

**Multiphysics effects and electronic properties of anisotropic
semiconductor quantum dots**

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Multiphysics Effects and Electronic Properties of Anisotropic Semiconductor Quantum Dots

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Abstract—In this paper we analyze a number of important coupled effects in semiconductor quantum dots with multiband models, including magneto-electromechanical coupling. We also demonstrate that the Rashba spin-orbit coupling may provide appreciable contributions to electronic properties of quantum dots by focusing on gate-controlled electron spins in quantum dots. In particular, we analyze the properties of anisotropic semiconductor quantum dots formed in the conduction band in the presence of the magnetic field. For this case, we formulate the Kane-type model and based on it we study the properties of dots by using both analytical and finite element techniques. It is shown that that in semiconductor quantum dots, the electron spin states in the phonon-induced spin-flip rate can be manipulated with the application of externally applied anisotropic gate potentials. The spin flip rates can be enhanced by such potentials, which can also reduce the level crossing points to lower quantum dot radii. We provide numerical examples providing further insight into these new findings where it is evident that these observed effects are due to the suppression of the g-factor towards bulk crystal. Based on these findings, the phonon induced spin-flip rate can be controlled through the application of spin-orbit coupling. Other coupled effects that affect the electronic properties of quantum dots are also discussed.

Keywords—Low dimensional nanostructures, quantum dots, coupled multiphysics effects, electron-phonon coupling, finite element method, electromechanics, band structure calculations, quantum-continuum coupling.

I. INTRODUCTION

A number of coupled multiphysics effects, such as electromechanical, can be used as tuning parameters for the optical response of low dimensional nanostructures, examples of which include quantum wires, rods, and dots. The latter objects have applications in diverse areas from photonics, optoelectronics and band gap engineering to biotechnological applications and medical engineering.

Although in the recent years some coupled effects, e.g. piezoelectric, have often been included in the studies of properties of low dimensional nanostructures, the influence of coupled magneto-thermo-electromechanical effects has barely been included in such studies. This often needs to be supplemented by accounting for the Rashba spin-orbit coupling that can be used as a key parameter in controlling the electron spin in low dimensional nanostructures and, as a result, can

profoundly influence their properties. Both of these contributions in the analysis of electronic properties of low dimensional nanostructures are considered in this paper (see details of the related models also in [1], [2]).

In our studies we focus on the so-called 0-dimensional nanostructures or quantum dots (QDs) where we consider several important examples (including, e.g., ferroelectric, piezomagnetic, and magnetoelectric nanostructures [2]). Based on these examples, we have analyzed the influence of magneto-thermo-electromechanical effects by using the fully coupled quantum-continuum models implemented via finite element methodology. In particular, we have shown that the influence of the mentioned coupled effects can be significant within the general fully coupled framework we developed. We have quantified this influence in each of the above three cases.

We note that a special consideration deserves the influence of thermal effects which are commonly neglected in similar studies in the literature [3]. There is a reason for that. Indeed, if we take magnetic quantum dots (in particular, GaN/BaTiO₃), we have confirmed that the influence of electromechanical effects on the band structure calculations (and hence on the electronic properties of these nanostructures) and the spin splitting energy are practically independent of temperature. Nevertheless, we have also demonstrated that in piezoelectric quantum dots (in particular, AlN/GaN), the influence of temperature on the electromechanical effects, electronic properties and spin splitting energy is significant. One of the observations is that in such piezoelectric quantum dots, the energy difference between ground and first excited state decreases with the increase of temperature.

Finally, we would like also to highlight our results on the spin splitting energy of ground and first excited states through the application of magnetic fields for several types of quantum dots with and without wetting layers. An interesting novel finding is that in the presence of wetting layers in the quantum dots, Kramer's degenerate eigenvalues and spin splitting energy occur at lower levels. Moreover, the divergence in the Zeeman spin splitting energy increases with the increase in magnetic field due to the Rashba spin-orbit coupling in both cases: quantum dots with wetting layers and without wetting layers. The calculated g-factor provides further insight into the issues discussed here.

A. Electron Spin States in Gated Quantum Dots

Recently, electron spin states in gated QDs in presence of magnetic fields along arbitrary direction have been measured experimentally [4]. The authors in Refs. [5], [6] by applying both computational and theoretical techniques, have shown that the spin-orbit coupling can be used as a control parameter in the electric/magnetic field tunability of the electron g-factor tensor. Long spin relaxation times have also been measured experimentally in both GaAs and InGaAs QDs by these authors.

