Derivation of electron spin relaxation rate by electron–phonon interaction using a new diagram method

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A formula for determining the electron spin relaxation rate of an electron–phonon system is derived using a new spring-loop diagram method. The result properly contains the distribution functions for the electrons and phonons. Therefore, all spin-flip and spin-conserving processes are explained from a microscopic point of view, and physical insight into the quantum dynamics of electron spin in a solid is obtained from the diagram. Photons and phonons are classified on the basis of their spin-flip and spin-conserving processes. This formula is used to calculate the electron spin relaxation rate \( \gamma \) in GaAs. The temperature \( T \) dependence of the relaxation rate obtained by comparison with the experimental result previously reported is \( \gamma \propto T^{1.94} \). © 2014 The Japan Society of Applied Physics

1. Introduction

Recently, intensive experimental and theoretical studies have concentrated on the electron spin dynamics of semiconductors from the viewpoint of both physics and applications.\(^1\)–\(^10\) It is important to understand the spin relaxation mechanism necessary for realizing useful spintronics devices. The perturbative approach is a popular method of gaining knowledge on spin dynamics. Despite considerable interest, however, a detailed theoretical study from a fully microscopic approach is only the first step made.\(^11\)–\(^17\) The Elliott–Yafet (EY) mechanism\(^18\),\(^19\) or D’yakonov–Perel’ (DP) mechanism\(^20\) contribute to the relaxation. For bulk III–V n-type semiconductors, such as GaAs, the DP and EY processes are the dominant spin-relaxation mechanisms at high and low temperatures, respectively.\(^21\),\(^22\)

On the other hand, the diagram method is a well-known scheme for calculating perturbative terms. The standard diagram method is a powerful tool for studying complex interacting systems in solid-state physics and can represent the trajectory of particles well in the intermediate states of scattering processes. On the other hand, the results obtained using the standard diagram contain the Fermi distribution function for electrons and the Planck distribution function for phonons in simple additive forms.\(^23\)–\(^26\) which violates the “population criterion”, meaning that they should be contained in multiplicative forms.\(^27\) How the Planck and Fermi distribution functions are included in the electron spin relaxation rate is important because the temperature dependence of the relaxation rate is caused by the distribution functions.

In this study, a formula for determining the electron spin relaxation rate in a system of electrons interacting with phonons is derived, i.e., \( \chi_{\pm}(\omega) = \frac{g^2 \mu_B^2}{\Omega_0} \sum \frac{(f_{\alpha-} - f_{\alpha+}) \gamma_\alpha(\omega)}{[\hbar \omega - g \mu_B B]^2 + \gamma_\alpha(\omega)^2} \) \((1)\)

where \( g \) is the electron g-factor, \( \mu_B \) is the Bohr magneton, \( \Omega_0 \) is the volume of the system, and \( f_{\alpha-} \) (\( f_{\alpha+} \)) is the Fermi distribution function for an electron in state \( \alpha \) with a down (up) spin. The effect of the electron–phonon interaction is included in the line shape function \( \gamma_\alpha(\omega) \), which is derived by a spring-loop diagram method.

The rules for deriving the line shape function by the diagram method are as follows.

Rule 1) Two implicit states with up and down spins are induced between the initial \( (\alpha-) \) and final \( (\alpha+) \) states by an electron–phonon interaction.

Rule 2) An implicit state is connected to the initial (or final) state by a proper interaction coupling factor \( (C\text{-factor}, C_{\alpha i,\beta j}(q)) \), which is represented by a spring (see Table I) and is defined as

\[ C_{\alpha i,\beta j}(q) = \langle \alpha|H_{qp}|\beta j \rangle, \]

where \( i, j = + \) (up spin) or \(-\) (down spin) and the electron–phonon interaction Hamiltonian \( H_{qp} \) depends on the mode of the phonons with the wave vector \( q \).

