\), the final result is therefore:
\[
\frac{d\hat{S}_k}{dt} = \Omega_k \times \hat{S}_k - \frac{2\pi n}{\hbar} \sum_p V_{kp}^2 \frac{1}{4} \sum_{\alpha \beta} \left\{ (1 - \alpha \beta \Omega_k \cdot \hat{\Omega}_p)(\hat{S}_k - \hat{S}_p) + \alpha \beta \Omega_k [\hat{\Omega}_p \cdot (\hat{S}_k - \hat{S}_p)] + \alpha \beta \hat{\Omega}_p [\Omega_k \cdot (\hat{S}_k - \hat{S}_p)] \right\} + \hbar (\alpha \Omega_k + \beta \hat{\Omega}_p)(f_k - f_p)\delta(E_{\alpha k} - E_{p\beta}). \tag{6}
\]
By taking the vector product with \(\Omega_k\), the odd part of Eq. (6) can be rewritten as:
\[
\Omega_k \times \frac{d\hat{S}_k^o}{dt} = \Omega_k \times (\hat{S}_k \times \hat{S}_k^c) - \frac{2\pi n V^2}{\hbar} \sum_p \sum_{\alpha \beta} \left[ \Omega_k \times \hat{S}_p^c - \frac{\hbar}{\pi} \sum_{\alpha \beta} \left\{ \Omega_k \cdot \hat{S}_p^c \Omega_k \cdot (\hat{S}_k \times \hat{S}_p^c) \right\} + \alpha \beta \Omega_k \cdot (\hat{S}_k \times \hat{S}_p^c) \delta(E_{\alpha k} - E_{p\beta}), \tag{7}
\]
where the summation over momenta has cancelled all terms odd in \(p\) and the identity \((\Omega_k \cdot \hat{\Omega}_p)(\Omega_k \cdot \hat{S}_p^c) - (\hat{\Omega}_k \cdot \Omega_p)(\hat{\Omega}_k \cdot \hat{S}_p^c) = [\hat{\Omega}_p \times \hat{S}_p^c - \hat{\Omega}_p \cdot (\hat{\Omega}_k \times \hat{S}_p^c)](k/p)\) has been used. From Eq. (7), the equation of motion of \(\hat{S}_k^c\) is instead given by:
\[
\frac{d\hat{S}_k^c}{dt} = \frac{2\pi n V^2}{\hbar} \sum_p \sum_{\alpha \beta} \left[ \hat{S}_k^c - \hat{S}_p^c \right] + \hbar \alpha \Omega_k f_k^o - \hbar \beta \Omega_k f_p^o \delta(E_{\alpha k} - E_{p\beta}), \tag{8}
\]
where \(f_k^o = \frac{1}{2}(f_k - f_{-k})\) is the odd part of \(f_k\).
By using Eqs. (5) the term \(\hat{\Omega}_k \times \hat{S}_k^c/dt\) in Eq. (8) can be eliminated in favor of \(\hat{S}_k^c\) and \(\hat{S}_k\). Next, by using Eq. (4), also the terms containing \(\hat{S}_k^c\) can be eliminated and Eq. (7) reduces to an equation of motion of the component \(\hat{S}_k^c\) only, that is sufficient to find the time evolution of \(S = \sum_k \hat{S}_k^c\). Let us consider the \(z\)-component of \(S, S_z\), for which the presence of \(f_k^o\) in Eq. (6) has no effect since these terms have zero component in the \(z\)-direction.
In this way, Eq. (7) reduces to:
\[ \int_0^\infty \frac{d k k}{2\pi} \left[ \frac{d^2 S^e_{zk}}{dt^2} + \left( \frac{\gamma R k^2}{4\tau^2_p} + \frac{\chi_k}{2} \right) S^e_{zk} + \frac{\Gamma_k}{\tau_p} \frac{d S^e_{zk}}{dt} \right] = 0, \]  
(10)
where \( S^e_{zk} = \int_0^\infty d\phi S^e_{zk}/2\pi \), with \( \phi \) being the angle between the directions of \( k \) and the \( x \)-axis, \( \tau^{-1}_p = \frac{2\pi}{\hbar} V^2 N_0 \) is the momentum relaxation rate for a two-dimensional electron gas with zero SO splitting and density of states (DOS) \( N_0 = m/2\pi\hbar^2 \), and:
\[ \Gamma_k = \frac{1}{4N_0} \sum_{\alpha\beta} \int_0^\infty \frac{dp}{2\pi} \left( 1 + \alpha\beta \right) \delta(E_{\alpha\alpha} - E_{\beta\beta}), \]
(11)
\[ \chi_k = \frac{1}{N_0} \sum_{\alpha\beta} \int_0^\infty \frac{dp}{2\pi} (\Gamma_k - \Gamma_p) \delta(E_{\alpha\alpha} - E_{\beta\beta}). \]
(12)

