Spin relaxation of a donor electron coupled to interface states

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An electron spin qubit in a silicon donor atom is a promising candidate for quantum information processing because of its long coherence time. To be sensed with a single-electron transistor, the donor atom is usually located near an interface, where the donor states can be coupled with interface states. Here we study the spin relaxation mechanisms arising from the coupling of a donor to confined interface states. We find that both Zeeman interaction and spin-orbit interaction can hybridize spin and orbital states, each contributing to phonon-assisted spin relaxation in addition to the spin relaxation for a bulk donor or a quantum dot. When the applied magnetic field $B$ is weak (compare to orbital spacing), the spin relaxation due to Zeeman interaction and spin-orbit interaction show the same $B^5$ dependence on the magnitude of $B$ field, but show different angular dependencies on the orientation of $B$ field. We find that there are peaks (hot-spots) in the $B$-dependent and detuning dependent spin relaxation due to strong hybridization of orbital states with opposite spin. We also find spin relaxation dips (cool-spots) due to the interference of different relaxation paths. The electrically tunable spin relaxation hot-spots and cool-spots can be useful for fast spin initialization and the preservation of quantum information during the transfer of spin qubit.

I. INTRODUCTION

Electron spin qubits in semiconductor donors or quantum dots (QDs) are promising candidates for quantum information processing because of the tunability of electronic states and compatibility with existing semiconductor fabrication technologies.\textsuperscript{1–4} Silicon as a host material for spin qubits is of particular interest because of the weak spin-orbit interaction (SOI) and the development of isotopic enrichment, which suppress both spin relaxation and pure dephasing.\textsuperscript{5–7} Long coherence time and high fidelity readout have been demonstrated experimentally for a spin qubit in isotopically enriched silicon.\textsuperscript{8} Furthermore, spin qubits in silicon donor atoms can be engineered by deterministic doping, where individual donor atoms can be placed with sub-nm precision by using scanning tunneling microscopy (STM) lithography.\textsuperscript{9}

For readout with a single-electron transistor, the donor atoms of interest are usually located near an interface.\textsuperscript{8 10 11} For example, in recent experiments with ion implanted phosphorus, the donors are separated about 10 nm from the interface.\textsuperscript{5} For these short separations, the interface states can couple to the donor state and alter the behavior of spin qubit in a donor. The interface states are QD-like states confined laterally by the nearby donor potential and vertically by an applied electric field at the interface. The resulting lateral confinement along the interface can be as large as 10 meV.\textsuperscript{12 13} It has been proposed to use the interface states to mediate dipole-dipole coupling between donor electrons\textsuperscript{14}, or to transfer spin qubit information between remote donor atoms\textsuperscript{15}, where electrons are transferred between donors and interface states by applying an electric field. Recently, STM experiment demonstrated the tunnel coupling between donor and a QD-like state.\textsuperscript{16}

Spin relaxation describes how spin decays from its excited state to ground state, which is a type of decoherence that cannot be substantially suppressed with the spin echo techniques. Spin relaxation is an important quantity for the characterization of quantum systems, such as donor systems\textsuperscript{5 6 10 17 20}, single QD system\textsuperscript{21–24} and double QD (DQD) systems\textsuperscript{25 28}. In a single bulk donor, spin relaxation is dominated by the Zeeman interaction, which hybridizes the donor ground orbital and excited orbitals with opposite spin.\textsuperscript{20–22} Spin relaxation in a single QD is dominated by SOI, which hybridizes the QD ground state with the excited states of opposite spin.\textsuperscript{21–23 33 36} For tunnel coupled donor-interface system, hybridization of donor ground orbital with QD-like interface states could give rise to additional electron spin relaxation. A recent study of electron spin relaxation in a flip-flop qubit shows that the interface state can induce a strong spin relaxation peak (hot-spot) based on the single valley approximation.\textsuperscript{37} Spin relaxation hot-spots are also studied in GaAs double QD\textsuperscript{38} and silicon QD\textsuperscript{23}. However, not much attention has been paid to the effect of destructive interference on spin relaxation.

In this work, we study spin relaxation of a donor coupled to QD-like interface states. We find that both Zeeman interaction and SOI can couple the donor ground state and QD states with opposite spin, and via phonon emission, will result in spin relaxation. When the applied magnetic field $B$ is small, we find that spin relaxation due to Zeeman interaction and SOI show the same $B^5$ dependence on the magnitude of $B$ field, but different dependencies on the orientation of $B$ field. Spin relaxation hot-spots are found due to the crossing of orbital states with opposite spin. We also find the spin relaxation cool-spots, where spin relaxation is suppressed due to the interference between different spin relaxation paths. The qubit operation near a spin relaxation hot-spot and cool-spot could be particularly interesting as a way to fast initialize spin qubit and preserve quantum information during co-
the electron spin Zeeman interaction, $H$ ing the valley and envelope degrees of freedom), $H$ and QD eigenstates. We are interested in the regime can be expressed in the basis of donor eigenstates and the lowest two QD states.

herent transfer of spin information between donor atoms via interface states.

The rest of the paper is organized as follows. In Sec. II, we set up the model Hamiltonian. In Sec. III, the effective spin-phonon interactions are obtained for two different spin hybridization mechanisms. In Sec. IV, we give spin relaxation expressions. In Sec. V, we show the numerical results of spin relaxation for various applied magnetic fields and detunings. In Sec. VI, we compare the result with spin relaxation in a single bulk donor and discuss possible consequences for experiments. Finally, we draw conclusions in Sec. VII.

II. SYSTEM HAMILTONIAN

We consider an electron spin of a phosphorus (P) donor atom in an isotopically enriched $^{28}$Si, where P donor electron is tunnel coupled to nearby QD-like interface states. Figure 1 shows a schematic diagram of the electric potential and energy levels of the system. The system Hamiltonian is given by

$$H = H_O + H_Z + H_{SO} + H_{EP},$$

where $H_O$ is the orbital part of the Hamiltonian (including the valley and envelope degrees of freedom), $H_Z$ is the electron spin Zeeman interaction, $H_{SO}$ is the SOI in effective mass theory, and $H_{EP}$ is the electron-phonon interaction. We will describe each term in detail in the following paragraphs.

