Spin relaxation in isotopically purified silicon quantum dots

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We investigate spin-flip processes of Si quantum dots due to spin-orbit coupling. We utilize the spin-orbit coupling constants related to bulk and structure inversion asymmetry obtained numerically for two dimensional heterostructures. We find that the spin-flip rate is very sensitive to these coupling constants. We investigate the nuclei-mediated spin-flip process and find the level of $^{29}$Si concentration for which this mechanism become dominant.

I. INTRODUCTION

The control of single-electron spin in nanoscale devices is a key element in the field of spintronics, where the spin degree of freedom is used for information transfer and processing. The vast majority of proposed spin devices are based on semiconductors $^{[1]}$, $^{[2]}$, $^{[3]}$, $^{[4]}$, where single-electron spin has been probed to be controllable by means of voltages applied to electrostatic gates $^{[5]}$. A promising technology for the implementation of quantum computation (QC) involves the storage of quantum information in the spin of electrons in quantum dots (QDs). The key requirement is that the lifetime of the spins is long compared with the time required for the operation of logic gates. This has motivated the development of QDs in Si-based materials $^{[6]}$, where spin-orbit coupling (SOC) is weak and isotopic enrichment can eliminate hyperfine coupling (HC). In such scenarios, processes limiting QC are dominated by SOC resulting from spatial inversion asymmetry. In typical solid state systems, macroscopic electric fields cause structure inversion asymmetry (SIA), giving rise to Rashba-type terms $^{[7]}$ of the form:

$$H_R = \alpha(\hat{\sigma}_x \hat{k}_y - \hat{\sigma}_y \hat{k}_x),$$

whereas fields resulting from the lack of an inversion center lead to bulk inversion asymmetry (BIA) and to the Dresselhaus term, $^{[9]}$:

$$H_D = \beta(\hat{\sigma}_y \hat{k}_x - \hat{\sigma}_x \hat{k}_y).$$

Here, $\sigma_i$ and $k_i$ denote spin and momentum operators, respectively, and $\alpha, \beta$ are the Rashba and Dresselhaus coupling constants, respectively. Although both SOC contributions have been noted for decades, their absolute value have been measured simultaneously only recently $^{[11]}$. The different theoretical models show controversy $^{[12]}$, with debated estimations for Rashba or Dresselhaus related parameters.

In this paper we calculate spin-flip rates for typical Si QD via higher-energy virtual state, involving also phonon emission. We define the regime for which SOC is the dominant source of relaxation as a function of $^{29}$Si isotope concentration. We utilize in our calculations the SOC parameters extracted numerically using for first time a model that includes atomic crystal symmetry, spin and interfaces built into the basis representation $^{[13]}$, that aims to clarify the existing controversy.

This paper is organized as follows: Sec. II contains a description of the model: we describe the electron-phonon interaction, and the spin-flip mechanism, namely SOC and hyperfine coupling (HC). In Sec. III we present our results, and finally, Sec. IV is devoted to conclusions.

II. METHODS

A. Model

We consider a QD formed in a two dimensional (2D) heterostructure with parabolic confinement. Spin-flip is considered via an orbital (or valley) state with energy $\hbar \omega_0$, as depicted in Fig. 1.

![FIG. 1: Schematic representation of a spin-flip process for a Si QD with one electron.](image)

In order to calculate the relevant transition rates for spin relaxation, we consider a perturbation given in general by $\delta H = H_{sf} + H_{ph}$, $H_{ph}$ corresponding to the electron-phonon coupling, and $H_{sf}$ to the mechanism causing a spin flip in the dot. The amplitude of a spin-flip event in the ground state then is given in second order perturbation theory,

$$\langle 1 \uparrow | \delta H | 1 \downarrow \rangle \approx \sum_n \left( \frac{|1 \uparrow \langle n \uparrow | H_{ph} | n \uparrow \rangle 1 \downarrow \rangle |}{E_n - E_1 + \Delta} \right),$$

where $\Delta$ is the energy exchanged with the bath. Here, $\uparrow, \downarrow$ denote the spin state and $n$ is the orbital degree of freedom. The orbitals are described in terms of Fock-Darwin states. The ground-state spin-flip rate $|1 \uparrow \rangle$ to $|1 \downarrow \rangle$ is then given by Fermi’s golden rule:

$$\Gamma_{\uparrow,\downarrow} = \frac{2\pi}{\hbar} |\langle 1 \uparrow | \delta H | 1 \downarrow \rangle|^2 \delta(E_i - E_f).$$
In this notation, $|1\rangle$ denotes the initial state of electron, nuclei and phonons, $|1\rangle \rightarrow |i\rangle = |i_n\rangle \otimes |i_{ph}\rangle$, likewise $|1\rangle \rightarrow |f\rangle = |1\rangle \otimes |f_n\rangle \otimes |f_{ph}\rangle$. Inserting Eq. (2) into (1) we obtain (setting $\Delta = 0$):

$$\Gamma_{1;1} = \frac{2\pi}{\hbar} \langle i | (f_{ph} H_{ph} | i_{ph} )^2 \delta (E_i - E_f) \langle 1 | H_{d} | 1 \rangle^2 (\hbar \omega_0)^2 \rangle. \quad (3)$$

