Hole spin relaxation in quantum dots

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We present results for relaxation of the spin of a hole in a cylindrical quantum dot due to acoustic phonon assisted spin flips at low temperatures with an applied magnetic field. The hole dispersion is calculated by numerical diagonalization of the Luttinger Hamiltonian and applying perturbation theory with respect to the magnetic field, and the hole-phonon coupling is described by the Bir-Pikus Hamiltonian. We find that the decoherence time for hole spins for dots ≤20 nm is on the order of $10^{-8}$ s. This is several orders smaller than the decoherence time due to phonon assisted processes for electron spins in similar dots and is comparable to the total decoherence time of an electron spin in a quantum dot, which is controlled by the hyperfine interaction with nuclei. We obtain the dependence of the relaxation rate of the hole spin on dot size and hole mass.

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I. INTRODUCTION

Recently considerable interest has been devoted to developing a theory for the relaxation of an electron spin localized in a quantum dot (QD). The problem is of importance for processing and transferring information coherently in structures of interest for quantum computation. It has been found that two processes are responsible for the loss of coherence of the electron spin. First, phonon assisted spin flips mediated by spin-orbit coupling give relaxation of coherence of the electron spin. In structures of interest for quantum computation. It has been found that two processes are responsible for the loss of coherence of the electron spin. First, phonon assisted spin flips mediated by spin-orbit coupling give relaxation of coherence of the electron spin.

II. VALENCE SUBBANDS AND HOLE-PHONON COUPLING

We consider a quantum dot (QD) obtained by deep etching of an InGaAs/GaAs quantum well. The valence subbands are studied by a standard four-band $\mathbf{k} \cdot \mathbf{p}$ effective-mass approach, which allows us to treat the interaction between light and heavy holes. In the effective-mass $\mathbf{k} \cdot \mathbf{p}$ method the dynamics of the holes is determined by its structure at the zone edge $\mathbf{k}=0$, and only small terms (up to $\mathbf{k}^2$) are present in the Hamiltonian. The total wave function $\Psi_{\mathbf{k}}$ is represented as a product of a Bloch function $\psi_{\mathbf{k}=0}$ and an envelope function $\phi_{\mathbf{k}}$, and therefore $\Psi_{\mathbf{k}} = \sum_{j} \phi_{\mathbf{k}} \psi_{\mathbf{k}=0}$, where $j$ runs over all bands. The basis states $\psi_{\mathbf{k}=0}$ used here have total angular momentum $J=\frac{1}{2}$ with projections $m_J=\pm\frac{1}{2}$ for the heavy holes and $m_J=\pm\frac{1}{2}$ for the light holes. In this basis the Hamiltonian has the form.
which describes the hole band mixing. Here
\[ P \pm Q = - \left( \gamma_1 \pm \gamma_2 \right) \frac{h^2 k_1^2}{2m_0} - \left( \gamma_1 \pm \gamma_2 \right) \frac{h^2 k_z^2}{2m_0}, \tag{2} \]

\[ S = 2 \sqrt{3} \gamma_2 \frac{h^2 k_z k_z}{2m_0}, \tag{3} \]

\[ R = \sqrt{3} \gamma_2 \frac{h^2 k_z^2}{2m_0}. \tag{4} \]

The coupling between the conduction electron and the hole bands is smaller, and it is not included here. We use the spherical approximation for the Luttinger coefficients. For the wave vector the conventions are \( k_z^2 = k_1^2 + k_2^2 \) and \( k_z = i k_y \). The magnetic field \( B \) is along the \( z \) axis, and it enters the Hamiltonian through the diagonal Zeeman terms and through the magnetic-field dependence of \( k = -i \Delta + eA/\hbar \), where \( A \) is the vector potential. A parameter \( \Lambda \) is included representing the spin-independent strain splitting between the heavy- and light-hole bands that originates from a lattice mismatch at the interfaces and it gives rise to the uniaxial strain.

For the structures considered here the three-dimensional confinement can be described by infinite wall potentials in the lateral direction with \( d/2 \) the radius of the dot and a confining potential along the \( z \) direction
\[ V_z = \begin{cases} 0, & |z| \leq c/2 \\ V_0, & |z| > c/2. \end{cases} \tag{5} \]

Here \( V_0 = -69.2 \text{ meV} \) is for the heavy-hole bands, and \( - (69.2 - \Lambda) \text{ meV} \) for the light-hole bands, which are chosen from \( \text{In}_{0.1}\text{Ga}_{0.9}\text{As} \), and \( \Lambda \) is taken to be \( \Lambda = 40 \text{ meV} \) (Ref. 13). The well width \( c \) is chosen to be 5 nm, and the QD is in a cylindrical form.