The orbital Hamiltonian of a coupled donor-QD system can be expressed in the basis of donor eigenstates and QD eigenstates. We are interested in the regime where the lowest two QD eigenstates are energetically close to the donor ground state, and since other donor or QD states are at least 10 meV higher, we will focus on the lowest three states: the ground state $|0\rangle$ of a single donor and the two lowest states $|1\rangle$ and $|2\rangle$ of the QD (see Appendix A). Thus, the effective three-level Hamiltonian (suppressing the spin degree of freedom) is

$$H_O = \epsilon_0 |0\rangle\langle 0| + \epsilon_1 |1\rangle\langle 1| + \epsilon_2 |2\rangle\langle 2| + t_{01} |0\rangle\langle 1| + t_{02} |0\rangle\langle 2| + h.c.,$$

where $\epsilon_n$ ($n=0, 1, 2$) is the energy of each orbital basis state $|n\rangle$, $t_{01}$ and $t_{02}$ are the tunneling matrix elements between the donor ground state and the two QD states. The energies $\epsilon_n$ can be parameterized as $\epsilon_0 = -\epsilon/2$, $\epsilon_1 = \epsilon/2$ and $\epsilon_2 = \epsilon/2 + E_{VS}$, where $\epsilon$ is the detuning between donor and QD ground state, and $E_{VS}$ is the valley splitting between two QD states. The detuning $\epsilon$ is tunable with a metallic gate, and valley splitting $E_{VS}$ ranges from tens of meV to a few meV depending on interface potential and interface roughness.

In the presence of a magnetic field, the electron spin Zeeman interaction is given by

$$H_Z = \frac{1}{2}\mu_B \sum_j P_j \vec{\sigma} \cdot \vec{g}(j) \cdot \vec{B},$$

where $P_j$ is the projection operator that selects the $j$th valley, $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ is a vector of the Pauli matrices ($z$-axis is along [001] direction), and $\vec{B} = B(\sin \theta_B \cos \phi_B, \sin \theta_B \sin \phi_B, \cos \theta_B)$ is the applied magnetic field. The anisotropic g-factor tensor $\vec{g}(j)$ is

$$\vec{g}(j) = g_{\perp} \vec{1} + g_{ani} \vec{U}(j),$$

where $g_{\perp}$ ($g_{||}$) is the g-factor perpendicular (parallel) to the valley ellipsoid, $g_{ani} = g_{||} - g_{\perp}$ measures the extent of g-factor anisotropy, $\vec{1}$ is an identity operator, and $\vec{U}(j)$ is an operator selecting the $|j\rangle$-th direction. Note that, the g-factor tensor could in principle be different for donor and QD, which can be considered in a more general form of Zeeman interaction in Appendix B.

The SOI couples the orbital and spin degrees of freedom and could affect the spin relaxation. We consider Rashba SOI,

$$H_{SO} = \alpha_{so}(p_x \sigma_y - p_y \sigma_x),$$

where $\alpha_{so}$ is Rashba SOI constant, and $p_x$ and $p_y$ are the in-plane momentum operators (interface direction is assumed to be [001]). The SOI due to the potential of the donor atom has been omitted since its effect on spin relaxation is small.

The energy dissipation for relaxation is provided by the electron-phonon interaction $H_{EP}$. In silicon, we have

$$H_{EP} = \sum_j \sum_{\vec{q} \lambda} e^{i \vec{q} \cdot \vec{r}} M^{(j)}_{\lambda \lambda} (b^{\dagger}_{-\vec{q} \lambda} + b_{\vec{q} \lambda}),$$
\[ M^{(j)}_{\Phi} = i \sqrt{\hbar q/2\rho_e v_\lambda} \Pi^{(j)}_{\Phi}, \]  
\[ \Pi^{(j)}_{\Phi} = e^{i\vec{b}_\Phi \lambda} \cdot (\Xi_d \hat{\tau} + \Xi_u \hat{U}^{(j)}_{\Phi}) \cdot \hat{q}, \]  

where \( P_j \) is the projection operator that selects the \( j \)th valley, \( \hat{b}_\Phi \) (\( \hat{b}_\Phi \)) is the creation (annihilate) operator of a phonon with wave vector \( \vec{q} \) and branch-index \( \lambda \), \( \lambda = t \) (longitudinal mode), \( t_1 \), or \( t_2 \) (transverse modes). \( \rho_e \) is the sample density (volume is set to unity), \( v_\lambda \) is phonon velocity, \( \hat{\tau} \) (longitudinal mode), \( \hat{\rho} \) and \( \hat{\lambda} \) are unit vectors of phonon polarization and wave vector, \( \Xi_d \) and \( \Xi_u \) are the dilation and uniaxial shear deformation potential constants, and the coefficient \( \Pi^{(j)}_{\Phi} \) is calculated and summarized in Appendix C.

### III. EFFECTIVE SPIN-PHONON INTERACTION

The electron-phonon interaction can dissipate the energy of the electron, however, it does not relax spin without a mechanism that hybridizes the electron spin and orbital state. To study spin relaxation, in principle, we should solve \( H_0 + H_Z + H_{SO} \) and find the corresponding eigenstates, where the states with different spins are hybridized. Then, by including electron-phonon interaction \( H_{EP} \), one can calculate the relaxation of the eigenstates. However, because we are interested in the spin degree of freedom, and because the hybridization of spin and orbital state is small, one can treat this perturbation theory without losing much accuracy. Suppose the orbital Hamiltonian is diagonalized as \( H_O = E_n |\vec{n}\rangle \langle \vec{n}| \),

\[ |\vec{n}\rangle = \sum_n \mathcal{C}_{\vec{n}n} |n\rangle, \]