These spin-flip rate measurements in QDs confirm theoretical predictions of the suppression of the phonon induced spin-flip rate by spin-orbit coupling with respect to the environment [7], [8], [9].

In the reminder of this paper, we focus on the anisotropic orbital effect on the phonon induced spin-flip rate for InAs quantum dots. Based on both theoretical and finite element numerical simulation methods, we find that the anisotropic potential enhances the spin flip rate and reduces the level crossing point to a lower quantum dot radius. Also we find that the anisotropic potential reduces the variation in the g-factor towards bulk crystal.

II. MATHEMATICAL MODEL

We consider 2D anisotropic semiconductor QDs formed in the conduction band in the presence of magnetic field B along z-direction. The total Hamiltonian $H = H_{xy} + H_{so}$ of an electron in the conduction band under the Kane model [10], [11] can be written as

$$H_{xy} = \frac{\vec{P}^2}{2m} + \frac{1}{2}m\omega_0^2(ax^2 + by^2) + \frac{\hbar}{2}\sigma_z\omega_z, \quad (1)$$

$$H_{so} = \frac{\alpha_R}{\hbar}(\sigma_x P_y - \sigma_y P_x) + \frac{\alpha_D}{\hbar}(-\sigma_x P_x + \sigma_y P_y), \quad (2)$$

$$\alpha_R = \gamma_R e E, \quad \alpha_D = 0.78\gamma_D \left(\frac{2me}{\hbar^2}\right)^{2/3} E^{2/3}, \quad (3)$$

where $\vec{P} = -i\hbar\nabla + e\vec{A}$ is the 2D electron momentum operator in the asymmetric gauge $\vec{A} = \frac{B}{\sqrt{a+b}}(-y\sqrt{b}, x\sqrt{a}, 0)$ and $\omega_z = g_0\mu_B B/\hbar$ is the Zeeman frequency. Also, m is the effective mass, μ_B is the Bohr magneton, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli spin matrices, $\omega_0 = \frac{\hbar}{m\ell_0^2}$ is the strength of the parabolic confining potential with quantum dot radius ℓ_0 . From Eq. 3, it can be calculated that the strength of the Rashba and Dresselhaus spin-orbit coupling becomes equal at the electric field, $E \approx 3 \times 10^3$ V/cm for InAs quantum dots. However, at this value of electric field, the rotational symmetry is not broken and the spin splitting energy mainly corresponds to the Zeeman spin splitting energy. Above this value of the electric field, only Rashba spin-orbit coupling has an appreciable contribution to the manipulation of spin states in quantum dots via the g-factor tensor and phonon induced spin flip rate.

We now turn to the calculation of the phonon induced spin relaxation rate in between two lowest energy states in QDs. The interaction between electron and piezo-phonon can

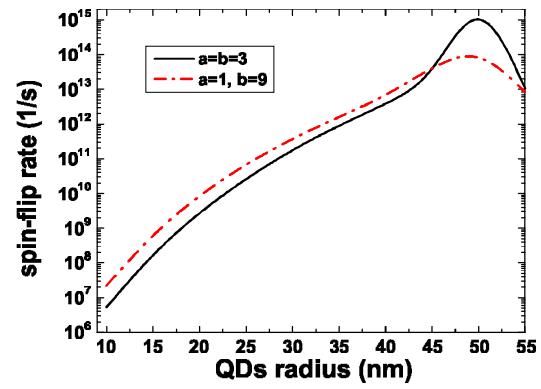


Fig. 1. (Color online) Phonon induced spin-flip rate due to spin-orbit admixture mechanism as a function of QDs radius. We choose the potentials characterized by $a = b = 3$ for symmetric QDs (solid line) and $a = 1$ & $b = 9$ for asymmetric QDs (dashed-dotted line). Also we choose $B = 1$ T and $E = 7 \times 10^5$ V/cm. The material constants for InAs QDs are chosen from Refs. [13] as $g_0 = -15$, $m = 0.0239$, $\gamma_R = 110$ Å², $\gamma_D = 130$ eVÅ³, $eh_{14} = 0.54 \times 10^{-5}$ erg/cm, $s_l = 4.2 \times 10^5$ cm/s, $s_t = 2.35 \times 10^5$ cm/s and $\rho = 5.6670$ g/cm³.