The hole-phonon interaction including the effects of strain from phonons is given by the Bir-Pikus Hamiltonian. The components of the strain tensor \( \epsilon \) in terms of normal-mode coordinates are
\[ \epsilon_{ij} = \sum_Q \frac{i}{2} \sqrt{\frac{\hbar}{2 \rho \omega_Q}} (Q_i \hat{\eta}_j + Q_j \hat{\eta}_i) e^{iQ \cdot r}. \tag{6} \]

Here \( \rho \) is the mass density of the material, \( Q \) is the phonon wave vector, \( \hat{\eta} \) is the phonon polarization, and \( \omega_Q \) is the phonon frequency.

The form of the hole-phonon interaction is similar to that in Eq. (1) but with matrix elements
\[ \begin{bmatrix} \frac{\hbar^2}{2m_0} \rho \omega_Q (Q_i \hat{\eta}_j + Q_j \hat{\eta}_i) e^{iQ \cdot r} & \epsilon_{ij} \end{bmatrix}, \tag{1} \]

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system has cylindrical symmetry, the Hamiltonian commutes with the operator \( F_z \) of the projection of the total angular momentum \( \mathbf{F} = \mathbf{L} + \mathbf{J} \), where \( \mathbf{J} \) is the Bloch angular momentum and \( \mathbf{L} \) is the envelope angular momentum. \( H_0 \) is diagonalized numerically for a given \( F_z \) using the following basis of envelope functions:

\[
\psi_{F_z=\pm3/2} = \frac{e^{i(F_z \pm 3/2)}}{\sqrt{2\pi}} R_{F_z=\pm3/2}(\rho) Z_{F_z=\pm3/2}(z),
\]

(12)

where the radial functions \( R(\rho) \) satisfy the boundary condition \( R(d/2) = 0 \) and \( d \) is the diameter of the dot. \( \psi_{F_z=\pm1/2} \) are the solutions of the Schrödinger equation in the vertical direction \( Z(z) \) expanded in an orthonormal basis set as

\[
Z_{m_j} = \sum_i b_i^m e_i^m(z),
\]

(15)

where \( b_i^m \) are the solutions of the Schrödinger equation

\[
\left[ \frac{\hbar^2 k_z^2}{2m_z} + V(z) \right] \xi_i(z) = E_i \xi_i(z).
\]

(16)

This expansion works for heterostructures with materials having similar material characteristics. The small differences in the effective masses within and outside of the quantum dot are neglected. To treat the continuum states and the bound states of the vertical well, the scheme of Ando\textsuperscript{14} is used by enclosing the dot into a large box with 100 times larger \( z \) extension. The eigenstates \( Z(z) \) are characterized by the index \( i \) for each band and by “parity.” The definite parity is a consequence of the symmetric form of the potential well.

In principle, one can perform the direct numerical diagonalization of the total Hamiltonian for \( B = 0 \). \( H_0 \) is diagonalized in the above basis set for a specific quantum number \( F_z \). For realistic quantum dots, however, the direct numerical evaluation of the matrix from Eq. (1) generally requires the expansion of the wave functions in large basis sets and diagonalization of very large matrices in order to obtain convergence.\textsuperscript{13} To overcome this, we apply a second expansion in \( H_0 \) with respect to the parallel wave vector \( k_z \) as in Ref. 13 where the lateral dimension of the dot is much greater than the vertical dimension. This method is especially useful for systems with lower dimensions. Then, the Hamiltonian for zero magnetic field is

\[
H_0 = H_0(k_z = 0) + H' = \frac{\hbar^2 k_z^2}{2m_z} \left[ \hat{h}_{+} + \hat{h}_{-} + \hat{h}_{2+}k_z^2 + \hat{h}_{2-}k_z^2 \right],
\]

(18)

where \( \hat{h}_{+} \) and \( \hat{h}_{+} \) can be found from the Hamiltonian in Eq. (1) and \( k_z \), \( k_z \) are evaluated by \( \pi/d \), where \( d \) is the lateral size of the dot. The energy spectrum and valence bands are calculated by treating \( H' \) perturbatively, using the method in Ref. 13 and they are characterized by the indices \( n_{\rho} \), \( n_z \), and parity. The unperturbed wave functions are those in Eqs. (12) and (13).

