Phonon modulation of the spin-orbit interaction as a spin relaxation mechanism in quantum dots

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We calculate the spin relaxation rates in a parabolic InSb quantum dot due to the spin interaction with acoustical phonons. We considered the deformation potential mechanism as the dominant electron-phonon coupling in the Pavlov-Firsov spin-phonon Hamiltonian. By studying suitable choices of magnetic field and lateral dot size, we determine regions where the spin relaxation rates can be practically suppressed. We analyze the behavior of the spin relaxation rates as a function of an external magnetic field and mean quantum dot radius. Effects of the spin admixture due to Dresselhaus contribution to spin-orbit interaction are also discussed.

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I. INTRODUCTION

The ability to manipulate and control processes that involve transitions between spin states is, at the moment, of extreme importance due to the recent applications in polarized spin electronics and quantum computation. Spin dephasing is the most critical aspect that should be considered in the elaboration of proposals of quantum computation based on single spin states as qubits in quantum dots (QDs). Currently, QDs of diverse geometries are considered as promising candidates for implementation of quantum computation devices because the electronic, magnetic, and optical properties can be controlled through the modern growth and nanofabrication techniques. Due to the long electron spin dephasing time experimentally reported,²⁻⁴ the spin of an electron localized in a QD has been suggested to realize a quantum bit. While for bulk and for two-dimensional (2D) systems the spin relaxation processes have been studied in some detail, the problem for QDs still requires deeper and further discussions. Several processes that can induce spin relaxation in semiconductors have been identified and were studied. At the moment, what remains in discussion is which between these processes is dominant in zero-dimensional systems. Some experimental results have shown good agreement with the theoretical predictions for 2D systems⁵ but, in general, the identification of the processes through direct comparison with the experimental results may become a formidable task. This problem is more critical for QDs, since few experimental results exist and the theoretical discussion of the spin relaxation mechanisms is still an open subject. Extensive theoretical works in QD systems have studied the main phonon mediated spin-flip mechanisms, including admixture processes due to spin-orbit coupling⁶ and phonon coupling due to interface motion (ripple mechanism). Spin relaxation rates depend strongly on the dot size, magnetic field strength, and temperature, as reported by several authors.^{6,8} It was shown that the quantum confinement produces, in general, a strong reduction of the QD relaxation rates.

In this work, we calculate the spin-flip transition rates, considering the phonon modulation of the spin-orbit interaction. For this purpose, we will use the spin-phonon interaction Hamiltonian proposed by Pavlov and Firsov. 9,10 In this model, the Hamiltonian describing the transitions with spin reversal, due to the scattering of electrons by phonons, can be written in a general form as

$$H_{ph} = V_{ph} + \gamma [\sigma \times \nabla V_{ph}] \cdot (\mathbf{p} + e/c\mathbf{A}), \tag{1}$$

where V_{ph} is the phonon operator, σ is the Pauli spin operator, γ is related to the strength of the electron-phonon interaction, $\bf p$ is the linear momentum operator, and $\bf A$ is the vectorial potential related to the external magnetic field $\bf B$. This model has the advantage of being easily adapted to the study of other interaction mechanisms with phonons.

II. THEORY

Based on the effective mass theory applied to the problem of the interaction of an electron with lattice vibrations, including the spin-orbit interaction and in the presence of an external magnetic field, Pavlov and Firsov^{9,10} have obtained the spin-phonon Hamiltonian that describes the transitions with spin reversal of the conduction band electrons due to scattering with longitudinal lattice vibrations as

$$H_{ph} = d(\mathbf{q}) \left(\frac{\hbar}{\rho_M V v q} \right)^{1/2} \times \left\{ e^{i\mathbf{q} \cdot \mathbf{r}} b_{\mathbf{q}} \begin{bmatrix} 0 & \hat{\mathbf{n}}^- \times \hat{\mathbf{e}}_{\mathbf{q}} \\ \hat{\mathbf{n}}^+ \times \hat{\mathbf{e}}_{\mathbf{q}} & 0 \end{bmatrix} \left(\frac{\mathbf{p}}{\hbar} + \frac{e\mathbf{A}}{\hbar c} + \mathbf{q} \right) + \text{H.c.} \right\},$$
(2)