Rule 3) Two implicit transition factors \( (T\text{-factors}, T_{\pm}(ai, \beta j)) \), exist. One forms a clockwise loop, \( T_{+}(ai, \beta j) \), and the other forms a counterclockwise loop, \( T_{-}(ai, \beta j) \) (see Table I). They are defined as follows:

\[ T_{\pm}(ai, \beta j) \equiv G_{ai,\beta j}(\pm\omega_q)P_{\pm}(ai, \beta j). \]

Here, the energy denominator factors \( (G\text{-factors}, G_{ai,\beta j}(\pm\omega_q)) \), are defined as follows:

\[ G_{ai,\beta j}(\pm\omega_q) = (\hbar \omega + E_{ai} - E_{\beta j} \mp \hbar \omega_q)^{-1}, \]

where \( \hbar \omega_q \) is the phonon energy. With \( G_{ai,\beta j}(\pm\omega_q) \), the energy conservation is satisfied, i.e., \( E_{\beta j} = E_{ai} + \hbar \omega \mp \hbar \omega_q \).
The population factors ($P$-factors), $P_+(ai, βi)$ for the clockwise loop and $P_-(ai, βi)$ for the counterclockwise loop, are defined as

\[ P_+(ai, βi) \equiv (1 + N_q)f_{ai}f_{βi} - N_qf_{ai}(1 - f_{βi}), \]
\[ P_-(ai, βi) \equiv N_qf_{ai}(1 - f_{βi}) - (1 + N_q)f_{ai}(1 - f_{βi}), \]

where $N_q$ is the Planck distribution function for a phonon with energy $\hbar\omega_q$. The red and blue loops denote the spin-flip and spin-conserving processes, respectively. In the loops, the right and left arrows (forward and backward processes) denote the photon absorption and emission processes. The solid (upper) and dotted (lower) half-circles correspond to the phonon emission and absorption processes, respectively.

Rule 4) A $C$-factor multiplied by a $T$-factor becomes an element in the line shape function.

Rule 5) Finally, by summing all the elements over all the phonon wave vectors and implicit states, the line shape function can be obtained.

In this study, the electron, photon, and phonon are considered. Table II lists the symbols and meanings.

### 3. Line shape function

In accordance with the rules, Fig. 1 shows all possible processes. The diagram for the line shape function has eight implicit transitions (loops) (Table III).

The implicit states are named as such because they are included only in the line shape function, not in the magnetic susceptibility. Although the implicit transitions are not measured directly, they should be considered in the calculations in the case of an electron system interacting with phonons. The springs show that each implicit state ($λ$ or $λ'$) is coupled with an initial spin-down state ($α−$) or a final spin-up state ($α+$). The red and blue springs show that the initial spin-down (final spin-up) state is coupled with the implicit spin-up state.
Here, dotted arrows indicate participation in the spin-emission process. Blue vertical dotted arrows and red vertical solid arrows represent absorption and emission processes, respectively. Table IV shows a summary of the meaning of arrows in Fig. 1.

From Fig. 1 and the rules, the line shape function can be obtained as follows:

\[
\gamma_{\alpha}(\omega)(f_{\alpha-} - f_{\alpha+}) = \sum_{q,r} \left[ T_+(\alpha-, \lambda+) + T_-(\alpha-, \lambda+) \right] |C_{\lambda+a}(q)|^2 \\
+ \sum_{q,r} C_{\alpha-\lambda}(q)^2 \left[ T_+(\lambda+, \alpha+) + T_-(\lambda+, \alpha+) \right] \\
+ \sum_{q,r} [T_+(\alpha-, \lambda-)] [T_-(\alpha-, \lambda-)] |C_{\lambda-a}(q)|^2 \\
+ \sum_{q,r} |C_{\alpha-\lambda}(q)|^2 \left[ T_+(\lambda-, \alpha+) + T_-(\lambda-, \alpha+) \right] \\
= A + B + C + D + E + F + G + H. \tag{7}
\]

Here, A–H are the same as those in Fig. 1. \(f_{\alpha-} - f_{\alpha+}\) means the transition from the initial state (\(\alpha-\)) to the final state (\(\alpha+\)). Equation (7) is the same as the results obtained using Kang–Choi’s projection-reduction method.\(^{17}\)

