Chapter 3
Spin Relaxation in GaAs Based Quantum Dots for Security and Quantum Information Processing Applications

S. Prabhakar and R. Melnik

Abstract We report new three-dimensional modeling results of the band structure calculation of $GaAs/Al_{0.3}Ga_{0.7}As$ quantum dots (QDs) in presence of externally applied magnetic and electric fields along z-direction. We explore the influence of spin-orbit coupling in the effective g-factor of electrons in such QDs for possible application in security devices, encrypted data and quantum information processing. We estimate the relaxation rate in QDs caused by piezo-phonons.

3.1 Introduction

Several research proposals for the design of robust semiconductor spintronic devices for quantum logic gates in quantum information processing and security applications is based on the accurate manipulation of the effective g-factor of electrons with electric fields and estimation of the spin relaxation rate [14–16, 20]. One may expect a larger spin relaxation or decohenrence time than the gate operation time for the possible implementation of quantum dots devices in quantum information processing [1, 2]. Authors in Refs. [6, 11] have measured long spin relaxation times of 0.85 ms in GaAs QDs by pulsed relaxation rate measurements and 20 ms in InGaAs QDs by optical orientation measurements. These experimental studies in QDs confirm that the manipulation of spin-flip rates by spin-orbit coupling is important for the design of spintronics logic and other devices [7, 9, 16].

The spin-orbit coupling consists of the Rashba [3] and the linear Dresselhaus [5] terms that arise from structural inversion asymmetry along the growth direction and the bulk inversion asymmetry of the crystal lattice [1, 2, 24]. The electric and magnetic fields tunability of the electron g-factor in gated III-V semiconductor QDs with the Rashba and Dresselhaus spin-orbit couplings were explored in

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Refs. [12, 15, 22–24]. It has also been noted that in-plane anisotropy due to gate potential also influences the effective Landé g-factor of electrons in QDs [15, 17, 27]. In this paper, we consider three-dimensional $GaAs/Al_{0.3}Ga_{0.7}As$ conical QDs that are epitaxially formed at the heterojunction. We study the variation in the g-factor of electrons with electric and magnetic fields. We also estimate the phonon mediated spin-flip rate of electron spin states.

The paper is organized as follows. In Sect. 3.2, we provide a description of the theoretical model of three-Dimensional semiconductor QDs in presence of externally applied electric and magnetic fields. In Sect. 3.3, we give details of the diagonalization technique used for finding the eigenvalues and eigenstates for electrons in QDs. In Sect. 3.4, we discuss the dependency of the effective g-factor and spin relaxation rate with magnetic fields. Finally, in Sect. 3.5, we summarize our results.

3.2 Theoretical Model

We consider a $GaAs/Al_{0.3}Ga_{0.7}As$ QD epitaxially formed at the heterojunction. In presence of magnetic field applied along z-direction, we write the total Hamiltonian of this quantum dot as: [1, 9, 19, 21, 24]

$$H = H_0 + H_R + H_D, \tag{3.1}$$

where H_R and H_D are Hamiltonians associated with the Rashba and Dresselhaus spin-orbit couplings and

$$H_0 = \frac{\mathbf{P}^2}{2m} + V(x, y, z) + eE_z z + \frac{1}{2} g_o \mu_B \sigma_z B, \tag{3.2}$$

where $\mathbf{P} = \mathbf{p} + e\mathbf{A}$ is the kinetic momentum operator, $\mathbf{p} = -i\hbar(\partial_x, \partial_y, \partial_z)$ is the canonical momentum operator, $\mathbf{A} = B(-y, x, 0)$ is the vector potential, m is the effective mass of the electron in the conduction band, μ_B is the Bohr magneton and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices. Also, $V(x, y, z)$ is the confinement potential which is zero in the GaAs region and 0.3 eV in the barrier material, and E_z is the applied external field along z-direction. The Hamiltonians associated with the Rashba and Dresselhaus spin-orbit couplings can be written as [3, 5, 24]

$$H_R = \frac{\alpha_R}{\hbar} \left(\sigma_x P_y - \sigma_y P_x\right), \tag{3.3}$$

$$H_D = \frac{\alpha_D}{\hbar} \left(-\sigma_x P_x + \sigma_y P_y\right), \tag{3.4}$$

where the strengths of the Rashba and Dresselhaus spin-orbit couplings are characterized by the parameters α_R and α_D. They are given by