A solution to Eq. (10) is obtained by equating to zero the expression within square brackets, which leads to a homogeneous differential equation of the second order for \( S^e_{zk}(t) \). In this way the functions \( \Gamma_k \) and \( \chi_k \) assume respectively the meaning of renormalization of the damping term and of shift of the (bare) precessional frequency \( \gamma_{Rk} \). It can be easily realized from Eqs. (10-12) that in the weak SO limit \( \varepsilon_F/\varepsilon_R \to \infty \), for which \( \Gamma_{zk} \to \frac{\gamma_{zk}^2}{2m} \), both the damping renormalization and the frequency shift are absent (\( \Gamma_k = 1 \) and \( \chi_k = 0 \)), indicating that these quantities stem from additional intra- and inter-band scattering channels opened when \( \varepsilon_F/\varepsilon_R \) is finite. Let us take a closer look at \( \Gamma_k \) and \( \chi_k \) by performing the integration over \( p \) in Eqs. (10-12):
\[ \Gamma_k = \left\{ \begin{array}{ll}
\frac{k R}{k R} & 0 \leq k \leq k R \\
1 + \frac{(2k R - k) k R}{(k R - k R)} & k R \leq k \leq 2k R \\
1 & 2k R \leq k
\end{array} \right. \]
(13)
\[ \chi_k = \left\{ \begin{array}{ll}
\frac{2k R^2 + 3k R k}{2k R - k R} & 0 \leq k \leq k R \\
\frac{(2k R - k R)^2}{k R - k R} & k R \leq k \leq 2k R \\
-\frac{(k R - k R)^2}{(k R - k R)(k R)} & 2k R \leq k \leq 3k R \\
-\frac{(3k R - k R)^2}{(k R - k R)(k R)} & 3k R \leq k \leq 4k R \\
0 & 4k R \leq k
\end{array} \right. \]
(14)

For \( k > 4k R \), \( \Gamma_k \) and \( \chi_k \) are the same as in the zero SO limit, while for lower momenta they acquire a strong \( k \) dependence (plotted in Fig. 1(c)) arising from the combined effect of the reduced dimensionality (\( D = 2 \)) and the SO interaction. In particular, the divergence of \( \Gamma_k \) at \( k = k R \) and those of \( \chi_k \) at \( k = k R \) and \( k = 3k R \) are due to scattering processes probing the SO induced van Hove singularity of the DOS of the lower sub-band which diverges as \( N_{\text{so}} - E \propto \sqrt{\varepsilon_F/E} \) [see Fig. 1(b)]. As it is shown below, such strong \( k \) dependence has important consequences on the spin polarization dynamics.

Let us now turn to evaluate the explicit time dependence of \( S_z \). From Eq. (10), a general solution for \( S^e_{zk}(t) \) is given by a linear combination of \( \exp\left(-\frac{\Gamma_z + \chi_{zk} t}{2\tau_p}\right) \), where \( \Sigma_k = \Gamma_k - \chi_k - (2\gamma R k)^2 \), whose coefficients are fixed by imposing some initial conditions. If at \( t = 0 \) electrons have been prepared with a non-equilibrium spin-state occupation but equilibrium distribution for each spin branch then, at the lowest order in the initial weak spin imbalance \( \delta \mu = (\mu_+ - \mu_-)/2 \), \( S^e_{zk}(0) \) is simply:
\[ S^e_{zk}(0) = -\frac{\delta \mu}{\gamma R k} \sum_a \alpha f_0(E_{a\alpha} - \mu), \]
(15)
where \( f_0(x) = (\exp(x/T) + 1)^{-1} \) is the Fermi distribution function, \( T \) is the temperature and \( \mu \geq 0 \) is the chemical potential. Furthermore, by imposing that \( \lim_{t \to \infty} |S_{zk}(t)| < \infty \) and by arbitrarily choosing \( dS_{zk}(0)/dt = 0 \) for \( \tau^{-1}_p = 0 \), at zero temperature \( (\mu = \varepsilon_F) \) \( S_z(t) \) is readily found to be:
\[ S_z(t) = -\frac{\delta \mu}{2\pi\gamma R} \int_{k < 0} dk \left\{ \theta(\Sigma_k - \Gamma^2_k) \left[ (1 - \frac{\Gamma_k}{\tau_p}) \exp\left( -\frac{\Gamma_k + \sqrt{\Sigma_k}}{2\tau_p} t \right) \right] + \theta(\Sigma_k - \Gamma^2_k) \left[ (1 - \frac{\Gamma_k}{\tau_p}) \exp\left( -\frac{\Gamma_k}{2\tau_p} t \right) \right] \right\}, \]
(16)
where \( \theta \) is the unit step function, \( k_{\geq} = k R(\sqrt{\varepsilon_F/\varepsilon_R} + 1) \) for \( \varepsilon_F/\varepsilon_R > 1 \) and \( k_{\geq} = k R(1 \pm \sqrt{\varepsilon_F/\varepsilon_R}) \) for \( \varepsilon_F/\varepsilon_R < 1 \) [see Fig. 1(a)]. For \( \varepsilon_F/\varepsilon_R \to \infty \), \( k_{\geq} \to k R \) and Eq. (16) reduces to the classical formula:
\[ S_z(t) = S_z(0) \exp\left( -\frac{t}{2\tau_p} \right) \exp\left( \frac{t}{2\tau_p} \right) \left( \frac{\varepsilon_F}{\varepsilon_R} \right)^{1/2} \]
(17)
where \( S_z(0) = -\hbar \delta \mu N_0 \) and \( \Omega R = \gamma R k F \) is the Rashba frequency which characterizes the (damped) spin precession behavior \( S_z(t) \approx S_z(0) \exp(-t/2\tau_p) \cos(\Omega R t) \) for \( 2\tau_p \Omega R \gg 1 \) and the DP relaxational decay \( S_z(t) \approx S_z(0) \exp(-t/2\tau_p \Omega R^2) \) for \( 2\tau_p \Omega R \ll 1 \).