where $b_{\mathbf{q}}$ ($b_{\mathbf{q}}^{\dagger}$) are annihilation (creation) phonon operators, and the magnetic vector potential \mathbf{A} is obtained in the symmetric gauge considering an external magnetic field \mathbf{B} oriented along the z axis. $\hat{\mathbf{n}}^{\pm} = \hat{\mathbf{x}} \pm i\hat{\mathbf{y}}$, where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unitary

vectors along the x and y axis. $\hat{\mathbf{e}}_q$ is a unit vector in the direction of the phonon polarization, \mathbf{q} is the phonon wave vector, \mathbf{p} is the momentum operator, v is the average sound velocity, ρ_M is the mass density, V is the system volume, and $d(\mathbf{q})$ is a deformation potential electron-phonon coupling constant \mathbf{q}

$$d(q) = \frac{\hbar^2 q^2}{2m^*} \frac{E_0}{E_g} \left(1 - \frac{m^*}{m_0} \right) f\left(\frac{E_g}{\Delta}\right), \tag{3}$$

where E_g =0.17 eV is the band gap for InSb, the electron effective mass m^* =0.013 m_0 , E_0 =7.0 eV is the deformation potential, Δ =0.81 eV is the spin-orbit splitting of the valence band, and f(x)=(1+2x)/[(1+ $\frac{3}{2}x$)(1+x)].

According to Eq. (2), we will restrict ourselves to the case of *bulk* phonon modes. The longitudinal acoustic phonons are described by plane waves of the form $\mathbf{u}_0\hat{\mathbf{e}}_q\exp^{i\mathbf{q}\cdot\mathbf{r}}$, where \mathbf{u}_0 is the normalization constant. We consider the phonon energy dispersion in the Debye approximation: $E_q = \hbar vq$, for InSb we use $v = 3.4 \times 10^3$ m/s. It is important to point out that the theoretical treatment of the spin-phonon interaction developed by Pavlov and Firsov^{9,10} can be easily adapted to several electron-phonon interaction processes. An appropriate choice of the electron-phonon coupling $d(\mathbf{q})$ allows us to adapt the transition matrix elements related to the Hamiltonian (2) for piezoacoustic or LO spin scattering.

$$f_{n,M,\sigma} = C_{n,M} \frac{\rho^{|M|}}{a^{|M|+1}} e^{-\rho^2/2a^2} e^{iM\varphi} L_n^{|M|} \left(\frac{\rho^2}{a^2}\right) \chi(\sigma), \tag{4}$$

where $C_{n,M} = \sqrt{n!/[\pi(n+|M|)!]}$, $L_n^{|M|}$ is the Laguerre polynomial, n (M) is the principal (azimuthal) quantum number, and $\chi(\sigma)$ is the spin wave function for the spin variable σ . The corresponding eigenenergies are

$$E_{n,M,\sigma} = (2n + \left| M \right| + 1)\hbar\Omega + (M/2)\hbar\omega_c + (\sigma/2)g\mu_B B, \eqno(5)$$

where $\Omega = (\omega_0^2 + \omega_c^2/4)^{1/2}$, μ_B is the Bohr magneton, $a = (\hbar/m\Omega)^{1/2}$ is the effective length, $\sigma = \pm 1$ for spin up and down, respectively, and $\omega_c = eB/m$.

In our model, we also consider the effects of the Dresselhaus contribution that provides additional admixture between spin states. For 2D systems, the linear Dresselhaus Hamiltonian can be written as

$$H_D = \frac{\beta}{\hbar} (\sigma_x p_x - \sigma_y p_y), \tag{6}$$

where $p_i = -i\hbar \nabla_i + (e/c)A_i$, with i=x,y, and β is the Dresselhaus coupling parameter for this confinement. If the confinement potential in the z direction is considered highly symmetrical, then $\nabla V_z \sim 0$ and the Rashba contribution can be safely ignored.

The spin relaxation rates (W) between the electronic states $(n,M,\uparrow(\downarrow)) \rightarrow (n',M',\downarrow(\uparrow))$, with emission of one acoustic phonon, are calculated from the Fermi golden rule.

