Electron spin relaxation in a semiconductor quantum well

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A fully microscopic theory of electron spin relaxation by the D'yakonov-Perel' type spin-orbit coupling is developed for a semiconductor quantum well in an ambient magnetic field applied perpendicular to the plane of the well. We derive Bloch equations for an electron spin in the well and determine explicit microscopic expressions for the spin relaxation times. The dependencies of the electron spin relaxation rates on magnetic field strength, temperature, and the lowest subband energy of the quantum well are analyzed.

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I. INTRODUCTION

Spin phenomenology in semiconductor structures has been at the focal point of research interest over the past few years in connection with proposals for spin-based quantum devices.¹ Spin implementation of quantum computation, optical switches, magnetic memory cells, etc., calls for a precise knowledge of spin dynamics and, in particular, the spin relaxation rates. The basic mechanisms responsible for spin relaxation are those of D'yakonov-Perel' (DP),^{2,3} Elliott-Yafet,⁴ and Bir-Aronov-Pikus.⁵ It was shown⁶ that for III-V and II-VI compounds, which are the most promising materials for device purposes, the DP mechanism dominates at moderate temperatures and low hole concentrations. The spin relaxation time due to the DP mechanism has generally been expressed in the semiphenomenological form^{2,3}

$$\frac{1}{\tau_s} = Q \frac{\alpha^2}{\hbar^2 \varepsilon_g} \tau_p T^3 \tag{1}$$

for bulk semiconductors, and

$$\frac{1}{\tau_s} = \frac{\alpha^2 \langle p_z^2 \rangle^2}{2\hbar^2 m^2 \varepsilon_g} \tau_p T \tag{2}$$

for quantum well structures, where α describes conduction band spin splitting due to lack of inversion symmetry ($\alpha = 0.07$ for GaAs), ε_g is the band gap, and *T* is the Kelvin temperature ($k_B = 1$). The numerical coefficient *Q* depends on the orbital scattering mechanism, and $\langle p_z^2 \rangle$ is the average square of momentum in the quantum well growth direction. It should be noted that these formulas involve the average momentum relaxation time τ_p as a phenomenological parameter.

In the present paper we develop a *fully microscopic* theory of spin dynamics and apply it to a quantum well structure in the presence of an external magnetic field, directed along the well growth direction, taking account of various scattering mechanisms. Our theory facilitates the microscopic determination of τ_p and its temperature and magnetic field dependencies in terms of the fundamental material parameters.

Our analysis involves the explicit recognition of the two stages in the relaxation process corresponding to the relaxation time hierarchies involved in (a) electron thermalization due to interaction with phonons, and (b) spin relaxation. In the first stage of solution (a) we determine the relaxation rates and fluctuation characteristics of electron orbital motion due to coupling to the phonon bath. Spin relaxation dynamics (the slowest process in the system) can be neglected in this stage.

The second stage (b) proceeds with analysis of the spin relaxation process due to spin-orbit interaction, wherein the orbital degrees of freedom are considered as an effective heat bath, having the characteristics determined in the first stage. A standard set of Bloch equations with two distinct relaxation times (longitudinal relaxation time T_1 , responsible for spin magnetic moment relaxation, and transverse relaxation time T_2 , responsible for decoherence) is derived in this second stage. In both stages of our analyses we employ the method proposed in Ref. 7 and developed in Refs. 8 and 9.

II. FORMULATION

The Hamiltonian of part (a) is given by

$$H = H_0 + U(\mathbf{r}_\perp, t) + H_{ph}, \qquad (3)$$

where the spin and its interactions are neglected in the first stage, and

$$H_0 = \frac{\hbar \,\omega_0}{2} + \frac{m V_x^2}{2} + \frac{m V_y^2}{2} \tag{4}$$

is the Hamiltonian of a two-dimensional electron in a quantum well with harmonic confinement in the *z* direction having a frequency ω_0 . We assume the temperature to be low enough so that only the lowest energy subband of the quantum well is occupied. In this case the motion of an electron can be described by means of two electron in-plane velocity components, which in the presence of a constant, uniform magnetic field directed along the *z* axis **B**=(0,0,*B*) are given by

$$V_{x} = \frac{1}{m} \left(p_{x} - \frac{e}{c} A_{x} \right), \quad V_{y} = \frac{1}{m} \left(p_{y} - \frac{e}{c} A_{y} \right),$$
$$[V_{x}, V_{y}]_{-} = -\frac{i\hbar\omega_{c}}{m}, \quad (5)$$

where $\mathbf{A} = (A_x, A_y, 0)$ is the vector potential, $B = (\partial/\partial x)A_y - (\partial/\partial y)A_x$, $\omega_c = |e|B/mc$ is the cyclotron frequency, and $[\ldots, \ldots]_-$ denotes a commutator. The phonon Hamiltonian has the form

$$H_{ph} = \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left(b_{\mathbf{k}}^{+} b_{\mathbf{k}} + \frac{1}{2} \right), \tag{6}$$

where $\hbar \omega_{\mathbf{k}}$ is the phonon energy and $b_{\mathbf{k}}^+$ and $b_{\mathbf{k}}$ are creation and annihilation operators, respectively. The term $U(\mathbf{r}_{\perp},t)$ in Eq. (3) describes the electron coupling to phonons and impurities.