The first term (A) in Eq. (7) or Fig. 1 can be interpreted as follows. Note that \(T_+(\alpha-, \lambda+) = G_{\alpha-, \lambda+}(\omega E_0) P_+(\alpha-, \lambda+)\). \(F_+(\alpha-, \lambda+)\) means an implicit transition between the initial spin-down state (\(\alpha-\)) and the implicit spin-up state (\(\lambda+\)). A phonon (filled purple square) is emitted to the spring (absorbed by an electron) during the solid (dotted) half-circle process. The transition forms a loop because the phonon emission process maintains a balance with the absorption process. The implicit spin-up state is coupled with the final spin-up state (\(\alpha+\)) by | \(C_{\lambda+a}(q)\) |^2. \(G_{\alpha-, \lambda+}(\omega E_0)\) means that the energy of the implicit spin-up state is determined by the energies of the initial spin-down state, photon, and phonon. Accordingly, an electron undergoes a spin-flip implicit transition with phonon emission (or absorption) from the initial spin-down state to the implicit spin-up state (or vice versa), which is coupled with the final spin-up state.

The second term (B) corresponds to the counterclockwise loop between the initial spin-down state (\(\alpha-\)) and the implicit spin-up state (\(\lambda+\)). In the third term (C), the initial spin-down state is coupled with the implicit spin-up state and a spin-conserving implicit transition occurs between the implicit spin-up state and the final spin-up state (\(\alpha+\)), where a phonon symbolized by the empty purple square plays a role. The other terms can be interpreted in a similar manner.

Figure 2 shows the net implicit transitions of the first four terms in Eq. (7) or Fig. 1. Loops [1], [2], [3], and [4] correspond to processes A, B, C, and D in Fig. 1 or Eq. (7), respectively. The meaning of the forward process from stage (a) to stage (c) is as follows. (i) An electron (empty black circle) in the initial spin-down state of loop [1] emits a phonon (filled purple square) to the spring and absorbs a
photons (filled green triangle). (ii) An electron in the initial spin-down state of loop [2] absorbs a phonon from the spring and absorbs a photon. (iii) An electron (filled black circle) in the implicit spin-up state of loop [3] emits a phonon (empty purple square) to the spring and absorbs a photon (empty green triangle). (iv) An electron in the implicit spin up state of loop [4] absorbs a phonon from the spring and absorbs a photon. From state (d) to stage (f) is the reverse process.

Figure 3 shows the net implicit transitions of the last four terms in Eq. (7) or Fig. 1. Loops [5], [6], [7], and [8] correspond to processes E, F, G, and H in Fig. 1 or Eq. (7), respectively. The symbols are the same as those in Fig. 2.

4. Application

To confirm the correctness of the method, the electron spin relaxation rate (γ) in GaAs is calculated using Eqs. (1) and (7). If the Lorentzian approximation is assumed for weak scattering, the relaxation rate is related to the line shape function as γ = 2Im(χ_0(ω))/ℏ, where Im denotes the “imaginary part”.

A system of electrons interacting with phonons through the phonon-modulated spin–orbit interaction is considered, for which the interaction Hamiltonian is given as18,19

$$H_{sp} = \frac{\hbar}{4m^*c^2}[∇V_{sp} × (p + eA)] · σ,$$

where e is the speed of light, p is the momentum operator of an electron with the effective mass m, A is the vector potential, V_{sp} is the electron–phonon interaction potential, and σ is the Pauli spin matrix. Piezoelectric phonon scattering is one of the main scattering mechanisms in III–V compounds such as GaAs. The acoustic strain induced by pressure in these materials gives rise to a macroscopic electric field, which is assumed to be proportional to the derivative of the atomic displacement given by

$$u = \sum_q \sqrt{\frac{\hbar}{2\rho_mΩ_qω_q}}(b_q + b_q^+e^{iq·r})\hat{ε}_q,$$

where ρ_m is the mass density, b_q (b_q^+) is the creation (annihilation) operator for a phonon with wave vector q, and \(\hat{ε}_q\) is the polarization vector. Equation (8) then becomes

$$H_{sp} = \sum_{j_{xx},x_{yy},x_{xy},x_{yx}} \sum_{a,b} \sum_q [I(q)]_{ab}a_{j_{xx}}^†a_{a,b}^*(h_q + b_q^+)(x_{xx}σ_x)\hat{ε}_q).$$