In the Hamiltonian (2), we only consider the deformation potential electron-phonon coupling; this is due to the large g factor in narrow gap InSb ($|g| \sim 51$). The dominant electron-phonon coupling for spin relaxation is the deformation potential mechanism. The piezoelectric coupling governs the spin relaxation processes in wide or intermediate gap semi-conductors. In the transition matrix elements calculation, we not only consider the linear term $i\mathbf{q} \cdot \mathbf{r}$ in the expansion of $\exp(i\mathbf{q} \cdot \mathbf{r})$, but also the integral representation of Bessel function is used in the evaluation of electron-phonon overlap integrals. The linear approximation of $\exp(i\mathbf{q} \cdot \mathbf{r})$ may be valid for spin inversion transitions in the spin polarized ground states of GaAs based QDs where, due to the small value of the electron g factor, only long wavelength phonons are involved.

III. RESULTS AND DISCUSSION

The calculations were performed for a parabolic InSb QD at $T \sim 0$ K. The material parameters for the InSb system are listed in Ref. 13. We only have considered electron transitions between ground state electron Zeeman levels $(0,0,\uparrow) \rightarrow (0,0,\downarrow)$ and $(0,1,\downarrow) \rightarrow (0,1,\uparrow)$. The temperature dependence for one-phonon emission rate is determined from $W=W_0(n_B+1)$, where n_B is the Bose-Einstein distribution function and W_0 is the rate at T=0 K. In the temperature regime $T \leq 10$ K, we obtain $n_B+1 \approx 1$ and $W \approx W_0$. For temperatures larger than a few Kelvin degrees (T>10 K), two-phonon processes become the dominant spin relaxation mechanism. These types of processes have not been considered in the present calculation.

In Fig. 1, we show the spin relaxation rates due to deformation potential electron-phonon mechanism, as a function of the external magnetic field B and considering some typical values for the effective lateral QD size, $r_0 = \sqrt{\hbar/m\omega_0}$.

Some interesting facts about these results should be pointed out:

(i) The rates show a strong dependence with the magnetic field. This fact can be explained from the dependence of the rates with the transition energy ΔE . In general, we obtain that $W \sim [g^* \mu_B B]^n = (\Delta E)^n$, n being an integer number that depends on the electron-phonon coupling process and g^* the effective g factor. As can be seen in Fig. 1, when the magnetic field increases, the rates also increase until a maximum near $B \sim 0.5$ T is reached. The position of this main maximum is defined from the transition energy conservation: $E_{nl\sigma'} - E_{n'l'\sigma'} = \hbar v q$.

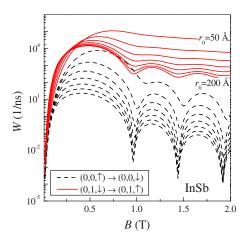
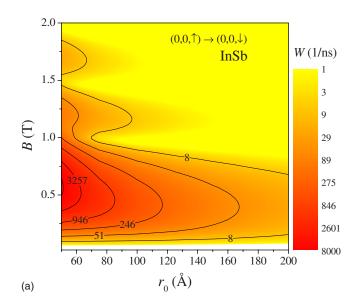


FIG. 1. (Color online) Spin relaxation rates W for a parabolic InSb QD considering the deformation potential coupling mechanism as a function of the magnetic field B. We consider the transitions $(0,0,\uparrow) \rightarrow (0,0,\downarrow)$ and $(0,1,\downarrow) \rightarrow (0,1,\uparrow)$, and several lateral dot radii r_0 =50, 75, 100, 125, 150, 175, and 200 Å (same r_0 ordering for both transitions).

(ii) The oscillatory behavior of the rates, observed for B>0.7 T, are mainly produced by the complex interplay between the spin admixture and electron-phonon overlap integrals. The phonon modulated Rashba interaction, given in Eqs. (1) and (2), produces level admixture according to the selection rules: $(n,M,\uparrow) \rightarrow (n,M+1,\downarrow)$, $(n,M,\downarrow) \rightarrow (n,M-1,\uparrow)$, and $(n,M,\uparrow(\downarrow)) \rightarrow (n,M,\downarrow(\uparrow))$. The last condition, which hybridizes states with different spin orientations at the same level M, is mainly responsible for the rate oscillations at B>0.7 T. For $\Delta M=0$ transitions, the Dresselhaus spin-orbit interaction, given in Eq. (6), is not able to produce spin admixture.