where \( E_n \) and \( |n\rangle \) are the orbital eigenenergies and eigenstates, and the orbital basis state \( |n\rangle \) can be expressed in terms of envelope and Bloch functions (see Appendix A). Then, we consider \( H = H_0 + H_h + H_{EP} \), where \( H_0 = H_O + \sum_n \langle \vec{n}| H_Z |\vec{n}\rangle \langle \vec{n}| \) \( |\vec{n}\rangle \) is the unperturbed part, and \( H_h + H_{EP} \) is the perturbation. \( H_h = \sum_n \delta_{\vec{n},\vec{n}'} \langle \vec{n}| H_Z |\vec{n}\rangle \langle \vec{n}| \) \( |\vec{n}\rangle \) + h.c.) + \( H_{SO} \) hybrids spin and orbital state, and \( H_{EP} \) provides energy dissipation of the system. To 2nd order of \( H_h + H_{EP} \), the effective spin-flip Hamiltonian is

\[ (H)_{\Phi \Phi}^{\dagger} = \frac{1}{2} \sum_{n \neq n'} \left\{ \begin{array}{c} (H_h)_{\Phi n} (H_{EP})_{\Phi n}^{\dagger} + (H_{EP})_{\Phi n} (H_h)_{\Phi n}^{\dagger} \end{array} \right\}, \]

where \( (H)_{\Phi n}^{\dagger} \approx \langle \vec{n}| H |\vec{n}'\rangle \) and \( E_Z \) is the ground orbital Zeeman splitting determined by \( \langle 0| H_Z |0\rangle \).

In the following subsections, we will obtain the matrix elements of \( H_Z, H_{SO} \) and \( H_{EP} \). We will use a simplified notation \( (H_h)_{\vec{n}\vec{n}'} \approx \langle \vec{n}| H |\vec{n}'\rangle \) for the matrix element in the diagonalized orbital basis, and \( H_{\vec{n}n'} \approx \langle \vec{n}| H |n'\rangle \) for the matrix element in the original orbital basis, where \( H_i \) can be \( H_Z, H_{SO} \) or \( H_{EP} \). We also use \( \vec{r} \) to denote the excited orbital states, i.e. \( \vec{r} \neq 0 \) is always assumed.

### A. Zeeman Interaction Induced Hybridization

Zeeman interaction induced spin relaxation is known to be the dominant spin relaxation mechanism in a single donor, where g-factor anisotropy leads to hybridization of spin-valley states. In a coupled donor-QD system, Zeeman interaction will also hybridize spin and orbital states \( |0\rangle, |1\rangle \) and \( |2\rangle \), and give rise to additional spin relaxation besides the relaxation in a single donor.

To find the matrix element of Zeeman interaction in the orbital eigenstates, we first express Zeeman interaction in the basis of donor ground state \( |0\rangle \) and QD ground states \( |1\rangle \) and \( |2\rangle \), then, Zeeman interaction is

\[ H_{Z,nn'} = \frac{1}{2} \mu_B \vec{\sigma} \cdot \vec{g}^{(n')} \cdot \vec{B}, \]

\[ \vec{g}^{(n')} = (g_\perp \hat{\tau} + g_{ani} \hat{\rho}_{n,n}) \delta_{nn'}, \]

\[ \hat{D}^{(nn')} = \sum_j \alpha_n^{(j)} \alpha_n'^{(j)} \hat{U}^{(j)}, \]

where \( \alpha_n^{(j)} \) is probability amplitude of state \( |n\rangle \) in the \( j \)th valley. Then, we can express Zeeman interaction in the basis of orbital eigenstates \( |\vec{n}\rangle \). From Eq. \( (7) \), \( |\vec{n}\rangle = \sum_n \mathcal{C}_{\vec{n}n} |n\rangle \), Zeeman interaction can be expressed in the basis of orbital eigenstates

\[ (H_Z)_{0\vec{n}} = \frac{1}{2} \mu_B \vec{\sigma} \cdot \vec{g}^{(0\vec{n})} \cdot \vec{B}, \]

\[ \vec{g}^{(0\vec{n})} = g_\parallel \hat{\tau}_\parallel + g_{ani} \sum_n \mathcal{C}_{\vec{n}n}^* \mathcal{C}_{\vec{n}n} \hat{D}^{(nn')}, \]

where the off-diagonal elements of \( \vec{g}^{(0\vec{n})} \) are zero, and the diagonal elements are

\[ \vec{g}^{(0\parallel)} = g_\parallel \hat{\tau}_\parallel + g_{ani} \sum_n \mathcal{C}_{\vec{n}n}^* \mathcal{C}_{\vec{n}n} \hat{D}_{zz} \]

where

\[ \vec{B} = \hat{B}_{zz} = \frac{1}{3} \hat{\tau}_z - \hat{U}^{(z)} \]

To find the effective spin-orbit hybridization term, we need to express Zeeman interaction in a new \( (X,Y,Z) \) coordinate system, where \( Z \) axis is along the spin quantization axis determined by \( \langle 0| H_Z |0\rangle \). However, since \( g_\perp \approx g_\parallel \approx 2 \gg g_{ani} \), the spin quantization can be taken approximately along the applied magnetic field. Therefore, in the new \( (X,Y,Z) \) coordinate, the spin-orbit hybridization term due to Zeeman interaction is

\[ (H_Z)_{0\vec{r}}^{\dagger} = \frac{1}{2} \mu_B B g_X \hat{\sigma}_X, \]
\[ g_X^r \approx g_{ani} C_{\theta 0} C_{\theta 0} \Delta_{XZ}, \tag{20} \]

where \( g_{ani} = 1 \) and \( \Delta_{XZ} = \frac{1}{2} \sin 2\theta_B \).

Eq. (20) indicates that the hybridization due to Zeeman interaction is proportional to \( C_{\theta 0} C_{\theta 0} \), the g-factor anisotropy \( g_{ani} \), and \( \Delta_{XZ} = \frac{1}{2} \sin 2\theta_B \). The hybridization is maximum when \( \theta_B = 45^\circ \), and is zero when \( \theta_B = 0^\circ \) or \( 90^\circ \). The hybridization becomes zero because the spin quantization direction (given by \( G_{\theta 0}^r \)) and the direction of spin operator (given by \( G_{\theta 0}^r : \vec{B} \)) in the hybridization term \( \langle HZ \rangle_{\theta r} \) are along the same direction as \( \vec{B} \), when \( \vec{B} \) is along the main axis of g-factor tensor. In this case, the transpose coupling of spin to phonon, which is responsible for spin relaxation, becomes zero.