The electron-phonon interaction is given by

$$U_{e-ph}(\mathbf{r}_{\perp},t) = -\sum_{\mathbf{k}} Q_{\mathbf{k}}(t) X_{\mathbf{k}}(t)$$
$$= -\frac{1}{L^{3/2}} \sum_{\mathbf{k}} Q_{\mathbf{k}}(t) f(k_z) e^{i\mathbf{k}_{\perp}\mathbf{r}_{\perp}}, \qquad (7)$$

where

$$Q_{\mathbf{k}}(t) = i\zeta [b_{\mathbf{k}}(t) - b_{-\mathbf{k}}^{+}(t)]$$
(8)

is the phonon heat bath variable (ζ is the strength of the electron-phonon coupling), and the electron variable conjugate to this operator is defined as

$$X_{\mathbf{k}}(t) = \frac{1}{L^{3/2}} f(k_z) e^{i\mathbf{k}_{\perp} \mathbf{r}_{\perp}(t)}.$$
(9)

Here L^3 is the volume of the crystal, $\mathbf{r}_{\perp} = (x, y)$, and $f(k_z) = \exp(-\hbar k_z^2/4m\omega_0)$ is the electron confinement form factor. The response function of uncoupled phonon heat bath variables, $\varphi_{\mathbf{k}}(t;t_1)$, and their correlation function, $M_{\mathbf{k}}(t;t_1)$, are given by

$$\varphi_{\mathbf{k}}(t;t_{1}) = \left\langle \frac{i}{\hbar} \left[Q_{\mathbf{k}}^{(0)}(t), Q_{-\mathbf{k}}^{(0)}(t_{1}) \right]_{-} \right\rangle \Theta(t-t_{1}) \quad (10)$$

and

$$M_{\mathbf{k}}(t;t_{1}) = \left\langle \frac{1}{2} [\mathcal{Q}_{\mathbf{k}}^{(0)}(t), \mathcal{Q}_{-\mathbf{k}}^{(0)}(t_{1})]_{+} \right\rangle,$$
(11)

where $Q_{\mathbf{k}}^{(0)}(t)$ are the *unperturbed* phonon variables, $\Theta(t - t_1)$ is the Heavyside unit step function, and $[\ldots, \ldots]_+$ denotes an anticommutator.

The electron-impurity interaction is described by

$$U_{e-i}(\mathbf{r}_{\perp}) = -\frac{1}{L^{3/2}} \sum_{\mathbf{k}} U_{\mathbf{k}} f(k_z) e^{i\mathbf{k}_{\perp}\mathbf{r}_{\perp}}, \qquad (12)$$

where $U_{\mathbf{k}}$ are the spatial Fourier components of the impurity potential with correlation function

$$\Phi_{\mathbf{k}} = \left\langle \frac{1}{2} \left[U_{\mathbf{k}}, U_{-\mathbf{k}} \right]_{+} \right\rangle. \tag{13}$$

In summary,

$$U(\mathbf{r},t) = U_{e-ph}(\mathbf{r}_{\perp},t) + U_{e-i}(\mathbf{r}_{\perp})$$
$$= -\sum_{\mathbf{k}} (Q_{\mathbf{k}}(t) + U_{\mathbf{k}})X_{\mathbf{k}}(t).$$
(14)

III. ORBITAL DYNAMICS

Employing the Hamiltonian of Eq. (3), we obtain Langevin-like operator equations of motion determining inplane electron dynamics, as given by (the derivation is presented in Appendix A)

$$\frac{d}{dt}V_{x}(t) + \omega_{c}V_{y}(t) + G_{x}[V_{x}(t);V_{y}(t)] = \xi_{x}(t),$$
$$\frac{d}{dt}V_{y}(t) - \omega_{c}V_{x}(t) + G_{y}[V_{x}(t);V_{y}(t)] = \xi_{y}(t), \quad (15)$$

with fluctuation sources $\xi_{x,y}(t)$ and collision terms $G_x[V_x(t);V_y(t)]$ given by Eqs. (A8) and (A9). It should be emphasized that the expressions for fluctuation sources [Eq. (A8)] are obtained from microscopic analysis, and it is possible to calculate their correlation functions of any order. In particular, the correlation function of the fluctuation sources (in the case of weak coupling or Gaussian statistics of the unperturbed phonon variables) is given by

$$K_{\alpha\beta}(t,t_{1}) = \left\langle \frac{1}{2} [\xi_{\alpha}(t),\xi_{\beta}(t_{1})]_{+} \right\rangle$$
$$= \frac{1}{m^{2}} \sum_{\mathbf{k}} k_{\alpha}k_{\beta}f^{2}(k_{z})$$
$$\times \left((M_{\mathbf{k}}(t,t_{1}) + \Phi_{\mathbf{k}}) \left\langle \frac{1}{2} [X_{\mathbf{k}}(t),X_{-\mathbf{k}}(t_{1})]_{+} \right\rangle \right.$$
$$\left. + R_{\mathbf{k}}(\tau) \left\langle \frac{1}{2} [X_{\mathbf{k}}(t),X_{-\mathbf{k}}(t_{1})]_{-} \right\rangle \right), \qquad (16)$$

where $R_{\mathbf{k}}(t-t_{1}) = \hbar [\varphi_{\mathbf{k}}(t-t_{1}) + \varphi_{\mathbf{k}}(t_{1}-t)]/2i$.

We can separate the electron velocity operator into its average and fluctuation parts,

$$V_{x,y}(t) = \langle V_{x,y}(t) \rangle + \widetilde{V}_{x,y}(t).$$
(17)

Due to relaxation processes only the fluctuating part is nonzero, $\langle V_{x,y}(t) \rangle = 0$, and the equations of motion for the fluctuating components take the forms

$$\frac{d}{dt}\widetilde{V}_{x}(t) + \omega_{c}\widetilde{V}_{y}(t) + G_{x}[V_{x}(t);V_{y}(t)] - \langle G_{x}[V_{x}(t);V_{y}(t)] \rangle = \xi_{x}(t),$$

$$\frac{d}{dt}\widetilde{V}_{y}(t) - \omega_{c}\widetilde{V}_{x}(t) + G_{y}[V_{x}(t);V_{y}(t)] - \langle G_{y}[V_{x}(t);V_{y}(t)] \rangle = \xi_{y}(t).$$
(18)