$$\alpha_\mathrm{R} = \gamma_\mathrm{R} eE, \qquad \alpha_\mathrm{D} = 0.78\gamma_\mathrm{D}\left(\frac{2me}{\hbar^2}\right)^{2/3} E^{2/3}, \tag{3.5}$$

where γ_R and γ_D are the Rashba and Dresselhaus coefficients. Now we write $H|\Psi\rangle = \varepsilon|\Psi\rangle$ in terms of a coupled eigenvalue problem, consisting of two equations, in the basis states $|\psi_1\rangle$ and $|\psi_2\rangle$ as

$$\begin{aligned}
&\Bigg[-\frac{\hbar^2}{2m}\left(\partial_x^2+\partial_y^2+\partial_z^2\right)+\frac{1}{8}m\omega_c^2\left(x^2+y^2\right)-\frac{i\hbar\omega_c}{2}\left(-y\partial_x+x\partial_y\right)+V(x,y,z)\\
&+eE_z z+\frac{1}{2}g_0\mu_\mathrm{B}B\sigma_z\Bigg]|\psi_1\rangle+\Bigg[\alpha_\mathrm{R}eE_z\{\partial_x-i\partial_y+\frac{m\omega_c}{2\hbar}(x-iy)\},\\
&+\alpha_\mathrm{D}\left\{i\partial_x-\partial_y+\frac{m\omega_c}{2\hbar}(y-ix)\right\}\Bigg]|\psi_2\rangle=\varepsilon|\psi_1\rangle,
\end{aligned} \tag{3.6}$$

$$\begin{aligned}
&\Bigg[-\frac{\hbar^2}{2m}\left(\partial_x^2+\partial_y^2+\partial_z^2\right)+\frac{1}{8}m\omega_c^2\left(x^2+y^2\right)-\frac{i\hbar\omega_c}{2}\left(-y\partial_x+x\partial_y\right)+V(x,y,z)\\
&+eE_z z+\frac{1}{2}g_0\mu_\mathrm{B}B\sigma_z\Bigg]|\psi_2\rangle+\Bigg[\alpha_\mathrm{R}eE_z\{-\partial_x+i\partial_y+\frac{m\omega_c}{2\hbar}(x+iy)\},\\
&+\alpha_\mathrm{D}\left\{-i\partial_x+\partial_y+\frac{m\omega_c}{2\hbar}(y+ix)\right\}\Bigg]|\psi_1\rangle=\varepsilon|\psi_2\rangle,
\end{aligned} \tag{3.7}$$

where $\omega_c = eB/m$.

We now turn to the calculation of the phonon induced spin relaxation rate at absolute zero temperature. Following Ref. [18], the interaction between electrons and piezo-phonons can be written as [9, 10, 13, 29]

$$u_{ph}^{\mathbf{q}\alpha}(\mathbf{r},t) = \sqrt{\frac{\hbar}{2\rho V\omega_{\mathbf{q}\alpha}}}\, e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_{q\alpha}t)} eA_{\mathbf{q}\alpha} b_{\mathbf{q}\alpha}^{\dagger} + \mathrm{H.c.} \tag{3.8}$$

Here, ρ is the crystal mass density, V is the volume of the QDs, $b_{\mathbf{q}\alpha}^{\dagger}$ creates an acoustic phonon with wave vector $\mathbf{q}$ and polarization $\hat{e}_\alpha$, where $\alpha = l, t_1, t_2$ are chosen as one longitudinal and two transverse modes of the induced phonon in the dots. Also, $A_{\mathbf{q}\alpha} = \hat{q}_i\hat{q}_k e\beta_{ijk} e_{\mathbf{q}\alpha}^j$ is the amplitude of the electric field created by phonon strain, where $\hat{\mathbf{q}} = \mathbf{q}/q$ and $e\beta_{ijk} = eh_{14}$ for $i \neq k, i \neq j, j \neq k$. The polarization directions of the induced phonon are $\hat{e}_l = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$,