Finally, if g-factor tensor \( \gamma^{ij}(r) \) is considered to be different between donor and QD, one can show that the only difference in the hybridization term is that \( g_{ani} \) is replaced by \( g_{\theta D,ani} \), which is the g-factor anisotropy in the QD (see Appendix D).

\[ \gamma^{ij}(r) \]

### B. SOI Induced Hybridization

The SOI could also hybridize the spin and orbital states. Together with electron-phonon interaction, it will induce spin relaxation. To evaluate the matrix element \( \langle HSO \rangle_{\theta r} \), i.e. \( (p_x)_{\theta r} \) and \( (p_y)_{\theta r} \), it is convenient to use the commutation relation \( [x, H_{XZ}] = i\hbar p_x/m^* \), where an average effective mass \( m^* = 0.315m_0 \) is chosen because of the presence of multiple valley states (see Appendix D). From the commutation relation, we have

\[ (p_x)_{\theta r} \approx m^* E_{\theta r} x_{\theta r}/(i\hbar), \tag{21} \]

where \( x_{\theta r} = \langle \theta | x | r \rangle \) and \( E_{\theta r} = E_r - E_\theta \) is the energy difference of the eigenstates in the absence of SOI. By using the single effective mass \( m^* \), the estimated matrix element could be different from actual values by at most a factor of three.

The matrix element \( x_{\theta r} \) can be written as

\[ x_{\theta r} = \sum_{nn'} C_{\theta 0}^n C_{\theta 0}^{n'} x_{nn'}^{(1)} + x_{nn'}^{(2)}, \tag{22} \]

where \( x_{nn'} \) is the matrix element in the original basis, and \( x_{nn'}^{(1)} \) ( \( x_{nn'}^{(2)} \)) contains only the terms with \( n' = n \) ( \( n' \neq n \)) in the summation. In \( x_{nn'}^{(2)} \), the terms of \( x_{01} \) and \( x_{02} \) are small because of the spatial separation of donor and QD states. The only contribution could come from \( x_{12} \) that couples two valley states of QD. The magnitude of \( x_{12} \) is on the order of 1 nm estimated in a recent experiment, and it should be even smaller for a flat interface. The term \( x_{nn'}^{(2)} \) will be omitted in the following discussion. For the term \( x_{nn'}^{(1)} \), one can show that

\[ x_{nn'}^{(1)} = C_{\theta 0}^n C_{\theta 0}^{n'} d_x, \]  

where \( d_x \) is the projection of a vector connecting the center of donor and center of QD on the x-axis. Thus,

\[ (p_x)_{\theta r} \approx C_{\theta 0}^n C_{\theta 0}^{n'} (\alpha_{so}/\alpha_{so}) E_{\theta r} \cos \phi_d, \tag{23} \]

where \( \alpha_{so} = \alpha_{so} m^* d_{ij}/(i\hbar) \), \( d_{ij} \) is the in-plane separation between donor and QD, \( \phi_d \) is introduced so that \( d_x = d_{ij} \cos \phi_d \) and \( d_y = d_{ij} \sin \phi_d \). Therefore, from Eq. (5),

\[ (H_{SO})_{\theta r}^{\uparrow\downarrow} = C_{\theta 0}^n C_{\theta 0}^{n'} (E_{\theta r} \sigma_{x}^{\uparrow\downarrow}), \]  

where \( \sigma_{x}^{\uparrow\downarrow} = (\sigma_{x}^{\uparrow} \cos \phi_d - \sigma_{z}^{\uparrow} \sin \phi_d) \). Similarly, we have

\[ (H_{SO})_{\theta r}^{\downarrow\uparrow} = -C_{\theta 0}^n C_{\theta 0}^{n'} (E_{\theta r} \sigma_{z}^{\downarrow\uparrow}), \tag{24} \]

where the minus sign indicates that there will be cancellation of two terms in Eq. (10) in the limit of zero magnetic field. This cancellation, known as Van-Vleck cancellation, will result in an extra \( E_Z^2 \) dependence (besides the contribution of \( E_Z^2 \) from phonon spectral density) for spin relaxation. The results also indicate that the hybridization due to SOI is proportional to \( \alpha_{so} \) and the lateral separation of the donor and QD. Interestingly, there is no coupling if the donor and QD are vertically aligned. In that case, \( (p_x)_{\theta r} \) and \( (p_x)_{\theta r} \) are zero, and hence the matrix elements of \( H_{SO} \) vanish.

### C. Electron-Phonon Matrix Elements

The electron-phonon interaction couples the ground \( |0\rangle \) and excited orbital states \( |\vec{r}\rangle \) (i.e. \( \vec{r} \neq 0 \)) with the same spin orientation. From Eq. (26), (27), (28) and (29), we have

\[ (H_{EP})_{\theta r}^{\uparrow\downarrow} = \sum_{\vec{q} \lambda} (M_{\vec{q} \lambda})_{\theta r}^{\uparrow\downarrow} (b_{\vec{q} \lambda}^+ + b_{\vec{q} \lambda}), \tag{26} \]

\[ (M_{\vec{q} \lambda})_{\theta r}^{\uparrow\downarrow} = \sum_{nn'} C_{\theta 0}^n C_{\theta 0}^{n'} M_{\vec{q} \lambda, nn'}, \tag{27} \]

\[ M_{\vec{q} \lambda, nn'} = \sum_j \alpha_n^{(j)} \alpha_n^{(j)} f_n^{(j)}(\vec{q}) M_{\vec{q} \lambda}^{(j)}, \tag{28} \]

where \( (H_{EP})_{\theta r} \) is the form factor \( f_n^{(j)}(\vec{q}) \) is

\[ f_n^{(j)}(\vec{q}) = \int d\vec{r} F_n^{(j)}(\vec{r}) F_n^{(j)}(\vec{r} e^{i\vec{q} \cdot r}), \tag{29} \]