Next, we apply perturbation theory with respect to the magnetic field through \( H_B \) for small \( B \) field. The wave function can be written as

\[
\psi_{F_z=\pm3/2} = \psi_{F_z=\pm3/2}^0 + \alpha_{1/2}(\pm1/2) \psi_{F_z=\pm1/2}^0 + \beta_{1/2}(\pm1/2) \psi_{F_z=\pm1/2}^0,
\]

(19)

\[
\psi_{F_z=\pm1/2} = \psi_{F_z=\pm1/2}^0 + \alpha_{3/2}(\pm3/2) \psi_{F_z=\pm3/2}^0 + \beta_{3/2}(\pm3/2) \psi_{F_z=\pm3/2}^0,
\]

(20)

where the \( \alpha \) and \( \beta \) coefficients are determined from \( H_B \) and they are all \( -heB/2m_0 \). The energies \( E_{F_z=\pm3/2} \) and \( E_{F_z=\pm1/2} \) are calculated up to the first order in the magnetic field \( B \).

### III. Scattering Rates for Hole Spins

To calculate the rate of the hole scattering between spin states we first determine the valence bands highest in energy using the method described in Sec. II. The calculation is done by numerical diagonalization of \( H_0 \) using the perturbative approach described above. For the QD’s studied here the two bands highest in energy preserve their heavy- and light-hole character, and they are degenerate for \( B = 0 \) with \( m_j = \pm 3/2 \). The perturbation \( H_B \) causes a splitting between the \( m_j = 3/2 \) and \( m_j = -3/2 \) bands, and the character of the bands becomes a mixture of heavy and light holes. The highest in energy bands have quantum numbers \( F_z = -3/2 \) for \( m_j = 3/2 \) and \( F_z = 3/2 \) for \( m_j = 3/2 \).

The transitions of interest for hole dephasing by spin flips are

\[
M_Q = \langle \psi_{F_z=3/2,m_j=-3/2,A}|H_Q|\psi_{F_z=-3/2,m_j=3/2,B} \rangle,
\]

(21)

where A and B stand for the parity of the bands. This expression has several terms due to the complex nature of the hole-phonon coupling \( H_Q \)—Eqs. (1), (7)–(10).

The scattering rates are calculated using the Fermi golden rule and the matrix element for the lowest transition from Eq. (21). Analytical results can be obtained if we consider the limit of small phonon wave vector \( Q \) in the exponential factor \( e^{iQ \cdot r} \approx (1 + iQ \cdot r) \) from the strain tensor \( \epsilon \). We have examined contributions from all types of acoustic phonon polarizations—longitudinal (LA) \( \tilde{\eta}_1 = Q/Q \) and the two transverse (TA) \( \tilde{\eta}_1 = (Q_x Q_z - Q_y Q_z - Q^2)/Q Q \) and \( \tilde{\eta}_2 = (Q_x - Q_z, 0)Q \), where \( Q = \sqrt{Q_x^2 + Q_y^2 + Q_z^2} \) and \( Q = Q_x^2 + Q_y^2 + Q_z^2 \). The result for the scattering rates are
where $\Delta E = (E_{F}^{0} - 3/2m_{0} = -3/2 = E_{F}^{0} - 3/2m_{0} = -1/2)$ is the energy difference between the heavy and light holes for $B = 0$. $\gamma_{hh} = \sqrt{2m_{0}^{\text{hh}}/\hbar^{2}}(\nu^{\text{hh}} - [E_{F}^{0}])$ with appropriate parameters for the heavy-hole subband. $K = 1.882$ is a numerical factor obtained from the numerical diagonalization of the hole bands, and $\tilde{s}$ is the sound velocity of InGaAs. The parameter $x_{i} = \frac{32}{3}, \frac{16}{3}, \frac{16}{3}$ for LA, TA1, and TA2 polarizations.