$\hat{e}_{t_1} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)$ and $\hat{e}_{t_2} = (-\sin\phi, \cos\phi, 0)$. Based on the Fermi Golden Rule, the phonon induced spin transition rate in the QDs is given by [10, 24]

$$\frac{1}{T_1} = \frac{2\pi}{\hbar}\int\frac{d^3\mathbf{q}}{(2\pi)^3}\sum_{\alpha=l,t}|M(\mathbf{q}\alpha)|^2\delta\left(\hbar s_\alpha\mathbf{q} - \varepsilon_f + \varepsilon_i\right), \tag{3.9}$$

where s_l,s_t are the longitudinal and transverse acoustic phonon velocities in QDs. Under the dipole approximation, we write (3.9) as [10, 25]

$$\frac{1}{T_1} = c\left(|M_x|^2 + |M_y|^2 + |M_z|^2\right), \tag{3.10}$$

where

$$c = \frac{2(eh_{14})^2\left(\varepsilon_f - \varepsilon_i\right)^3}{35\pi\hbar^4\rho}\left(\frac{1}{s_l^5} + \frac{4}{3}\frac{1}{s_t^5}\right), \tag{3.11}$$

$$M_x = \langle\psi_i|x|\psi_f\rangle, \tag{3.12}$$

$$M_y = \langle\psi_i|y|\psi_f\rangle, \tag{3.13}$$

$$M_z = \langle\psi_i|z|\psi_f\rangle. \tag{3.14}$$

In the above expression, we use $c = c_l I_{xl} + 2c_t I_{xt}$, where $c_\alpha = \frac{q^2e^2}{(2\pi)^2\hbar^2 s_\alpha}|\varepsilon_{q\alpha}|^2$, $|\varepsilon_{q\alpha}|^2 = \frac{q^2\hbar}{2\rho\omega_{q\alpha}}$. For longitudinal phonon modes similar to Refs. [7, 10], we have $|A_{q,l}|^2 = 36h_{14}^2\cos^2\theta\sin^4\theta\sin^2\phi\cos^2\phi$. Likewise, for transverse phonon modes, we have $|A_{q,t}|^2 = 2h_{14}^2[\cos^2\theta\sin^2\theta + \sin^4\theta\left(1 - 9\cos^2\theta\right)\sin^2\phi\cos^2\phi]$.

3.3 Computational Method

The geometry of GaAs conical QDs with wetting layer is shown in Fig. 3.1. The QDs are surrounded by host barrier material $Al_{0.3}Ga_{0.7}As$. We diagonalize the total Hamiltonian H using the finite-element method [4]. In typical examples reported here, the geometry contains on the order of 56729 elements. We impose Dirichlet boundary conditions at the outside boundaries to let the wavefunction to vanish and Neumann boundary conditions at the internal boundaries to let the wavefunction to follow continuity equation. Then we find eigenvalues and eigenfunctions by solving two coupled equations (3.6) and (3.7).

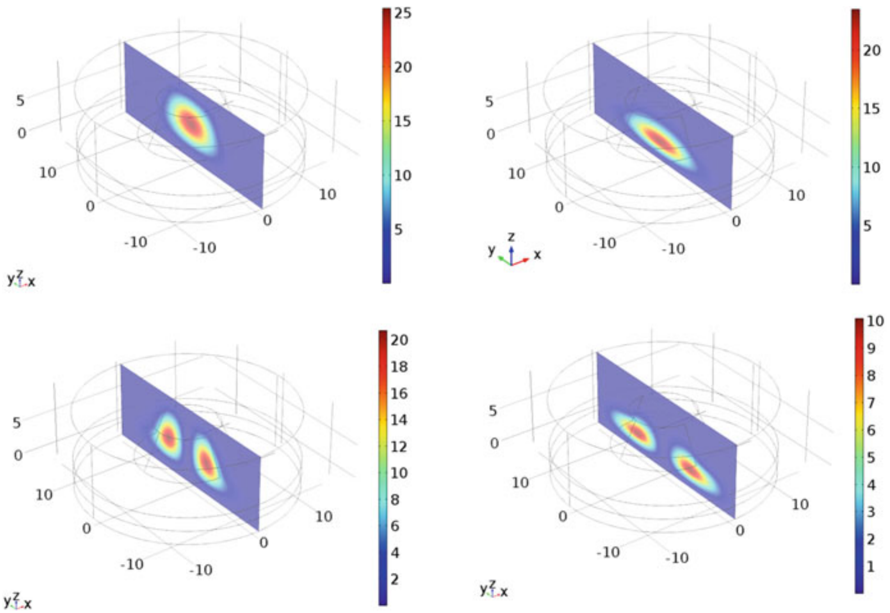

Fig. 3.1 Illustration of ground state wavefunctions (*upper panel*) and first excited state wavefunctions (*lower panel*) of electrons in GaAs/AlGaAs QDs. *Left column* QD wavefunctions correspond to the externally applied electric field, $E_z = 0.001$ V/nm, while *right column* QD wavefunctions correspond to the externally applied electric field, $E_z = 0.1$ V/nm. Evidently, penetration of wavefunctions from the QD region to the barrier materials leads to the variation in the Lande g-factor of electrons that can be utilized to design spintronic devices for security and quantum information processing