where \( F_n^{(j)}(\vec{r}) \) is the envelope function in the \( j \)th valley. For spin splitting around \( \omega_Z \approx 1 \text{ GHz} \), \( |\vec{q}| = \omega_Z/v_j \approx \mu m^{-1} \). Thus, the wavelength of phonons which are on resonance with the spin splitting is much larger than the geometrical size of the donor-QD system. In the limit of long wave phonons, we have \( \exp(i\vec{q} \cdot \vec{r}) \approx 1 \) and \( f_n^{(j)}(\vec{q}) \approx \delta_{nn'} \). Therefore,

\[ M_{\vec{q} \lambda, nn'} = \sum_j |\alpha_n^{(j)}|^2 M_{\vec{q} \lambda}^{(j)}, \tag{30} \]
where $M_{\mathcal{Q},22} = M_{\mathcal{Q},11} \neq M_{\mathcal{Q},00}$. Because of the orthogonal relation $\sum_n C_{\alpha n}^* C_{\bar{r} n} = 0$, we have

$$
(M_{\mathcal{Q} \lambda})_{\bar{r} \bar{r}'} = C_{\alpha 0}^* C_{\bar{r} 0} M_{\mathcal{Q} \lambda,00},
$$

(31)

$$
M_{\mathcal{Q} \lambda}' = i \sqrt{\hbar q / 2 \rho_c} \alpha \Pi_{\mathcal{Q} \lambda}',
$$

(32)

$$
\Pi_{\mathcal{Q} \lambda}' = \Xi_{\alpha} e^{i(q_{\mathcal{Q} \lambda} \cdot \vec{\Delta} \cdot \vec{q})},
$$

(33)

where $M_{\mathcal{Q} \lambda}' = M_{\mathcal{Q} \lambda,00} - M_{\mathcal{Q} \lambda,11}$, $\Pi_{\mathcal{Q} \lambda}' = \Xi_{\alpha} (1/3 - \cos^2 \vartheta)$, and $\Pi_{\mathcal{Q} \lambda,22} = 0$ (see Appendix C). Therefore, in the long wave limit, the electron-phonon interaction matrix elements between orbital eigenstates is proportional to the extent of mixing of donor and QD states $C_{\alpha 0}^* C_{\bar{r} 0}$, and proportional to the uniaxial shear deformation potential constant $\Xi_{\alpha}$.

The matrix element $M_{\mathcal{Q} \lambda}' \propto \omega_\mathcal{Q}^{1/2}$ is similar to the case of an electron in a bulk donor, but different from the case of a single QD. For an electron in a single QD, the electron-phonon interaction matrix element scales as $\omega_\mathcal{Q}^{3/2}$, where the extra $\omega_\mathcal{Q}$ is because of the dipole interaction needed to couple the ground and excited states. Thus, for the same hybridization mechanism of SOI, the phonon-induced spin relaxation in a QD has an extra $B^2$ dependence compared to the spin relaxation studied here.\[36\]

D. Summary of Effective Spin-Phonon Interactions

With the form of the electron-phonon interaction matrix elements, the effective spin-phonon Hamiltonian is

$$
(H_1)_{00}^{\uparrow \downarrow} = \frac{H_{EP}}{2} \sum_{\bar{r}} -E_{\bar{r} 0} H_{\bar{r}}^+ + E_{\bar{r}} H_{\bar{r}}^-, \quad (34)
$$

$$
H_{\mathrm{EP}}^{\uparrow \downarrow} = \sum_{\mathcal{Q} \lambda} M_{\mathcal{Q} \lambda}' (b_{\mathcal{Q} \lambda}^\dagger b_{\mathcal{Q} \lambda} + b_{\mathcal{Q} \lambda}^\dagger b_{\mathcal{Q} \lambda}^\dagger), \quad (35)
$$

$$
H_{\uparrow}^+ = C_{\alpha 0}^* C_{\bar{r} 0} (H_{\bar{r}})_{00}^{\uparrow} + C_{\alpha 0}^* C_{\bar{r} 0} (H_{\bar{r}})_{\bar{r} 0}^{\uparrow}, \quad (36)
$$

$$
H_{\downarrow}^- = C_{\alpha 0}^* C_{\bar{r} 0} (H_{\bar{r}})_{00}^{\downarrow} + C_{\alpha 0}^* C_{\bar{r} 0} (H_{\bar{r}})_{\bar{r} 0}^{\uparrow}. \quad (37)
$$

There are two possible hybridization mechanisms, i.e., $H_2$ and $H_{SO}$, however, we will study separately each hybridization mechanism, and will neglect interference of these two hybridization terms.

When $H_{\bar{r}} = H_Z$, we have $H_{\bar{r}}^-$ vanishes due to the same sign and magnitude of matrix elements of $(H_Z)_{0\bar{r}}^{\uparrow \downarrow}$ and $(H_Z)_{\bar{r} 0}^{\uparrow \downarrow}$. While

$$
H_{\bar{r}}^+ = |C_{\bar{r} 0}^* C_{\alpha 0}|^2 g_{an} \Delta_{\mathrm{XZ}} \mu_{BB}, \quad (38)
$$

where $\sigma_{\chi}^{\uparrow \downarrow} = 1$ in the $(X,Y,Z)$ coordinate. Therefore, the effective spin-flip Hamiltonian due to Zeeman interaction and electron-phonon interaction is

$$
(H_Z + H_{EP})_{00}^{\uparrow \downarrow} = -\frac{g'_{\chi}}{2} \Delta_{\mathrm{XZ}} \eta_Z E_Z H_{EP}, \quad (39)
$$

$$
\eta_Z = \sum_{r=1,2} \frac{E_{\bar{r} 0} |C_{\alpha 0}^* C_{\bar{r} 0}|^2}{E_{\bar{r} 0}^2 - E_Z^2}, \quad (40)
$$

where $g' \equiv g_{ani}/g_{ff}$ is the rescaled $g$-factor anisotropy and the coefficient $\eta_Z$ accounts for contributions from different orbitals to the effective spin-phonon interaction.