To further simplify Eqs. (18), we have to calculate the (anti)commutators involved in Eqs. (16), (A8), and (A9). This procedure is presented in Appendix B resulting in the following simplified equations:

$$\left(\frac{d}{dt} + \gamma_0\right) \widetilde{V}_x(t) + (\omega_c + \delta) \widetilde{V}_y(t) = \xi_x(t),$$
$$\left(\frac{d}{dt} + \gamma_0\right) \widetilde{V}_y(t) - (\omega_c - \delta) \widetilde{V}_x(t) = \xi_y(t), \qquad (19)$$

where the damping rate, $\gamma_0 = \gamma_x = \gamma_y$, and the frequency shift, $\delta = \delta_x = \delta_y$, are given by

$$\gamma_{x,y} = \frac{1}{mL^3} \sum_{\mathbf{k}} k_{x,y}^2 f^2(k_z) \\ \times \int_0^{+\infty} d\tau \tau \left\{ (M_{\mathbf{k}}(\tau) + \Phi_{\mathbf{k}}) \frac{2}{\hbar} \sin\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \\ + \varphi_{\mathbf{k}}(\tau) \cos\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right\} \exp\left\{-\frac{\tau^2}{2\tau_c^2(\mathbf{k}_\perp)}\right\}$$
(20)

and

$$\delta_{x,y} = \frac{1}{mL^3} \sum_{\mathbf{k}} k_x k_y f^2(k_z) \\ \times \int_0^{+\infty} d\tau \tau \left\{ (M_{\mathbf{k}}(\tau) + \Phi_{\mathbf{k}}) \frac{2}{\hbar} \sin\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \\ + \varphi_{\mathbf{k}}(\tau) \cos\left(\frac{\hbar k_\perp^2}{2m}\tau\right) \right\} \exp\left\{-\frac{\tau^2}{2\tau_c^2(\mathbf{k}_\perp)}\right\}.$$
(21)

Here, $\tau = t - t_1$ and $\tau_c^2(\mathbf{k}_{\perp})$ is given by Eq. (B11). It follows from Eq. (19) that the Fourier transforms of velocity correlation functions are given by

$$\left\langle \frac{1}{2} [V_{\alpha}(\omega); V_{\beta}]_{+} \right\rangle = \int d\tau e^{i\omega\tau} \left\langle \frac{1}{2} [V_{\alpha}(t+\tau), V_{\beta}(t)]_{+} \right\rangle,$$

$$\alpha, \beta = x, y, \qquad (22)$$

$$\left\langle \frac{1}{2} [V_x(\omega); V_x]_+ \right\rangle = \left\langle \frac{1}{2} [V_y(\omega); V_y]_+ \right\rangle$$
$$= \frac{K(\omega)}{2} \left(\frac{1}{(\omega - \omega_c)^2 + \gamma_0^2} + \frac{1}{(\omega + \omega_c)^2 + \gamma_0^2} \right), \quad (23)$$

$$\frac{1}{2} [V_x(\omega); V_y]_+ \rangle = -\left\langle \frac{1}{2} [V_y(\omega); V_x]_+ \right\rangle$$
$$= \frac{K(\omega)}{2i} \left(\frac{1}{(\omega - \omega_c)^2 + \gamma_0^2} - \frac{1}{(\omega + \omega_c)^2 + \gamma_0^2} \right), \quad (24)$$

where we neglected terms of the of order $\delta/\omega_c \ll 1$. The correlation function of the fluctuation forces is defined as $K(\omega) = K_{\alpha\alpha}(\omega)$, where

$$K_{\alpha\beta}(\omega) = \int dt \,\tau e^{i\omega\tau} K_{\alpha\beta}(t+\tau,t)$$

$$= \frac{1}{m^2} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} k_{\alpha} k_{\beta} f^2(k_z)$$

$$\times \int_0^{+\infty} d\tau \tau \bigg\{ (M_{\mathbf{k}}(\tau) + \Phi_{\mathbf{k}}) \sin\bigg(\frac{\hbar k_{\perp}^2}{2m} \tau\bigg)$$

$$- iR_{\mathbf{k}}(\tau) \cos\bigg(\frac{\hbar k_{\perp}^2}{2m} \tau\bigg) \bigg\} \exp\bigg\{ -\frac{\tau^2}{2\tau_c^2(\mathbf{k}_{\perp})} \bigg\}.$$

(25)

To carry out the τ - and **k**-integrations in Eqs. (20) and (25), we have to employ explicit expressions for the response and correlation functions for a particular scattering mechanism. In the present paper we consider polar optical phonons, deformational acoustic phonons and charged impurities as possible scattering mechanisms. Their corresponding response and correlation functions are listed below.

Optical phonons

$$\varphi_{\mathbf{k}}^{OP}(\tau) = \frac{4\pi\Omega_{0}e^{2}}{k^{2}\epsilon^{*}}\sin(\Omega_{0}\tau)\eta(\tau),$$
$$M_{\mathbf{k}}^{OP}(\tau) = \frac{\hbar}{2}\frac{4\pi\Omega_{0}e^{2}}{k^{2}\epsilon^{*}}\cos(\Omega_{0}\tau)\coth\left(\frac{\hbar\Omega_{0}}{2k_{B}T}\right), \quad (26)$$

where Ω_0 is the optical phonon frequency, $1/\epsilon^* = 1/\epsilon_{\infty} - 1/\epsilon_0$, (ϵ_{∞} and ϵ_0 are the hf and static permittivities of the crystal, respectively).

Deformational acoustic phonons

$$\varphi_{\mathbf{k}}^{AP}(\tau) = \frac{D^2 k}{\rho u} \sin(uk\tau) \,\eta(\tau),$$
$$M_{\mathbf{k}}^{AP}(\tau) = \frac{\hbar}{2} \frac{D^2 k}{\rho u} \cos(uk\tau) \coth\left(\frac{\hbar uk}{2k_B T}\right), \qquad (27)$$

where D is the deformation potential, ρ is the crystal density, and u is the sound velocity.