We note that the phonon and the spin-flip parts can be factorized, so we define $\Gamma_{1;1} = \Gamma_{ph} \times \xi^2$, with

$$\Gamma_{ph} = \frac{2\pi}{\hbar} \langle i | (f_{ph} H_{ph} | f )^2 \delta (E_i - E_f) \rangle; \quad \xi^2 = \frac{\langle 1 | H_{d} | 1 \rangle^2 (\hbar \omega_0)^2 \rangle}{(\hbar \omega_0)^2}. \quad (4)$$

Hence, $\Gamma_{ph}$ and $\xi$ can be treated separately. $\Gamma_{ph}$ describes the phonon-emission process, coupling two orbitals via electron-phonon deformation potential, and $\xi$ includes the spin-flip process. We give next a detailed description of both terms.

### B. Phonon-electron coupling

For Si under compressive stress along [001], the electron interacts with a phonon of momentum $q$ via deformation potentials $[14, 15, 16]$. The Hamiltonian reads:

$$H_{ph} = \sum_q \sum_\epsilon \left[ a_q^+ e^{-iq\epsilon} + a_q e^{iq\epsilon} \right] \hat{q} \left( \mathbf{\Xi}_d \hat{e}_\epsilon \hat{q}_x + \mathbf{\Xi}_d \hat{e}_\epsilon \hat{q}_y + \mathbf{\Xi}_d + \mathbf{\Xi}_u \right) \hat{e}_\epsilon \hat{q}_z \quad (5)$$

where $\langle n_q - 1 | a_q^+ a_q | n_q \rangle = \sqrt{\langle m_q / 2 M_c \omega_q \rangle}$, $M_c$ is the mass of the unit cell and $\hbar \omega_q$ the phonon energy. Here, $s$ denotes the polarization of the phonon (two transverse and one longitudinal), $q$ is the wavevector, $\mathbf{\Xi}_u$ and $\mathbf{\Xi}_d$ are the electron-phonon coupling parameters in Si (see table I). This is slightly simpler than the corresponding Hamiltonian in GaAs because of the absence of the piezoelectric coupling in Si. In order to calculate $\Gamma_{ph}$, we use the electric dipole (ED) approximation, $e^{iq\epsilon} \approx 1 + iq\epsilon$ (valid in the range of 0.1-0.2 meV, which is roughly the phonon energy involved in this relaxation process).

For the process depicted in Fig. 1 mixing of $s$-orbitals occur at 0-th order in ED (to lowest order). We summarize in Table I the parameters relevant for the computation of $\Gamma_{1;1}$ used throughout the text. Using the 0-th order ED approximation, $\langle 1 | H_{d} | 1 \rangle \approx 1$, we obtain for the electron-phonon coupling:

$$\hat{H}_{ph} \approx \sum_q \left[ a_q^+ a_q^\dagger \right] \left( \mathbf{\Xi}_d \hat{e}_\epsilon \hat{q}_x + \mathbf{\Xi}_d \hat{e}_\epsilon \hat{q}_y + \mathbf{\Xi}_d + \mathbf{\Xi}_u \right) \hat{e}_\epsilon \hat{q}_z, \quad (6)$$

which, using (4), gives the rate:

$$\Gamma_{ph}^{D} \approx \frac{(n_q + 1)}{2 \rho_{Si}(2\pi)^2} \sum_{\epsilon} \int_{0}^{2\pi} d\phi \int_{0}^{\infty} d\omega \int_{0}^{\infty} dq_s \frac{q_s^4}{\omega_{qs}^2} \left( \mathbf{\Xi}_d \hat{e}_\epsilon \hat{q}_x + \mathbf{\Xi}_d \hat{e}_\epsilon \hat{q}_y + \mathbf{\Xi}_d + \mathbf{\Xi}_u \right) \delta (\hbar \omega_{qs} - \hbar \omega_0). \quad (7)$$

where $n_q + 1 \approx 1$ in the range of low temperatures considered, and $\rho_{Si}$ is the density of Si (see table I). $\hat{e}_\epsilon$ is the $i$-th component of the unitary polarization vectors and $s$ denotes the polarization, $s = l, t_1, t_2$.