When $H_{\bar{r}} = H_{SO}$, $H_{\bar{r}}^+$ vanishes due to the different signs of matrix elements of $(H_{SO})_{00}^{\uparrow \downarrow}$ and $(H_{SO})_{\bar{r} 0}^{\uparrow \downarrow}$. While

$$
H_{\bar{r}}^- = 2 |C_{\bar{r} 0}^* C_{\alpha 0}|^2 \sigma_{\chi}^{\uparrow \downarrow} \eta_{SO} E_Z H_{EP}, \quad (41)
$$

Therefore, the effective spin flip Hamiltonian due to SOI and electron-phonon interaction is

$$
(H_{SO} + H_{EP})_{00}^{\uparrow \downarrow} = a_{so} \sigma_{\chi}^{\uparrow \downarrow} \eta_{SO} E_Z H_{EP}, \quad (42)
$$

where $\eta_{SO} = \eta_Z$. $H_{\bar{r}}$ and $H_{SO}$ are different and the cancellation of terms is different, however, the final effective spin-phonon interaction Hamiltonians are similar. The $g$-factor anisotropy in Zeeman interaction is a result in part of the microscopic SOI, so both mechanisms originate from SOI, one from microscopic SOI not in the effective mass theory, the other from the SOI in the effective mass theory. Both hybridizations show the same dependence with $E_Z$. They also show the same dependence on the hybridization of orbital states $\eta_{SO} = \eta_Z$. The only difference is the angular dependencies with magnetic field due to the difference between $\Delta_{\mathrm{XZ}}$ and $\sigma_{\chi}^{\uparrow \downarrow}$.

The strength of spin-phonon interaction for both mechanisms is proportional to $\eta_Z$, which depends on the energies of spin-orbital states. $\eta_Z$ can be strongly enhanced, when the spin state is in resonant with the orbital states, where a corresponding spin relaxation hot-spot appears. $\eta_Z$ can also be zero, when contributions from different orbitals cancel with each other, where spin relaxation is strongly suppressed (spin relaxation cool-spot).

IV. SPIN RELAXATION

The spin relaxation time is given by $1/T_1 = W_{1^+} + W_{1^-}$, where $W_{1^+} = \Gamma [n(\omega_\mathcal{Q}) + 1]$ is the rate for transition from the higher-energy (spin-up) state to lower energy (spin-down) state (emitting phonon) and $W_{1^-} = \Gamma [n(\omega_\mathcal{Q}) + 1]$ is the rate for the opposite transition (absorbing phonon), where $\Gamma = 2 \hbar \sum_{\mathcal{Q} \lambda} \langle |H_{00}^{\uparrow \downarrow}|^2 \delta(E_Z - \hbar \omega_\mathcal{Q}) \rangle$. Considering the zero temperature limit, the spin relaxation rate is given by

$$
1/T_1 = \Gamma_{Z-ph} + \Gamma_{SO-ph}, \quad (43)
$$
where $\Gamma_{Z-ph}$ is the spin relaxation due to Zeeman interaction and phonon noise, and $\Gamma_{SO-ph}$ is the spin relaxation due to SOI and phonon noise. We find that

$$\Gamma_{Z-ph} = \frac{1}{4} \left(g' \eta_{Z} \Delta_{XZ} \right)^2 \left(\hbar \omega_{Z}\right) \Gamma_{ph}(\omega_{Z}),$$

$$\Gamma_{SO-ph} = \left|a_{so} \eta_{SO} \sigma_{z}^{x}_{\eta} \right|^2 \left(\hbar \omega_{Z}\right) \Gamma_{ph}(\omega_{Z}),$$

$$\Gamma_{ph}(\omega_{Z}) = \frac{1}{4 \pi \hbar \rho_{c} v_{x}^{e}} \sum_{\lambda} \frac{\omega_{\lambda}^{2}}{v_{\lambda}^{e}} \int_{0}^{\pi} d\theta \sin \phi \Pi_{\lambda}(\phi),$$

where $\omega_{Z} = E_{Z}/\hbar$ is the electron Zeeman frequency.

The analytical expressions indicate that both spin relaxation mechanisms show the same $B^2$ (or $\omega_{Z}^2$) dependence on the magnitude of the applied magnetic field. They also show the same dependence on the hybridization of orbital states since $\eta_{SO} = \eta_{Z}$. The two mechanisms show different angular dependencies on the orientation of the applied magnetic field. They also show different magnitudes depending on other parameters. Spin relaxation due to Zeeman interaction shows $g_{ani}^2$ dependence on the g-factor anisotropy, while spin relaxation due to Zeeman interaction shows $\alpha_{so}^2$ dependence on the SOI strength and $|d_{\parallel}|^2$ dependence on the lateral separation of the donor and the QD. The spin relaxation due to Zeeman interaction shows $\Delta_{XZ}^2 = \sin^2(2\theta_B)$ dependence on the orientation of the applied magnetic field, while the spin relaxation due to SOI shows $|\sigma_{z}^{x}_{\eta}|^2 = 1 - \sin^2 \theta_B \cos^2(\phi_B - \phi_d)$ dependencies on the orientation of the applied magnetic field and $\phi_d$ of the lateral separation with respect to the [100] direction.

V. SPIN RELAXATION RATE

In the following, we report the numerical results of spin relaxation as a function of (the magnitude and orientation of) the applied magnetic field and detuning of the donor and QD ground states. Unless indicated, we choose the following values for parameters: $t_{01} = t_{02} = 0.1$ meV, $E_{VS} = 0.3$ meV, $\Xi_{d} = 5.0$ eV, $\Xi_{u} = 8.77$ eV, $g_{ani} = 0.001$, $\alpha_{so} = 45$ m/s, and $|d_{\parallel}| = 2$ nm.