Static charged impurities have only a correlation function, given by

and

 \tilde{K}

$$\Phi_{\mathbf{k}} = \frac{2e^4 n_t^*}{\pi \epsilon_0^2 (k^2 + r_0^{-2})^2},$$
(28)

where r_0 is the screening radius, $n_t^* = \sum_{\alpha} n_{\alpha} Z_a^2$, n_{α} is the impurity concentration for species α , and Z_{α} is their charge number.

We neglect the cross correlations of scattering processes and, consequently, they are additive in both the damping rate and in the correlation function of the fluctuation sources:

$$\gamma_0 = \gamma_0^{OP} + \gamma_0^I + \gamma_0^{AP},$$

$$(\omega) = \tilde{K}^{OP}(\omega) + \tilde{K}^I(\omega) + \tilde{K}^{AP}(\omega).$$
(29)

Substituting the corresponding response and correlation functions in Eqs. (20) and (25), we obtain the contributions of polar optic phonons as

$$\gamma_{0}^{OP} = \frac{1}{\sqrt{2\pi}} \frac{\Omega_{0} e^{2}}{m \epsilon^{*}} \int_{0}^{+\infty} dk_{\perp} k_{\perp}^{3} \int_{0}^{+\infty} dk_{z} \frac{\tau_{c}^{3}(k_{\perp}) f^{2}(k_{z})}{k^{2}} \\ \times \left\{ (N_{0}+1)(\omega_{\perp}+\Omega_{0}) \exp\left[-\frac{1}{2}(\omega_{\perp}+\Omega_{0})^{2} \tau_{c}^{2}(k_{\perp})\right] \\ + N_{0}(\omega_{\perp}-\Omega_{0}) \exp\left[-\frac{1}{2}(\omega_{\perp}-\Omega_{0})^{2} \tau_{c}^{2}(k_{\perp})\right] \right\}$$
(30)

and

$$\begin{split} \tilde{K}^{OP}(\omega) &= \frac{1}{2\sqrt{2\pi}} \frac{\hbar\Omega_{0}e^{2}}{m^{2}\epsilon^{*}} \int_{0}^{+\infty} dk_{\perp}k_{\perp}^{3} \int_{0}^{+\infty} dk_{z} \frac{\tau_{c}(k_{\perp})f^{2}(k_{z})}{k^{2}} \\ &\times \bigg\{ (N_{0}+1) \bigg(\exp\bigg[-\frac{1}{2}(\omega+\omega_{\perp}+\Omega_{0})^{2}\tau_{c}^{2}(k_{\perp}) \bigg] \\ &+ \exp\bigg[-\frac{1}{2}(\omega-\omega_{\perp}-\Omega_{0})^{2}\tau_{c}^{2}(k_{\perp}) \bigg] \bigg) \\ &+ N_{0} \bigg(\exp\bigg[-\frac{1}{2}(\omega+\omega_{\perp}-\Omega_{0})^{2}\tau_{c}^{2}(k_{\perp}) \bigg] \bigg) \\ &+ \exp\bigg[-\frac{1}{2}(\omega-\omega_{\perp}+\Omega_{0})^{2}\tau_{c}^{2}(k_{\perp}) \bigg] \bigg\}; \quad (31)$$

the contributions of deformational acoustic phonons as

$$\gamma_{0}^{AP} = \frac{1}{4\pi\sqrt{2\pi}} \frac{D^{2}}{m\rho u} \int_{0}^{+\infty} dk_{\perp} k_{\perp}^{3} \int_{0}^{+\infty} dk_{z} k \tau_{c}^{3}(k_{\perp}) f^{2}(k_{z}) \\ \times \left\{ (N_{k}+1)(\omega_{\perp}+uk) \exp\left[-\frac{1}{2}(\omega_{\perp}+uk)^{2} \tau_{c}^{2}(k_{\perp})\right] \right. \\ \left. + N_{k}(\omega_{\perp}-uk) \exp\left[-\frac{1}{2}(\omega_{\perp}-uk)^{2} \tau_{c}^{2}(k_{\perp})\right] \right\}$$
(32)

and

$$\widetilde{K}^{AP}(\omega) = \frac{1}{8\pi\sqrt{2\pi}} \frac{\hbar D^2}{m^2 \rho u} \int_0^{+\infty} dk_{\perp} k_{\perp}^3 \int_0^{+\infty} dk_z k \, \tau_c(k_{\perp}) f^2(k_z) \\ \times \left\{ (N_k + 1) \left(\exp\left[-\frac{1}{2} (\omega + \omega_{\perp} + uk)^2 \tau_c^2(k_{\perp}) \right] \right) \\ + \exp\left[-\frac{1}{2} (\omega - \omega_{\perp} - uk)^2 \tau_c^2(k_{\perp}) \right] \right) \\ + N_k \left(\exp\left[-\frac{1}{2} (\omega + \omega_{\perp} - uk)^2 \tau_c^2(k_{\perp}) \right] \right) \\ + \exp\left[-\frac{1}{2} (\omega - \omega_{\perp} + uk)^2 \tau_c^2(k_{\perp}) \right] \right) \right\};$$
(33)

and, finally, the contributions of the charged impurities as

$$\gamma_{0}^{I} = \frac{1}{2\pi^{2}\sqrt{2\pi}} \frac{e^{4}n_{t}^{*}}{m^{2}\epsilon_{0}^{2}} \int_{0}^{+\infty} dk_{\perp} k_{\perp}^{5} \int_{0}^{+\infty} dk_{z} \frac{\tau_{c}^{3}(k_{\perp})f^{2}(k_{z})}{(k^{2}+r_{0}^{-2})^{2}} \\ \times \exp\left(-\frac{\omega_{\perp}^{2}\tau_{c}^{2}(k_{\perp})}{2}\right)$$
(34)