As pointed out before, spin-flips can be provided by two different mechanisms, the HC with the $^{29}$Si nuclei and the SO coupling. For an isotopically-purified sample, we expect SO to be the dominant spin-flip mechanism. Hence, we first evaluate SO mediated spin-flip and then consider the $^{29}$Si concentration at which the HC mediated spin-flip rate becomes comparable to the SO mediated one.

### C. Spin orbit coupling

For the process depicted in Fig. 1 mixing of $s$-orbitals occur at 0-th order in ED (to lowest order). We summarize in Table I the parameters relevant for the computation of $\Gamma_{1;1}$ used throughout the text. Using the 0-th order ED approximation, $\langle 1 | H_{d} | 1 \rangle \approx 1$, we obtain for the electron-phonon coupling:

$$\hat{H}_{SO} = \frac{1}{\hbar} \left[ (\beta + \alpha) \hat{\sigma}_+ \hat{\sigma}_{-} + (\beta - \alpha) \hat{\sigma}_{-} \hat{\sigma}_{+} \right]. \quad (9)$$

We note that the SO term does not commute with $\hat{H}_0$. This implies that the spin does not remain fixed during the motion of the electron, apart from an apparent homogeneous shift of the
momentum to first order, which would not change observables (other than just a shift in the energy levels). To get rid of such terms fixed by gauge invariance, it is convenient to apply the transformation of Aleiner et al., \( \hat{U} = \exp\left(i\gamma_0 \hat{q}_+ \hat{\sigma}_- + i\gamma_1 \hat{q}_- \hat{\sigma}_+\right) \). \((\hat{q}_\pm)\) is the operator along the directions \( \hat{\varepsilon}_\pm \), which allows to see how the levels split in the presence of \( \hat{H}_{SO} \). Using the Zassenhaus formula, \( e^{A+B} \simeq e^A e^{-\frac{1}{2}[A,B]} \ldots \), we factorize \( \hat{U} \) to second order in SOC:

\[
\hat{U} = e^{(i\gamma_0 \hat{q}_+ \hat{\sigma}_- + i\gamma_1 \hat{q}_- \hat{\sigma}_+)} \simeq e^{i\gamma_0 \hat{q}_+ \hat{\sigma}_-} e^{i\gamma_1 \hat{q}_- \hat{\sigma}_+} e^{\frac{1}{2} i\gamma_0 \hat{q}_+ \hat{\sigma}_- \hat{q}_-. \hat{\sigma}_+} .
\]

(11)

Retaining terms to third order in SOC, the momentum transform as:

\[
\hat{U}^+ \hat{P}_+ \hat{U} \simeq \hat{P}_+ + i\gamma_1 \hat{q}_- \hat{\sigma}_- - i\gamma_2 \hat{q}_- \hat{\sigma}_+ - 2i\gamma_1 \gamma_2 \hat{q}_- \hat{\sigma}_- \hat{\sigma}_+ ,
\]

and likewise:

\[
\hat{U}^+ \hat{P}_- \hat{U} \simeq \hat{P}_- + i\gamma_1 \hat{q}_+ \hat{\sigma}_+ + i\gamma_2 \hat{q}_+ \hat{\sigma}_- - 2i\gamma_1 \gamma_2 \hat{q}_+ \hat{\sigma}_+ \hat{\sigma}_- .
\]

so that the total Hamiltonian, \( \hat{H} = \hat{H}_0 + \hat{H}_{SO} \), transforms as \( \hat{H}' = \hat{U}^+ \hat{H} \hat{U} \). Considering terms up to third-order in SOC:

\[
\hat{H}' \simeq \hat{H}_0 + \frac{\hbar}{m_1l_2} \left[ \hat{q}_+ \hat{\sigma}_- \hat{q}_- \hat{\sigma}_+ \right] + \frac{2\hbar}{m_1l_2} \hat{q}_- \hat{\sigma}_- \left[ \frac{\hat{p}_+ \hat{\sigma}_+}{l_1} - \frac{\hat{p}_- \hat{\sigma}_-}{l_2} \right] = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 ,
\]