A. $|B|$ dependence

Figure 2 shows the spin relaxation rate $1/T_1$ due to each mechanism as a function of the magnitude of the applied magnetic field for detuning $\epsilon = -1$ meV. Since the g-factor anisotropy is unknown, we choose two possible values for $g_{ani}$, i.e. $g_{ani} = 0.01$ (black solid line) as indicated by recent tight-binding calculations[47] and $g_{ani} = 0.001$ (red line) as has been used in literature[30, 32]. For SOI, the lateral shift $d_{\parallel}$ of QD relative to donor can be tuned experimentally, we choose $d_{\parallel} = 1$ nm (blue dotted line) and $d_{\parallel} = 2$ nm (purple dot-dashed line). We choose

![FIG. 2: Spin relaxation as a function of magnetic field when detuning $\epsilon = -1$ meV. We show spin relaxation due to Zeeman interaction when $g_{ani} = 0.01$ (black solid line) and $g_{ani} = 0.001$ (red solid line), and spin relaxation due to SOI when $d_{\parallel} = 1$ nm (blue dotted line) and $d_{\parallel} = 2$ nm (purple dot-dashed line).](image)

FIG. 3: Energy diagram as a function of magnetic field when detuning $\epsilon = -1$ meV. The ground orbital spin-up state crosses twice (marked as filled black dots) with two excited orbital spin-down states, which is responsible for the spin relaxation hot-spots in Fig. 2. At the spin relaxation cool-spot (marked as an empty circle), a schematic diagram shows two possible spin relaxation paths (dashed and dotted lines).

![FIG. 3: Energy diagram as a function of magnetic field when detuning $\epsilon = -1$ meV. The ground orbital spin-up state crosses twice (marked as filled black dots) with two excited orbital spin-down states, which is responsible for the spin relaxation hot-spots in Fig. 2. At the spin relaxation cool-spot (marked as an empty circle), a schematic diagram shows two possible spin relaxation paths (dashed and dotted lines).](image)

FIG. 4: A general schematic energy diagram at the spin relaxation cool-spot. There are two possible spin relaxation paths (dashed and dotted lines) indicated by lines with arrows, whose interference leads to the suppression of spin relaxation.

![FIG. 4: A general schematic energy diagram at the spin relaxation cool-spot. There are two possible spin relaxation paths (dashed and dotted lines) indicated by lines with arrows, whose interference leads to the suppression of spin relaxation.](image)
the polar angle of magnetic field as $\theta_B = \pi/4$, and the azimuthal angle $\phi_B = 0$. We choose $\phi_d = 0$ for the angle of the in-plane QD shift $d'_\parallel$ relative to [100]. When $g_{ani} = 0.01$, the spin relaxation rate increases from 0.02 $s^{-1}$ to 100 $s^{-1}$ with the applied magnetic field increasing from $B = 1$ T to $B = 5$ T, due to the $B^5$ dependence of spin relaxation at smaller magnetic fields. As $B$ further increases, spin relaxation peaks (spin relaxation hot-spot) appear due to strong spin-orbit hybridization that occurs when the ground orbital state $|\bar{0}\rangle$ crosses with one of the two excited orbital states $|\bar{r}\rangle$ with opposite spin orientation. Interestingly, there is also a spin relaxation dip (cool-spot) between two peaks due to the destructive interference of different spin relaxation paths.

Figure 3 shows the energy diagram as a function of magnetic field when detuning $\epsilon = -1$ meV. The Zeeman splitting for each orbital eigenstate increases with magnetic field. For small detunings, the ground orbital spin-up state can cross twice (marked as filled black dots) with two excited orbital spin-down states in the B field range considered, which is responsible for the spin relaxation hot-spots in Fig. 2. At the magnetic field marked as an empty circle, there is a spin relaxation cool-spot, where a schematic diagram is also shown for the energy levels and the spin relaxation paths.

Figure 4 shows a general schematic diagram of energy levels at the spin relaxation cool-spot and the two possible spin relaxation paths (dashed and dotted lines). The relaxation is possible when spin-up ground state $|G\uparrow\rangle$ is hybridized with spin-down excited states. When there are two available spin-down excited states $|Ex1\downarrow\rangle$ or $|Ex2\downarrow\rangle$, the two spin relaxation path can have destructive interference, and the spin relaxation is suppressed.

Figure 5 shows the spin relaxation rate $1/T_1$ due to each mechanism as a function of the applied magnetic field for detuning $\epsilon = 1$ meV, where the QD states are lower than donor ground state. We show spin relaxation due to Zeeman interaction when $g_{ani} = 0.001$ (black solid line), and spin relaxation due to SOI when $d'_\parallel = 2$ nm (red dashed line).

In Figure 5, there is a dip very close to the first peak. To understand the dip position, we study the condition of destructive interference. According to Eq. (40), an interference dip appears when $E_{10}^2|C_{10}'|^2 + E_{20}^2|C_{20}'|^2 = 0$. For $\epsilon = 1$ meV, we have $E_{10} \approx E_{VS} = 0.3$ meV, $E_{20} \approx \epsilon = 1$ meV, $|C_{00}| \approx |C_{10}| \approx |C_{20}| \approx 1$. Therefore, the condition for destructive interference is
FIG. 8: Spin relaxation as a function of the polar angle $\theta_B$ of the applied magnetic field when detuning $\epsilon = 0$ meV and $B = 0.5$ T. We show spin relaxation due to Zeeman interaction (black solid line) with $\theta_B = \pi/4$ and $\phi_B = 0$, and spin relaxation due to SOI when $d_1 = 2$ nm with $\phi_B - \phi_d = 0$ (red dashed line), $\phi_B - \phi_d = \pi/4$ (blue dotted line), and $\phi_B - \phi_d = \pi/2$ (purple dot-dashed line).

$E_Z \approx \sqrt{E_{VS}^2 + \epsilon E_{VS}} \frac{C_{01}}{E_{20}} \approx \frac{E_{VS} + t_{02}^2}{2\epsilon}$, and the distance between the peak and dip is $t_{02}^2/(2\epsilon) \sim 5$ meV (or 43 mT), which explains the tiny separation of the peak and dip in the figure.