3.4 Results and Discussions

In Fig. 3.1, we have plotted probability distribution, $|\psi_1|^2 + |\psi_2|^2$ (arbitrary unit) of ground (upper panel) and first excited state (lower panel) wavefunctions of electron at $E_z = 0.001$ V/nm (left panel) and $E_z = 0.1$ V/nm (right panel). As we can see, the penetration of electron wavefunctions into the barrier material is enhanced for larger values of the applied electric field along z-direction. This leads to the variation in the effective g-factor (see also Fig. 3.3) of electrons in GaAs/$Al_{0.3}Ga_{0.7}As$ QDs that can be utilized to design quantum logic gates for applications in security and quantum information processing. In Fig. 3.2, we have plotted a cross section along z-direction of the edge potential and probability distribution ($|\psi_1|^2 + |\psi_2|^2$) of ground state

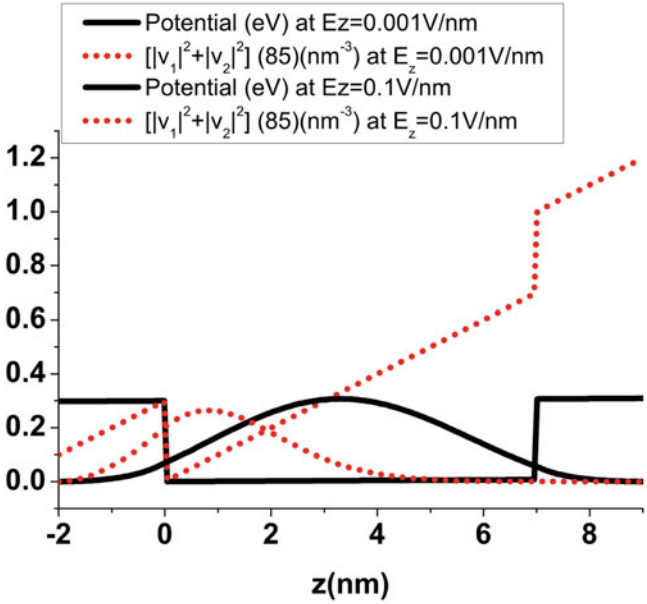

Fig. 3.2 Conduction band edge and its corresponding normalized wavefunctions vs distance from $GaAs/Al_{0.3}Ga_{0.7}As$. Again, penetration of wavefunctions in the barrier material at large electric fields can be seen (also see Ref. [8])

wavefunctions of electrons at $E_z = 0.001\,\mathrm{V/nm}$ (left panel) and $E_z = 0.1\,\mathrm{V/nm}$ (right panel). Here we again see that the penetration of electron wavefunctions into the barrier material is enhanced for larger values of the applied electric field along z-direction (for experiment results, see Ref. [8]). In Fig. 3.3 (upper panel), we have plotted the effective g-factor, $g = (\varepsilon_1 - \varepsilon_2)/\mu_B B$ of electron vs magnetic fields. Here, the variation of effective g-factor of electrons in quantum dots with electric field can be seen and can be applied to make quantum logic gates for application in spintronic devices. At large magnetic fields, we find the level crossing due to admixture of spin and orbital states (see lower panel of Fig. 3.3). In Fig. 3.4, we have plotted piezo-phonon mediated spin and orbital relaxation vs magnetic fields in $GaAs/Al_{0.3}Ga_{0.7}As$ QDs at $E_z = 0.1\,\mathrm{V/nm}$. We see that the relaxation rate is enhanced with magnetic fields and can approach to the orbital relaxation rate at large magnetic fields where the decoherence time is greatly reduced due to the level crossing of orbital and spin states. Such an ideal location should be avoided during the design of spintronic devices for application in security and quantum information processing (Table 3.1).