Here, \(X_{ab} \equiv \langle a|X|b\rangle\), \(a_{j_{xx}}^†\) is the creation (annihilation) operator for an electron in the state \(|a,s_a\rangle\) with spin \(s_a\), \(X_{xx}\) is the spinor, and

$$I(q) = \frac{\hbar D_q}{4m^*c^2}[∇e^{iq·r} × (p + eA)],$$

where

$$D_q = \frac{e^2q^2}{2\rho_mΩ_qω_q},$$

Here, \(q_d = n_ee^2/εε_0κ_T\) is the reciprocal of the Debye screening length, where \(ε\) is the static dielectric constant and \(n_e\) is the number density of electrons. In Eq. (12), the proportionality constant (piezoelectric constant) \(P_{pe}\) is used as a fitting parameter.

Figure 4 shows the temperature dependence of the electron spin relaxation rate by piezoelectric phonon scattering in GaAs for \(n_e = 2.7 × 10^{11} m^{-3}\), \(P_{pe} = 2.4 × 10^{24} eV/m\), and \(f = 30\ GHz\), which is the frequency of the incident electromagnetic wave. The result (solid red line) was fitted to the
the results reported by Römer et al.\textsuperscript{10}) the spin
Relativistic motion of the electron around the nucleus causes
5. Discussion and conclusions
experimental result reported by Römer et al.,\textsuperscript{10}) adding the
rate is proportional to the inverse of the relaxation time (\(\tau\)). Therefore, when an external static magnetic
field caused by the current due to an
electric action. Therefore, when an external static magnetic
field, \(B\), is applied, the electron spin magnetic moments exhibit precession by \(\mu_s \times B\) and their directions can be flipped by \(\mu_s \times B\).

The experimental results for the spin relaxation rate could be explained by the formulae developed in this study, and the spin-flip and spin-conserving processes could be analyzed properly using the present diagram. Therefore, a proper theory, which is physically acceptable and generally applicable, can be derived by Kang–Choi’s projection-reduction method. The present diagram should be discerned from the Feynman’s diagram\textsuperscript{28,29} because the present diagram does not represent the trajectories of the particles in the intermediate stages of the scattering processes. This diagram could be called the “KC spring-loop diagram” because all the contributions to the self-energy terms can be grouped into the topologically distinct spring-loop diagrams based on the electron–phonon population topology. It is expected that the present method will be applicable to other electron transition phenomena, e.g., random spin–orbit coupling.\textsuperscript{30}

Fig. 4. (Color online) Temperature dependence of the rate of electron spin relaxation due to piezoelectric phonon scattering in GaAs for \(f = 30\) GHz, \(n_e = 2.7 \times 10^{21}\) m\(^{-3}\), and \(P_{pe} = 2.4 \times 10^{24}\) eV/m. The black triangles show the results reported by Römer et al.\textsuperscript{10})

Relativistic motion of the electron around the nucleus causes the spin–orbit interaction, \(H' = -\mu_s \cdot \mathbf{B}_{\text{ef}}\). Here, \(\mu_s = g\mu_B \sigma/2\) is the spin magnetic dipole moment of the electron and \(\mathbf{B}_{\text{ef}} = \mathbf{E} \times \mathbf{v}/c^2\) is the magnetic field caused by the current due to an electron moving with velocity \(\mathbf{v}\) around the nucleus, where the electric field \(\mathbf{E}\) is related to the electron–phonon interaction potential energy \(V_{\text{ep}}\) as \(\mathbf{E} = -\nabla V_{\text{ep}}\). The direction of \(\mu_s\) deviates slightly from the \(z\)-axis because the direction of \(\nabla V_{\text{ep}}\), i.e., \(\mathbf{B}_{\text{ef}}\), is changed by the electron–phonon interaction. Therefore, when an external static magnetic field, \(\mathbf{B} = Bz\), and a time-varying magnetic field in the incident electromagnetic wave, \(\mathbf{B}_i = B_1 \cos \omega t (i = x, y)\), are applied,

the electron spin magnetic moments exhibit precession by \(\mu_s \times \mathbf{B}\) and their directions can be flipped by \(\mu_s \times \mathbf{B}\).

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