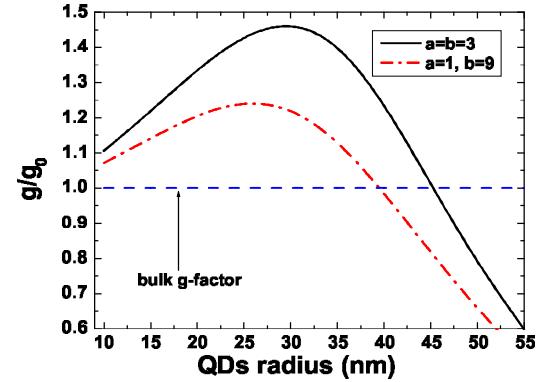


Fig. 2. (Color online) g-factor vs. QDs radius at the potentials characterized by $a = b = 3$ (solid line) for isotropic QDs and $a = 1, b = 9$ (dashed-dotted line) for anisotropic QDs. We choose $E = 7 \times 10^5$ V/cm and $B = 1$ T.

be written as [8], [11], [12]

$$u_{ph}^{\mathbf{q}\alpha}(\mathbf{r}, t) = \sqrt{\frac{\hbar}{2\rho V\omega_{\mathbf{q}\alpha}}} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}\alpha}t)} e^{A_{\mathbf{q}\alpha} b_{\mathbf{q}\alpha}^\dagger} + H.c. \quad (4)$$

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}_α , 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

ransition rate in the QDs is given by [13], [11]

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} \int \frac{d^3 q}{(2\pi)^3} \sum_{\alpha=l,t} |M(q\alpha)|^2 \delta(\hbar s_\alpha q - \Delta), \quad (5)$$

where s_l, s_t are the longitudinal and transverse acoustic phonon velocities in QDs. The matrix elements $M(q\alpha)$ for the spin-flip rate between the Zeeman sublevels with the emission of phonon $q\alpha$ have been calculated perturbatively [11], [14]. Also $\Delta = E_2 - E_1$ is the energy difference between the two lowest states in the quantum dots including spin-orbit coupling.

III. RESULTS AND DISCUSSIONS

In Fig. 1, we quantify the influence of anisotropic gate potentials on the phonon induced spin-flip rate as a function of quantum dot radius in both symmetric and asymmetric InAs QDs. It can be seen that the anisotropic potential ($a = 1, b = 9$) enhances the spin-flip rate compared to that of symmetric potentials ($a = b = 3$). Note that we chose the above confining potentials in such a way that the areas of the symmetric and asymmetric QDs are held constant.

The level crossing takes into account, due to mixing, the Zeeman spin states $|0, 0, -\rangle$ and $|0, 1, +\rangle$ in QDs. The level crossing point, determined by the condition $\hbar(\omega_+ - \omega_-) = |g_0|\mu_B B$, for anisotropic QDs is smaller than for the case of isotropic QDs (given that the area of the QDs in both cases is constant). By applying both theoretical and numerical methods in Fig. 1, we report that the anisotropic potential in the spin-flip rate reduces the level crossing point to a smaller QD radius.

In Fig. 2, we study the g -factor vs quantum dot radius in both isotropic and anisotropic quantum dots. It can be seen that the anisotropic potential reduces the variation in the g -factor towards bulk crystal (see dashed-dotted line) compared to isotropic quantum dots (see solid line). This tells us that the anisotropic potential leads to the quenching effect in the orbital angular momentum [15] that pushes the g -factor of an electron towards the bulk crystal.

IV. CONCLUSIONS

To conclude, we have provided details on some of the most important coupled effects that affect electronic properties of anisotropic semiconductor quantum dots. This includes magneto-electromechanical effects and spin-orbit coupling. We have also shown that the electron spin states in the phonon induced spin-flip rate can be manipulated with the application of externally applied anisotropic gate potentials in QDs. The anisotropic potential causes the reduction of the g -factor towards bulk crystal that causes the enhancement of the spin-

flip rate and reduces the level crossing point to a lower QD radius. The phonon induced spin-flip rate can be tuned with the application of the Rashba spin-orbit coupling in QDs.

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