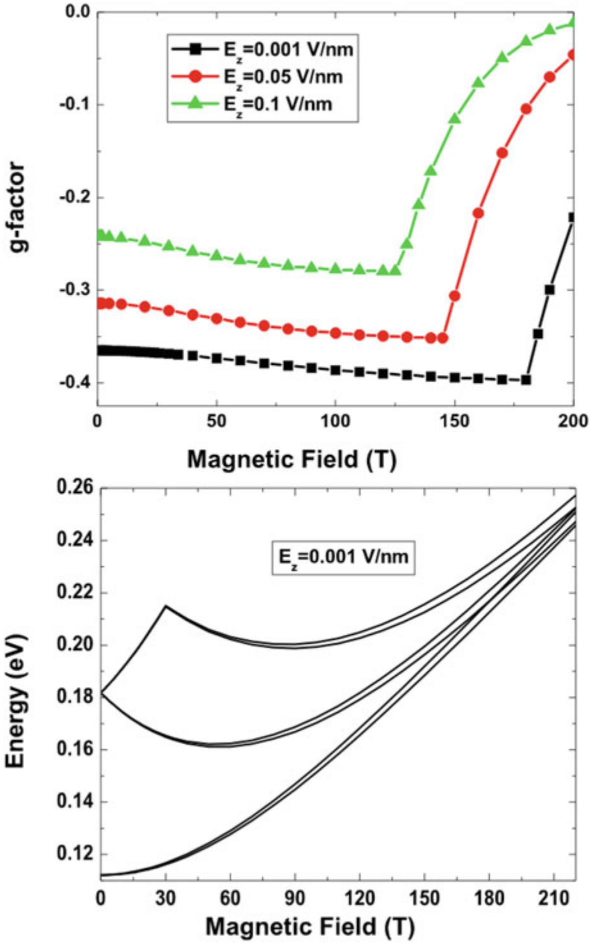

Fig. 3.3 (*upper*) Electron effective g-factor vs magnetic field in $GaAs/Al_{0.3}Ga_{0.7}As$ QDs. Level crossing can be observed at large magnetic fields which vary with the applied external electric fields along z-direction. (*lower*) Band diagram of electron in $GaAs/Al_{0.3}Ga_{0.7}As$ QDs vs magnetic field. The band crossing is seen at large magnetic field, $B \approx 185\,\mathrm{T}$

3.5 Conclusion

Based on finite element implementation, we have provided three-dimensional modeling results for the tuning of the effective g-factor of electrons with spin orbit coupling in $GaAs/Al_{0.3}Ga_{0.7}As$ QDs and shown that the level crossing can be observed at large magnetic fields due to the admixture of spin and orbit states. We also estimated the relaxation rate caused by piezo-phonon and shown that the spin-hot spot can be observed at the level crossing point. Decoherence time is greatly reduced at the level crossing point. Thus, We suggest to avoid such an ideal location in the design of GaAs based QD devices for possible applications in spintronics, security, encrypted data and quantum information processing.

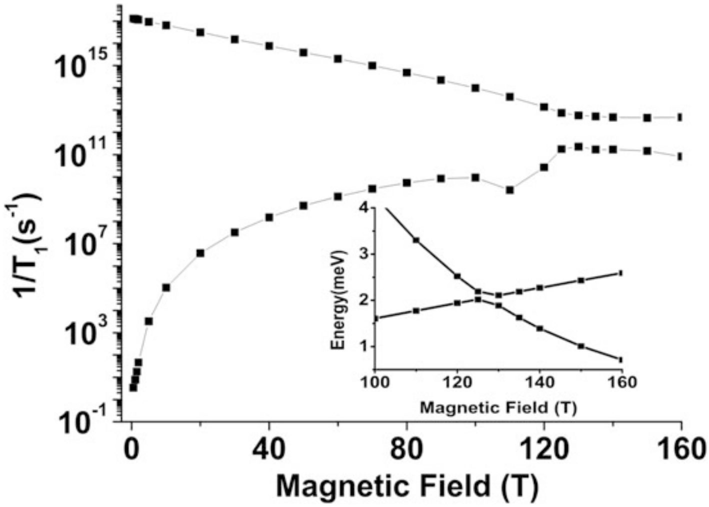

Fig. 3.4 Piezo-phonon mediated spin relaxation vs magnetic fields in $GaAs/Al_{0.3}Ga_{0.7}As$ QDs at $E_z = 0.1\,V/nm$

Table 3.1 The material constants used in our calculations are taken from Refs. [19, 26, 28]

Parameters	GaAs	$Al_{0.3}Ga_{0.7}As$
g_0	-0.44	0.4
m	$0.067m_0$	$0.088m_0$
α_R [nm^2]	0.044	0.022
α_D [eVnm^3]	0.026	0.0076
eh_{14} [10^{-5} erg/cm]	2.34	0.54
s_l [10^5 cm/s]	5.14	
s_t [10^5 cm/s]	3.03	
ρ [g/cm^3]	5.3176	

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