(12)

where we have defined \( \gamma_1 = m(\alpha - \beta) / h \equiv l_1^{-1} \) and \( \gamma_2 = -m(\alpha + \beta) / h \equiv l_2^{-1} \), with \( l_{1,2} \) characterizing the length scale associated with the strength of the SOC for electrons moving along the crystallographic directions. This choice allows us to cancel out the linear terms in momentum. The second term of Eq. (12) gives an effective magnetic field that can be expressed as:

\[
\hat{H}_1 = i\hbar_1 [\hat{a}_1 \hat{a}_2 - \hat{a}_2 \hat{a}_1] \hat{\sigma}_z ,
\]

(13)

where we have defined:

\[
\hbar_1 = \frac{2m}{\hbar} (\alpha^2 - \beta^2) \left( \sqrt{\frac{\hbar}{\omega_2}} + \sqrt{\frac{\hbar}{\omega_1}} \right) .
\]

We note that \( \hat{H}_1 \) does not break the Kramers degeneracy, and hence, does not contribute to spin-flip. However, the last term of Eq. (12) does break Kramers degeneracy, allowing spin-flip terms. In second quantization, we have:

\[
\hat{H}_2 = \frac{\gamma_1}{\hbar} [\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_1 + \hat{a}_1^\dagger (1 - \hat{a}_2 \hat{a}_1) \hat{a}_2 \hat{a}_1] + \frac{\gamma_2}{\hbar} [\hat{a}_2^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_2 + \hat{a}_2^\dagger (1 - \hat{a}_1 \hat{a}_2) \hat{a}_1 \hat{a}_2],
\]

(14)

where we have defined:

\[
\gamma_1 = (\beta - \alpha)^2 (\beta + \alpha) m \sqrt{\frac{2m}{\hbar \omega_1}}, \quad \gamma_2 = (\beta + \alpha)^2 (\beta - \alpha) m \sqrt{\frac{2m}{\hbar \omega_2}}.
\]

We then conclude that, for SOC, \( \zeta_{SO} \approx \gamma_1^2 / \hbar \omega \), from which we can proceed to calculate \( \Gamma_{1,1} \), using (14) and (8) in (4). We emphasize that this term is third order in SOC, and applying Fermi Golden’s rule, the spin-flip rate will appear in sixth order. Hence, \( \Gamma_{1,1} \) is very sensitive to the SOC parameters, so it is critical to determine them to a high degree of precision.

**D. Hyperfine Coupling.**

For an electronic spin in a QD and in the presence of nuclear spins, a contact interaction Hamiltonian can be assumed as a perturbation,

\[
\hat{H}_{hc} = \sum_{j} \frac{4\mu_0}{3I} \eta_s I \hat{c}(\mathbf{r}_j - \mathbf{R}_j) = A \sum_{j} \eta_s I \hat{c}(\mathbf{r}_j - \mathbf{R}_j)
\]

(15)

where \( \hat{c} \) and \( \eta_s I \) denote the spin and position of the \( j \)-th electron (\( j \)-th nuclei), and \( A \) is the hyperfine coupling constant. We now use (15) as the spin-flip mechanism to calculate \( \zeta \) of Eq. (4):

\[
|\langle 1 | \hat{H}_{hc} | 2 \rangle |^2 = A^2 \sum_{j} \left| \langle \uparrow | \hat{c} \hat{\sigma}(\mathbf{r}_j - \mathbf{R}_j) \downarrow \rangle \right|^2.
\]

Next we substitute the sum over \( j \) by an integral over the nuclei with a density \( \rho_n \):

\[
|\langle 1 | \hat{H}_{hc} | 2 \rangle |^2 = A^2 \rho_n \int \mathrm{d}^3 \mathbf{r}_j \left| \Phi_1 (\mathbf{r}_j) \right|^2 \left| \Phi_2 (\mathbf{r}_j) \right|^2.
\]

which can be easily performed assuming Fock-Darwin states for \( \Phi_j \), resulting:

\[
\zeta_{hc} = \frac{3A^2 \rho_n}{8\sqrt{\hbar \omega (\hbar \omega_1)^2}}.
\]

(16)

Using (16) together with Eq. (8) in (4), we can thus obtain the spin-flip rate due to HC. Typical values for \( \eta_{SO} \) of 186 have been reported [18, 19, 20], yielding \( A \approx 2 \times 10^{-7} \text{eVnm}^{-3} \). Only about 4% of the nuclei have spin, so \( C_n \approx 0.04 \times 8 / \sqrt{v_0} \approx 2 \text{nm}^{-3} (v_0 \approx 0.17 \text{nm}^3) \), is the unit cell volume for Si). It is important to note that \( \Gamma_{1,1} \) is proportional to \( C_n \), i.e., to the total number of nuclei \( N_n \) with which the electrons interact. This is consistent with the simple picture that the relaxation rate is proportional to the mean-square fluctuations in the random hyperfine field. Formulas for spin relaxation rates due to HC that give an apparent proportionality to \( N_n^{-1/2} \) are common in
the literature, and have given rise to the incorrect notion that some sort of motional narrowing is at work. This is not possible, since the fluctuations in the nuclear spin system are slow. In any case the rate must vanish as \( N_n \rightarrow 0 \).