As it is shown in Fig. 1, the g^* -factor effects are particulary important for the ground-state Zeeman transition. For small magnetic fields, $g^* \rightarrow g_{\text{bulk}}$ and we may neglect the spin admixture effects. Therefore, the spin relaxation shows no oscillations and becomes almost independent of r_0 . This small QD size dependence is in agreement with the experimental observations of Gupta $et\ al.^{14}$

- (iii) The rate's dependence on the lateral QD size r_0 is related to the interplay effects between the spatial and magnetic confinements. These competing effects are contained in the electron-phonon overlap integral, $I \propto \int f_{n',l',\sigma'}^*(\rho) \exp(i\mathbf{q} \cdot \mathbf{r}) f_{n,l,\sigma}(\rho) d\mathbf{r}$. For large fields, the magnetic confinement causes a gradual decrease in the overlap integral as the r_0 increases. For small magnetic fields, the spatial confinement is dominant. Thus, when r_0 diminishes, the wave functions become more localized and the overlap integral should increase. This effects explain the behavior of the spin transition $(0,1,\downarrow) \rightarrow (0,1,\uparrow)$ shown in Fig. 1 (red lines). The Zeeman ground-state rates (black lines) are strongly dependent on ΔE and, for small B, the rates are weakly dependent on I.
- (iv) The same rates calculated for GaAs (not shown here) are, in general, 1 order of magnitude smaller than InSb rates. As we expected, the relaxation via piezoelectric coupling is more efficient than via the deformation potential phonon processes.



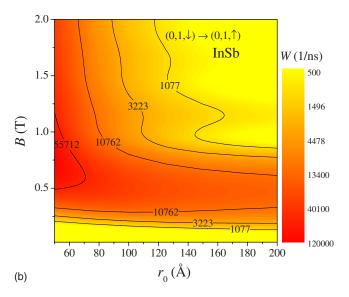


FIG. 2. (Color online) Contour plot of the spin relaxation rates as a function of magnetic field B and lateral size r_0 for transitions (a) $(0,0,\uparrow) \rightarrow (0,0,\downarrow)$ and (b) $(0,1,\downarrow) \rightarrow (0,1,\uparrow)$.

In Fig. 2(a), we have plotted the spin relaxation rates for the ground-state Zeeman transition as a function of r_0 and B. We clearly identify a region of strong spin coherence, defined by B > 1 T and $r_0 > 100$ Å. In this regime, the relaxation times τ are in the nanosecond order, and this is an important feature for spin qubit engineering. In the B < 0.1 T regime, the relaxation times are approximately a few microseconds. This spin frozen region is not robust against the temperature and will disappear whenever the thermal energy is larger than the spin transition energy. The plot in Fig. 2(b) shows the spin rates for $(0,1,\downarrow) \rightarrow (0,1,\uparrow)$ transition. As in the previous case, the strong coherence regime is defined approximately by B > 1 T and $r_0 > 100$ Å. However, the relaxation times, in this region, are 2 orders of magnitude faster than for $(0,0,\uparrow) \rightarrow (0,0,\downarrow)$ transition.

In conclusion, in this work we presented the calculation of spin relaxation rates via electron-phonon interaction. The model used in our work allows us to estimate the magnitude of the scattering rates considering the most important contributions to the spin relaxation through acoustic deformation potential interaction. The rates exhibit a strong dependence on the magnetic field and on the lateral QD size. We identify regimes of strong spin coherence; for magnetic field B > 1 T and for lateral sizes $r_0 > 100$ Å, we obtain relaxation times approximately $10^{-2} - 1.0$ ns. The Zeeman ground-state transition $(0,0,\uparrow) \rightarrow (0,0,\downarrow)$ exhibits longer spin coherence times than the high energy transitions, which is important for spin qubit applications. The magnitudes of the calculated rates are compatible with those obtained experimentally. For a more rigorous analysis of the spin relaxation process, many

other effects should be considered, like the anisotropy of the electron g factor and the effects of the spatial confinement on the acoustic phonons. These two issues are still under intense discussion and should be considered for a more precise determination of the spin relaxation times.

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