and

$$\widetilde{K}^{I}(\omega) = \frac{1}{2\pi^{2}\sqrt{2\pi}} \frac{e^{4}n_{t}^{*}}{m^{2}\epsilon_{0}^{2}} \int_{0}^{+\infty} dk_{\perp} k_{\perp}^{3} \int_{0}^{+\infty} dk_{z} \frac{\tau_{c}(k_{\perp})f^{2}(k_{z})}{(k^{2}+r_{0}^{-2})^{2}} \\ \times \left(\exp\left[-\frac{1}{2}(\omega+\omega_{\perp})^{2}\tau_{c}^{2}(k_{\perp}) \right] \right.$$

$$\left. + \exp\left[-\frac{1}{2}(\omega-\omega_{\perp})^{2}\tau_{c}^{2}(k_{\perp}) \right] \right).$$
(35)

In all these formulas we use the notation $k = \sqrt{k_{\perp}^2 + k_z^2}$ and $\omega_{\perp} = \hbar k_{\perp}^2/2m$. $N_0 = [\exp(-\hbar\Omega_0/T) - 1]^{-1}$ and $N_k = [\exp(-\hbar uk/T) - 1]^{-1}$ are Bose distribution functions for the optical and acoustic phonons, respectively. The level of thermal velocity fluctuations, $\langle V_x^2 \rangle$, can be determined self-consistently using $\langle V_x^2 \rangle = \tilde{K}(\omega_c)/2\gamma_0$.⁸

IV. SPIN DYNAMICS

In the second stage we analyze spin relaxation due to DP interaction between spin and electron orbital motion. The corresponding spin interaction Hamiltonian is given by^{2,3}

$$H_{spin} = \mu_B(\vec{\sigma} \cdot \vec{B}) + \frac{\hbar}{2}(\vec{\sigma} \cdot \vec{\Omega}), \qquad (36)$$

where $\mu_B(\vec{\sigma} \cdot \vec{B})$ is the Zeeman splitting Hamiltonian term, μ_B is the Bohr magneton, and

$$\vec{\Omega} = \frac{\alpha \tilde{\varkappa}}{\hbar m^{3/2} \sqrt{2\varepsilon_g}},\tag{37}$$

with

$$\varkappa_{x} = m^{3} V_{x} (V_{y}^{2} - V_{z}^{2}), \quad \varkappa_{y} = m^{3} V_{y} (V_{z}^{2} - V_{x}^{2}),$$

$$\varkappa_{z} = m^{3} V_{z} (V_{x}^{2} - V_{y}^{2}).$$
(38)

For a quantum well strongly confined in the $\langle 001 \rangle$ direction, H_{DP} can be simplified as³

$$H_{DP} = -\sigma_x Q_x(t) - \sigma_y Q_y(t), \qquad (39)$$

where

$$Q_x(t) = \lambda V_x(t), \quad Q_y(t) = -\lambda V_y(t) \tag{40}$$

and

$$\lambda = \frac{\alpha \langle p_z^2 \rangle}{2\sqrt{2m\varepsilon_g}},\tag{41}$$

with $\langle p_z^2 \rangle = m \hbar \omega_0 / 2$ if the confinement is parabolic.

Considering orbital motion to play the role of an effective heat bath with correlation functions given by Eqs. (23) and (24), and employing a second application of the method of Refs. 7–9, we obtain a set of Bloch equations for the average spin projections as

$$\frac{d}{dt} \langle \sigma_x(t) \rangle = -\frac{\langle \sigma_x(t) \rangle}{T_2} - (\omega_B + \delta_x) \langle \sigma_y(t) \rangle,$$

$$\frac{d}{dt} \langle \sigma_y(t) \rangle = (\omega_B + \delta_y) \langle \sigma_x(t) \rangle - \frac{\langle \sigma_y(t) \rangle}{T_2},$$

$$\frac{d}{dt} \langle \sigma_z(t) \rangle = \frac{\sigma_z^0 - \langle \sigma_z(t) \rangle}{T_1},$$
(42)

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices and $\sigma_z^0 = -\tanh(\hbar\omega_B/2T)$ is the equilibrium *z*-component of spin. $\omega_B = g\mu_B B/\hbar$, $\mu_B = |e|\hbar/2m_0c$ is the Bohr magneton, and the *g* factor is -0.44 for GaAs. It should be emphasized that we determine the relaxation times T_1 and T_2 microscopically as

$$T_1 = \frac{\tau_s}{2}, \quad T_2 = \tau_s \,, \tag{43}$$

where

$$\frac{1}{\tau_s} = \frac{2\lambda^2}{\hbar^2} \frac{\tilde{K}(\omega_B)}{(\omega_B - \omega_c)^2 + \gamma_0^2}.$$
(44)

While this result is reminiscent of a formula obtained by Ivchenko for bulk semiconductors,¹⁰ that differs from the present quantum well case under consideration here in that the Ivchenko result has a sum of several Lorentzians and involves numerical constants in place of our relaxation rate γ_0 and numerator function $\tilde{K}(\omega)$ which have magnetic field and temperature dependencies that are explicitly determined by Eq. (29) on the microscopic basis. It is evident from Eq. (44), that the effect of magnetic field on spin relaxation is twofold: First, there is magnetic field dependence of the fluctuation source correlator, $\tilde{K}(\omega_B)$, associated with electron transitions between energy levels having different spin. Second, the difference between the frequencies ω_B and ω_c is involved in the denominator of Eq. (44), which occurs be-



FIG. 1. Dependencies of the relaxation rate on the energy of the lowest level of the quantum well; (a) for temperature T=40 K and two magnetic field strengths, (b) for temperature T=300 K (the same curve for both magnetic field strengths).

cause of deviations of electron effective mass and g factor in semiconductors from the free electron values. The temperature dependence can also be separated into two parts: (i) via electron thermal fluctuations (this contribution is linear with increasing temperature), and (ii) via temperature dependence of the momentum relaxation rate, $\gamma_0 = \gamma_0(T)$.