Equation (22) for spin relaxation rates allows us to determine the dependences on several physical parameters. From Eq. (22) the scattering rate is proportional to $B^{7}$. One is also able to see how the size of the QD affects $\Gamma$. The dependence on the lateral size comes from the $d^{4}$ and $\Delta E^{-2}$ parameters. The relaxation rate as a function of the dot diameter is shown in Fig. 1. The figure shows that after a diameter $d_{0} \approx 20$ nm the scattering starts to increase nonlinearly leading to a nonlinear decrease of the coherence time. Below $d_{0}$ the rate is nearly a constant with a coherence time $\approx \mu s$. For the QD’s studied here the two bands closest to the Fermi level preserve their heavy- and light-hole character, and the bands closest to $E_{F}$ are degenerate for $B = 0$ with $m_{j} = \pm 3/2$.

Figure 1 also shows that both the longitudinal and transverse polarizations are important with the TA scattering rate slightly larger. The scattering rates will increase at small diameters due to coupling to interface motion, but these effects are not included here. Holes can interact with the LA phonons through the $P_{Q}$, $Q_{Q}$, and $R_{Q}$ terms from the Bir-Pikus Hamiltonian. The interaction with the TA phonons comes from the terms $R_{Q}$ and $S_{Q}$ through the $\varepsilon_{xy}$, $\varepsilon_{yz}$, and $\varepsilon_{xz}$ components of the strain tensor. The height of the dot, $c$, enters $\gamma_{hh}$. Here we use $c = 5$ nm, and it is not changed in the calculation.

A comparison can be made with the phonon induced relaxation rates of an electron spin in a QD. For an electron spin the relaxation rate is about 4 orders smaller than the rate for holes with lowest value for electrons on the order of $10^{-3} - 10^{-4}$ s$^{-1}$. The electron scattering rate $\sim R^{4}$, where $R$ is the radius of the QD (Ref. 2) and it goes as $\sim m_{e}^{3}$. The explicit dependences of $\Gamma$ on size and mass is difficult to obtain for the holes because of the complicated diagonalization procedure. The radial mass is contained in $\Delta E$ and $K$ through the numerical diagonalization. The mass along $z$ axis is contained in $\gamma_{hh}$ and $K$. For the sake of argument, if we take the hole energy to have a similar size and mass dependences as the electron energy, $E \sim 1/mR^{2}$, and use Eq. (22) we see that the hole scattering rate is $\sim m_{h}^{3}/m_{c}$, where the electron mass is much less than the hole mass, the electron will have much slower relaxation than the hole. This could explain the dramatic difference in the value for the decoherence time for the electron ($\sim 10^{-3} - 10^{-4}$ s) and that for the hole ($\sim 10^{-8}$ s). In general the coherence time is longer for smaller dots for both holes and electrons.

We give the scattering as a function of temperature in Fig. 2. The temperature dependence comes from the phonon occupation factor $N_{Q}$ in $\Gamma$ in Eq. (11). The scattering rate is temperature independent up to $T \sim 0.5$ K. For higher $T$ it increases linearly with $T$ from $N_{Q}$.

IV. DISCUSSION

In this paper we have given calculations of the scattering rates for relaxation of holes in cylindrical (deep etched) quantum dots due to the emission and absorption of acoustic phonons via the deformation potential interaction mediated by the spin-orbit interaction described by the Bir-Pikus Hamiltonian. A magnetic field is applied in the $z$ direction. The Luttinger Hamiltonian was solved by numerical diagonalization for $B = 0$, and the magnetic field is introduced with perturbation theory. In this way we determine the valence bands closest to the Fermi level and their energies.

The Bir-Pikus Hamiltonian for strained structures is used
to calculate the hole-phonon relaxation rates. The calculation includes both longitudinal and transverse acoustic phonons. The relaxation rates as functions of magnetic field, lateral size of the dot and temperature were determined. We find that the decoherence time due to hole relaxation is lower for smaller dots and for dots \( \lesssim 20 \) nm dots is of the order of \( 10^{-8} \) s. Corresponding spin-flip rates for electrons in quantum dots due to phonon scattering were found to be several orders of magnitude smaller.

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11 The Luttinger parameters are \( \gamma_1 = 7.65, \quad \bar{\gamma}_2 = 2.41, \quad \text{and} \quad \bar{\gamma}_3 = 3.28 \). In the spherical-approximation \( \gamma_2 = (\bar{\gamma}_2 + \bar{\gamma}_3)/2 \). The other Luttinger parameter is \( \kappa = 1.2 \).