These formulas are correct, but they generally involve other parameters that actually vary with \( N_n \).

III. RESULTS

We considered a typical QD formed as in [6] with a level separation of \( \hbar \omega_0 = 0.2 \text{meV} \). The \( \alpha \) and \( \beta \) parameters where extracted numerically using NEMO-3D [26] on nanoHUB.org computational resources [27]. In NEMO-3D, atoms are represented explicitly in the \( sp^3d^5s^* \) tight-binding model, and the valence force field (VFF) method is employed to minimize strain [28]. NEMO-3D enables the calculation of localized states on a QW and their in-plane dispersion relation with a very high degree of precision, allowing to extract the splittings along the in-plane directions in momentum space [13]. For now, we note that the \( \alpha \) value is well defined and depends on external electric fields applied to the sample, whereas the Dresselhaus, \( \beta \), depends strongly on the atomistic details of the interface.

![Graph showing \( \Gamma_{\uparrow\downarrow} \) as a function of Si isotope purification degree. The horizontal lines correspond to \( \Gamma_{\uparrow\downarrow} \) due to SOC, for various values of Dresselhaus coupling parameter, \( \beta \).](image)

**FIG. 3:** \( \Gamma_{\uparrow\downarrow} \) as a function of \( ^{29}\text{Si} \) isotope purification degree. The horizontal lines correspond to \( \Gamma_{\uparrow\downarrow} \) due to SOC, for various values of Dresselhaus coupling parameter, \( \beta \).

Fig. [3] shows the calculated values for \( \Gamma_{\uparrow\downarrow} \) via both mechanism, HC and SOC. The parallel lines correspond to \( \Gamma_{\uparrow\downarrow}^{\text{SOC}} \) for different possible values of \( \beta \), whereas the thick solid line represents the spin-flip due to HC mechanism, \( \Gamma_{\uparrow\downarrow}^{\text{HC}} \), as a function of \( ^{29}\text{Si} \) isotope purification degree. Using our numerical value for \( \alpha \) and a few different values for \( \beta \), we find that for natural Si, the HC dominates. We note that these depend strongly on the sample, so a Si sample with dominating SOC is possible. In particular, for a Si/SiGe heterostructure, the \( \Gamma_{\uparrow\downarrow}^{\text{HC}} \) value corresponds to the horizontal solid line of Fig. [3] We can see that a purification of about 80% of the \(^{29}\text{Si} \) isotope will cause SOC to become dominant. In contrast, for a similar QD formed in a Si membrane, with purification of \( \sim 99\% \) we obtain SOC as the dominant mechanism, increasing the relaxation time by almost two orders of magnitude.

**FIG. 4:** Regions where SOC (shaded) or HC (light) are the dominant mechanism of relaxation as a function of Dresselhaus parameter, \( \beta \), and degree of \(^{29}\text{Si} \) isotope purification: for small \( \beta \), a larger isotopic purification degree is needed, and hence, larger relaxation times can be achieved.

**FIG. 4:**

In summary, we have calculated the dominant rates for phonon-assisted spin-flip relaxation for the ground state of a single-electron Si QD. \( \Gamma_{\uparrow\downarrow} \) is found to be of the order of tens of seconds, very sensitive to SOC. We observe that choosing a sample with small SOC, as pure Si membranes, can lead to spin lifetimes of up to a few hours. QDs fabricated in Si/SiGe heterostructures are more limited by SOC, and purifications of only about 80% would give spin lifetimes of a few minutes. Due to weak spin-orbit and HC, Si offers very long coherence times, which are required for solid state qubits.

**IV. CONCLUSIONS**

In summary, we have calculated the dominant rates for phonon-assisted spin-flip relaxation for the ground state of a single-electron Si QD. \( \Gamma_{\uparrow\downarrow} \) is found to be of the order of tens of seconds, very sensitive to SOC. We observe that choosing a sample with small SOC, as pure Si membranes, can lead to spin lifetimes of up to a few hours. QDs fabricated in Si/SiGe heterostructures are more limited by SOC, and purifications of only about 80% would give spin lifetimes of a few minutes. Due to weak spin-orbit and HC, Si offers very long coherence times, which are required for solid state qubits.

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