In the absence of a magnetic field $(\omega_c = \omega_B = 0, \langle V_x^2 \rangle = \tilde{K}(0)/2\gamma_0 = T/m)$, we recover Eq. (2) as the zero field limit:

$$\frac{1}{\tau_s}\Big|_{B=0} = \frac{4\lambda^2}{\hbar^2} \frac{1}{\gamma_0} \frac{\tilde{K}(0)}{2\gamma_0} = \frac{4\lambda^2}{\hbar^2} \frac{1}{\gamma_0} \langle V_x^2 \rangle = \frac{4\lambda^2}{\hbar^2} \frac{1}{\gamma_0} \frac{T}{m}$$
$$= \frac{\alpha^2 \langle P_z^2 \rangle^2}{2\hbar^2 m^2 \varepsilon_g} \frac{1}{\gamma_0} T, \qquad (45)$$

wherein our microscopic analysis yields the phenomenological constant τ_p of Eqs. (1) and (2) as $\tau_p \rightarrow 1/\gamma_0$.

Figures 1(a) and 1(b) exhibit the dependence of the relaxation rate on the energy of the lowest electronic subband of the quantum well (which is given by $E_0 = \hbar \omega_0/2$ for the case



FIG. 2. Dependence of the relaxation rate on magnetic field strength for various temperatures.

of harmonic confinement) for various temperatures and magnetic field strengths. It is evident from these figures that at low temperature the applied magnetic field suppresses spin relaxation, whereas at higher temperatures the momentum relaxation rate dominates in the denominator of Eq. (44), and there is a negligible magnetic field dependence in this case. In these calculations we have employed the following set of parameters for a GaAs-based quantum well: electron effective mass $m = 0.067m_0$, $1/\epsilon^* = 0.0069$, optical phonon energy $\hbar \Omega_0 = 0.035$ eV, deformation potential D = 8.6 eV, density $\rho = 5.4 \text{ g cm}^{-3}$, sound velocity $u = 5 \times 10^5 \text{ cm s}^{-1}$, impurity concentration $n_t^* = 10^{17} \text{ cm}^{-3}$, and static permittivity $\epsilon_0 = 13$. It should be emphasized that our microscopic calculations yield a quantitative agreement with the experimental results of Ref. 6. The full magnetic field dependence (up to 1000 Gs) of the spin relaxation rate is presented in Fig. 2 for $\hbar \omega_0 = 0.01$ eV. This dependence has the well-known² Lorentzian shape, evident in Eq. (44), and for a reasonable range of magnetic field strength it is not affected by the magnetic field dependence of the velocity fluctuations, which are embedded in the function $\tilde{K}(\omega_B)$. [However, for the case of dilute magnetic semiconductors having a large electron g factor, to which our general analysis is also applicable, the magnetic field dependence of the function $\tilde{K}(\omega_R)$ can be of crucial importance.] The magnetic field dependence for the case of bulk semiconductors (represented by a sum of several Lorentzians) was obtained in Ref. 10 and is also reconfirmed by our microscopic analysis.¹¹

The temperature dependence of the spin relaxation rate is shown in Fig. 3. The nonmonotonic behavior is due to the dominance of different scattering mechanisms in different temperature ranges. At low temperatures (before the peak), the momentum scattering rate is determined by impurities and is almost independent of temperature, and, consequently, we have almost linear growth of the spin relaxation rate with increasing temperature, as predicted by Eq. (2). However, as temperature further increases, optical phonons become the dominant scattering mechanism and, with this, the momentum scattering time becomes temperature dependent, result-



FIG. 3. Temperature dependence of the relaxation rate for various magnetic field strengths.

ing in suppression of the relaxation rate. It is important to note that in the temperature range in which phonons dominate, the relaxation rate is almost independent of the magnetic field, whereas at low temperatures the magnetic field shifts the peak and gives rise to deviations from linear behavior.

V. CONCLUSIONS

In conclusion, we have developed a fully microscopic theory of electron-spin relaxation in semiconductors by the D'yakonov-Perel' mechanism. We have applied this theory to a quantum well structure with a magnetic field in the growth direction. A set of Bloch equations for a spin system has been derived with microscopically determined longitudinal, T_1 , and transverse, T_2 , relaxation times, which are related as $T_1=T_2/2$ for the quantum well structure grown in the $\langle 001 \rangle$ direction.³ The well-known semiphenomenological expression for the spin relaxation rate³ emerges as the zeromagnetic field limit of our result. Furthermore, we have analyzed the dependencies of the electron-spin relaxation rate on the energy of the lowest quantum well subband, on the magnetic field strength, and on temperature, obtaining a *quantitative* agreement with the experimental results.