For finite values of \( \varepsilon_F/\varepsilon_R \), Eq. (16) starts to deviate from the classical regime (17). Let us first consider \( \varepsilon_F/\varepsilon_R > 25 \). In this case, the integration over \( k \) in
The surprising result of Eq. (20) provides the rather interesting prediction that, for sufficiently strong SO interaction and momentum scattering, the spin polarization decays as a power law rather than exponentially. In this case therefore the memory of the initial spin polarization can be much longer lived than in the DP regime, as shown in Fig. 2(a). Another striking feature is that obtained in the extreme $\epsilon_F/\epsilon_R \ll 1$ limit in which the integration of Eq. (16) becomes restricted to a narrow region around $k = k_R$ where both $\Gamma_k$ and $\chi_k$ diverge as $1/|k - k_R|$, so that Eq. (16) becomes:

$$S_z(t) \propto \exp\left(-\frac{t}{8\tau_p}\right), \quad (21)$$

indicating that for extremely strong SO interaction, momentum scattering increases the spin polarization decay. The power decay of (20) and the fast relaxation regime of (21) are plotted in Fig. 2(b) from a numerical integration of Eq. (16) for $\tau_p = 3.3$ fs, $\epsilon_F = 5$ meV and $\epsilon_R$ ranging from 50 meV down to 1 meV.

To conclude, the kinetic equations describing the time evolution of the spin polarization have been formulated for arbitrary strength of the SO interaction. Explicit solutions for quantum wells with Rashba-like SO interactions predict the failure of the DP relaxation formula for sufficiently strong SO couplings. In particular, the memory of the initial spin state can be strongly enhanced or reduced depending on $\epsilon_F/\epsilon_R$, suggesting an alternative route for spin manipulation in spintronic applications.

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[1] G. Prinz, Phys. Today 48 (4), 58 (1995).
[2] I. Žutić, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004).
[3] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990).
[4] J. Schiemann, J. C. Egués, and D. Loss, Phys. Rev. Lett. 90, 146801 (2003).
[5] I. I. Rashba, Sov. Phys. Solid State 2, 1224 (1960).
[6] G. Dresselhaus, Phys. Rev. 100, 580 (1955).
[7] M. I. Dyakonov and V. I. Perel, Fiz. Tverd. Tela 13, 3581 (1971) [Sov. Phys. Solid State 13, 3023 (1971)].
[8] J. Sinova et al., Phys. Rev. Lett. 92, 126603 (2004).
[9] Y. S. Gui et al., Phys. Rev. B 70, 115328 (2004).
[10] E. Rothenberg, J. W. Chung, and S. D. Kevan, Phys. Rev. Lett. 82, 4066 (1999).
[11] Yu. M. Koroteev et al., Phys. Rev. Lett. 93 046403 (2004).
[12] E. Bauer et al., Phys. Rev. Lett. 92, 027003 (2004).
[13] K. V. Samokhin, E. S. Zijlstra, and S. K. Bose, Phys. Rev. B 69, 094514 (2004).
[14] M. W. Wu, J. Phys. Soc. Japan 70, 2195 (2001).
[15] M. M. Glazov and E. L. Ivchenko, J. Supercond. 16, 735 (2003).
[16] F. X. Bronold, A. Saxena, and D. L. Smith, Phys. Rev. B 70, 245210 (2004).
[17] E. L. Ivchenko, Yu. B. Lyanda-Geller, and G. E. Pikus, Zh. Eksp. Teor. Fiz. 98, 989 (1990) [Sov. Phys. JETP 71, 550 (1990)].
[18] A. A. Burkov, A. S. Núñez, and A. H. MacDonald, Phys. Rev. B 70, 155308 (2004).
[19] C. Lechner and U. Rössler, cond-mat/0412370 (2004).
[20] K. Blum, Density Matrix Theory and Applications (Plenum, New York, 1981).
[21] T. Kuhn and F. Rossi, Phys. Rev. B 46, 7496 (1992).
[22] The following results are equally valid for quantum wells with zero Rashba interaction but with a Dresselhaus coupling of the form \( \Omega_k = (\gamma_D k_x, -\gamma_D k_y, 0) \).