APPENDIX A

The derivation of Langevin-like equations for electron velocity operators, Eq. (15) presented here follows the approach developed in our previous works.^{7–9} We start from Heisenberg equations of motion for electron position and velocity operators for the Hamiltonian of Eq. (3), as

$$\frac{d}{dt}x(t) = \frac{1}{i\hbar}[x(t),H]_{-} = V_{x}(t),$$

$$\frac{d}{dt}y(t) = \frac{1}{i\hbar}[y(t),H]_{-} = V_{y}(t), \qquad (A1)$$

$$\frac{d}{dt}V_x(t) = \frac{1}{i\hbar}[V_x(t),H]_-$$
$$= -\omega_c V_y(t) + \frac{1}{m}\sum_{\mathbf{k}}ik_x[Q_{\mathbf{k}}(t) + U_{\mathbf{k}}]X_{\mathbf{k}}(t),$$
$$\frac{d}{dt}V_y(t) = \frac{1}{i\hbar}[V_y(t),H]_-$$

$$=\omega_c V_x(t) + \frac{1}{m} \sum_{\mathbf{k}} i k_y [Q_{\mathbf{k}}(t) + U_{\mathbf{k}}] X_{\mathbf{k}}(t).$$

If the coupling between the electron subsystem and heat bath is weak, or in the case of Gaussian statistics of unperturbed heat bath variables, the fully coupled Heisenberg heat bath variable is given by⁷

$$Q_{\mathbf{k}}(t) = Q_{\mathbf{k}}^{(0)}(t) + \int_{-\infty}^{t} dt_{1} \varphi_{\mathbf{k}}(t;t_{1}) X_{-\mathbf{k}}(t_{1}), \qquad (A2)$$

where the response function of the phonon heat bath $\varphi_{\mathbf{k}}(t;t_1)$ is defined by Eq. (10). Substituting Eq. (A2) into Eq. (A1), we have to take into account the fact that only the fully coupled heat bath variable commutes with the electron variable taken at equal times. Accordingly, we perform a symmetrization of both terms of Eq. (A2) with the electron variables, with the results

$$\begin{split} \frac{d}{dt} V_{x}(t) &+ \omega_{c} V_{y}(t) \\ &= \frac{1}{m} \sum_{\mathbf{k}} i k_{x} \bigg(\frac{1}{2} [U_{\mathbf{k}}, X_{\mathbf{k}}(t)]_{+} + \frac{1}{2} [Q_{\mathbf{k}}^{(0)}(t), X_{\mathbf{k}}(t)]_{+} \\ &+ \int_{-\infty}^{t} dt_{1} \varphi_{\mathbf{k}}(t; t_{1}) \frac{1}{2} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{+} \bigg), \end{split}$$

$$= \frac{1}{m} \sum_{\mathbf{k}} i k_{y} \left(\frac{1}{2} [U_{\mathbf{k}}, X_{\mathbf{k}}(t)]_{+} + \frac{1}{2} [Q_{\mathbf{k}}^{(0)}(t), X_{\mathbf{k}}(t)]_{+} \right. \\ \left. + \int_{-\infty}^{t} dt_{1} \varphi_{\mathbf{k}}(t; t_{1}) \frac{1}{2} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{+} \right).$$
(A3)

To eliminate the unperturbed phonon/impurity variables we employ the Furutsu-Novikov theorem¹²

$$\left\langle \frac{1}{2} [\mathcal{Q}_{\mathbf{k}}^{(0)}(t), X_{\mathbf{k}}(t)]_{+} \right\rangle = \int_{-\infty}^{+\infty} dt_{1} M_{\mathbf{k}}(t; t_{1}) \left\langle \frac{\delta X_{\mathbf{k}}(t)}{\delta \mathcal{Q}_{-\mathbf{k}}^{(0)}(t_{1})} \right\rangle,$$
(A4)

where the correlation function $M_{\mathbf{k}}(t;t_1)$ of free phonon variables is given by Eq. (11), and $\delta/\delta Q^{(0)}(t_1)$ is the functional derivative with respect to the uncoupled heat bath variable $Q^{(0)}(t_1)$. Equation (A4) can be derived by an application of the Wick theorem, assuming the operator $X_{\mathbf{k}}(t)$ to be a functional of $\{Q^{(0)}(t_1)\}$ with $t_1 \leq t$ (see Ref. 7). This expression

is exact only for Gaussian statistics of the variables $Q^{(0)}(t)$, and it also can be applied in the case of weak coupling. For the case of strong coupling, Eq. (A4) requires modification to include functional derivatives of all orders. The functional derivative on the right-hand side of Eq. (A4) is proportional to the commutator⁷ in the form

$$\left\langle \frac{\delta X_{\mathbf{k}}(t)}{\delta Q_{-\mathbf{k}}^{(0)}(t)} \right\rangle = \left\langle \frac{i}{\hbar} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_1)]_{-} \right\rangle \Theta(t - t_1), \quad (A5)$$

with the following result:

$$\frac{1}{2} [\mathcal{Q}_{\mathbf{k}}^{(0)}(t), X_{\mathbf{k}}(t)]_{+} \rangle = \int_{-\infty}^{t} dt_{1} M_{\mathbf{k}}(t; t_{1}) \\
\times \left\langle \frac{i}{\hbar} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{-} \right\rangle.$$
(A6)

An analogous treatment of the electron-impurity correlation term yields

$$\left\langle \frac{1}{2} [U_{\mathbf{k}}(t), X_{\mathbf{k}}(t)]_{+} \right\rangle = \int_{-\infty}^{t} dt_{1} \Phi_{\mathbf{k}} \left\langle \frac{i}{\hbar} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{-} \right\rangle,$$
(A7)

where $\Phi_{\mathbf{k}}$ is the impurity potential correlation function given by Eq. (13). We also introduce fluctuation source operators defined as

$$\xi_{x,y}(t) = \frac{1}{m} \sum_{\mathbf{k}} i k_{x,y} \left(\frac{1}{2} [\mathcal{Q}_{\mathbf{k}}^{(0)}(t) + U_{\mathbf{k}}, X_{\mathbf{k}}(t)]_{+} - \int_{-\infty}^{t} dt_{1} [M_{\mathbf{k}}(t;t_{1}) + \Phi_{\mathbf{k}}] \frac{i}{\hbar} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{-} \right),$$
(A8)

with zero average, $\langle \xi_{x,y}(t) \rangle = 0$, and collision terms defined as

$$G_{x,y}[V_{x}(t);V_{y}(t)] = -\frac{1}{m} \sum_{\mathbf{k}} ik_{x,y} \int_{-\infty}^{t} dt_{1} \Big([M_{\mathbf{k}}(t;t_{1}) + \Phi_{\mathbf{k}}] \\ \times \frac{i}{\hbar} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{-} + \varphi_{\mathbf{k}}(t;t_{1}) \frac{1}{2} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{+} \Big),$$
(A9)

resulting in the Langevin-like equations of Eq. (15).

APPENDIX B:

In this appendix we determine the commutators $[X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_1)]_{\pm}$ involved in Eqs. (16), (A8), and (A9). We assume that there is finite correlation time, τ_c , of the electron-phonon interaction (which will be obtained self-consistently). For the case of weak coupling, the commutators can be calculated using the free, uncoupled evolution of the electron velocity operators during τ_c , as given by

$$x(t) = x(t_1) + V_x(t_1) \frac{\sin[\omega_c(t-t_1)]}{\omega_c} - V_y(t_1) \frac{1 - \cos[\omega_c(t-t_1)]}{\omega_c},$$
 (B1)

$$y(t) = y(t_1) + V_x(t_1) \frac{1 - \cos[\omega_c(t - t_1)]}{\omega_c}$$
$$+ V_y(t_1) \frac{\sin[\omega_c(t - t_1)]}{\omega_c}.$$

This allows to us determine the following commutator:

$$[i\mathbf{k}_{\perp}\mathbf{r}_{\perp}(t), -i\mathbf{k}_{\perp}\mathbf{r}_{\perp}(t_{1})]_{-} = -\frac{i\hbar k_{\perp}^{2}}{m\omega_{c}}\sin[\omega_{c}(t-t_{1})],$$
(B2)

where $k_{\perp} = |\mathbf{k}_{\perp}| = \sqrt{k_x^2 + k_y^2}$ is the magnitude of the transverse wave vector. With the operator equation (Baker-Campbell-Hausdorff identity)

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{-1/2[\hat{A},\hat{B}]_{-}},$$
 (B3)

(which is valid, when $[\hat{A}, \hat{B}]_{-}$ is a *c* number) we obtain

$$\frac{i}{\hbar} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{-} = \frac{2}{\hbar L^{3}} f^{2}(k_{z}) \exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})]\} \\ \times \sin\left(\frac{\hbar k_{\perp}^{2}}{2m\omega_{c}} \sin[\omega_{c}(t-t_{1})]\right),$$

$$\frac{1}{2} [X_{\mathbf{k}}(t), X_{-\mathbf{k}}(t_{1})]_{+} = \frac{1}{L^{3}} f^{2}(k_{z}) \exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})]\} \\ \times \cos\left(\frac{\hbar k_{\perp}^{2}}{2m\omega_{c}} \sin[\omega_{c}(t-t_{1})]\right).$$
(B4)

We assume the coordinate fluctuations to be approximately Gaussian (see Ref. 8 for the corresponding discussion) and, consequently, obtain

$$\langle \exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})]\}\rangle = \exp\left\{-\frac{1}{2}\langle (\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})])^{2}\rangle\right\}$$
(B5)

and

$$\exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t)-\mathbf{r}_{\perp}(t_{1})]\}-\langle\exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t)-\mathbf{r}_{\perp}(t_{1})]\}\rangle$$
$$\approx i\mathbf{k}_{\perp}(\mathbf{r}_{\perp}(t)-\mathbf{r}_{\perp}(t_{1}))\langle\exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t)-\mathbf{r}_{\perp}(t_{1})]\}\rangle.$$
(B6)

With these simplifications we have

$$G_{x,y}[V_{x}(t);V_{y}(t)] - \langle G_{x,y}[V_{x}(t);V_{y}(t)] \rangle$$

$$= -\frac{1}{mL^{3}} \sum_{\mathbf{k}} ik_{x,y}f^{2}(k_{z}) \int_{-\infty}^{t} dt_{1} \Big\{ [M_{\mathbf{k}}(t;t_{1}) + \Phi_{\mathbf{k}}] \\ \times \frac{2}{\hbar} \sin \Big(\frac{\hbar k_{\perp}^{2}}{2m\omega_{c}} \sin [\omega_{c}(t-t_{1})] \Big) \\ + \varphi_{\mathbf{k}}(t;t_{1}) \cos \Big(\frac{\hbar k_{\perp}^{2}}{2m\omega_{c}} \sin [\omega_{c}(t-t_{1})] \Big) \Big\} \\ \times i\mathbf{k}_{\perp} [\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})] \langle \exp\{i\mathbf{k}_{\perp} [\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})] \} \rangle.$$
(B7)

We make the further assumption that the correlation time of the electron-phonon interaction, τ_c , is much less than the period of the cyclotron oscillations, i.e. $\omega_c \tau_c \ll 1$ (the same approximation was used in Ref. 10). This is reasonable for semiconductors at moderate magnetic fields and not too low temperatures, and it leads to

$$\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_1)] \approx k_x V_x(t)(t - t_1) + k_y V_y(t)(t - t_1),$$
(B8)

$$\frac{i\hbar k_{\perp}^2}{2m\omega_c}\sin[\omega_c(t-t_1)] \approx \frac{i\hbar k_{\perp}^2}{2m}(t-t_1), \qquad (B9)$$

and

$$\langle \exp\{i\mathbf{k}_{\perp}[\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_{1})]\}\rangle = \exp\left\{-\frac{(t-t_{1})^{2}}{2\tau_{c}^{2}(\mathbf{k}_{\perp})}\right\},$$
(B10)

where

$$\tau_c^{-2}(\mathbf{k}_{\perp}) = k_x^2 \langle V_x^2(t) \rangle + k_y^2 \langle V_y^2(t) \rangle + k_x k_y \langle [V_x(t), V_y(t)]_+ \rangle.$$
(B11)

The resulting simplified stochastic equations for the fluctuating velocity components take the form given by Eq. (19).

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