Figure 6 shows the corresponding energy diagram when $\epsilon = 1$ meV. The level crossings, which is responsible for the spin relaxation hot-spots, are marked as filled dots. The spin relaxation cool-spot (marked as an empty circle) is due to destructive interference of relaxation paths, which is shown schematically in the Figure.

Figure 7 shows the same plot as Figure 5 when the detuning $\epsilon = 0$ meV, where the donor state is in resonance with the lower QD state and the hybridized orbital states are split by the tunneling coupling. When B is small, the spin relaxation shows again the $B^2$ dependence. However, due to the stronger orbital hybridization, the spin relaxation rate at $B = 1$ T is much faster than the case of $\epsilon = -1$ meV or $\epsilon = 1$ meV. Two spin relaxation peaks and one spin relaxation dip appear similarly as before.

B. $\theta_B$, $\phi_B$ dependencies

Besides the dependence on the magnitude of the applied magnetic field, we also study the dependence on the orientation of the applied magnetic field.

Figure 8 shows the spin relaxation rate $1/T_1$ due to each mechanism as a function of the polar angle $\theta_B$ of the applied magnetic field when detuning $\epsilon = 0$ meV and $B = 0.5$ T. We show spin relaxation due to Zeeman interaction when $g_{ani} = 0.001$ (black solid line), and spin relaxation due to SOI when $d_1 = 2$ nm (red dashed line). We choose the azimuthal angle $\phi_B = 0$ for spin relaxation due to Zeeman interaction (black solid line), and $\phi_B - \phi_d = 0$, $\phi_B - \phi_d = \pi/4$ and $\phi_B - \phi_d = \pi/2$ for spin relaxation due to SOI. The spin relaxation due to Zeeman interaction goes to zero when the polar angle $\theta_B = 0$ or $\pi/2$, i.e. when the magnetic field is in-plane or out-of-plane, and it is maximum when $\theta_B = \pi/4$. The spin relaxation due to Zeeman interaction vanishes at certain orientations of magnetic field due to the vanishing of hybridization as discussed above. However, spin relaxation due to SOI becomes maximum when $\theta_B = 0$ (in-plane) and minimum when $\theta_B = \pi/2$ (out-of-plane).

Figure 9 shows the spin relaxation rate $1/T_1$ due to each mechanism as a function of the azimuthal angle $\phi_B$ when detuning $\epsilon = 0$ meV, $B = 0.5$ T and $\theta_B = \pi/4$. We show spin relaxation due to Zeeman interaction (black solid line), and spin relaxation due to SOI when $d_1 = 2$ nm with $\phi_B = 0$ (red dashed line), $\phi_B = \pi/4$ (blue dotted line), and $\phi_B = \pi/2$ (purple dot-dashed line).

Figure 10 shows the same plot as Figure 5 when the detuning $\epsilon = 0$ meV and $\theta_B = \pi/4$. We show spin relaxation due to Zeeman interaction (black solid line), and spin relaxation due to SOI when $d_1 = 2$ nm with $\phi_B = 0$ (red dashed line), $\phi_B = \pi/4$ (blue dotted line), and $\phi_B = \pi/2$ (purple dot-dashed line).
use the same $g_{ani}$ for Zeeman interaction mechanism and the same $d_{||}$ for the SOI mechanism as in Figure 8. We choose $\phi_d = 0$, $\phi_d = \pi/4$ and $\phi_d = \pi/2$ for spin relaxation due to SOI. Since the spin relaxation due to Zeeman interaction is maximized when $\theta_B = \pi/4$, it dominates over the spin relaxation due to SOI. As shown in the figure, the spin relaxation due to Zeeman interaction shows no dependence with $\phi_B$.

Figure 10 shows the spin relaxation rate $1/T_1$ due to each mechanism as a function of the azimuthal angle $\phi_B$ when detuning $\epsilon = 0$ meV, $B = 0.5$ T and $\theta_B = \pi/2$. We use the same $g_{ani}$ and $d_{||}$ as in Figure 8 and 9. The spin relaxation due to Zeeman interaction is suppressed when $\theta_B = \pi/2$, and the spin relaxation due to SOI dominates. We choose $\phi_d = 0$, $\phi_d = \pi/4$ and $\phi_d = \pi/2$ for spin relaxation due to SOI. Spin relaxation due to SOI depends on $\phi_B - \phi_d$, as previously indicated. The rate is minimum when $\phi_B = \phi_d$ and maximum when $\vec{B}$ and $\vec{d}$ are orthogonal. For in-plane B, the relaxation can be completely suppressed when $\phi_B = \phi_d$. By changing the angle of the QD shift relative to the donor with an electric field, we can modify the dependence of spin relaxation with azimuthal angle $\phi_B$ of the applied magnetic field. Thus, the electric field (in-plane) dependence of spin relaxation can be applied to tell whether the relaxation is dominated by Zeeman interaction or SOI.

C. Detuning dependence

Figure 11 shows the spin relaxation rate $1/T_1$ as a function of detuning between donor and interface states when the applied magnetic field $B = 0.5$ T. We use the same $g_{ani}$ and $d_{||}$ as before. We choose $\theta_B = \pi/4$, $\phi_B = 0$ and $\phi_d = 0$. Figure 11 shows that there is a broad transition of spin relaxation from negative to positive detuning for both spin relaxation mechanisms. There is no sharp peak because the orbital splitting is always larger than the spin Zeeman splitting, so that hotspot cannot happen in this case.

Figure 12 shows the spin relaxation rate $1/T_1$ as a function of the detuning when $B = 5$ T. We choose the same value for other parameters as in Figure 11. Figure 12 shows that there are multiple peaks as the detuning goes from negative to positive values, which result from the multiple crossings of ground orbital states with spin up and the excited orbital states with spin down. Interestingly, there is also spin relaxation dip at certain detuning is due to the destructive interference of two possible paths of spin relaxation.

FIG. 11: Spin relaxation as a function of detuning when $B = 0.5$ T. We show spin relaxation due to Zeeman interaction when $g_{ani} = 0.001$ (black solid line), and spin relaxation due to SOI when $d_{||} = 2$ nm (red dashed line). $\theta_B = \pi/4$, $\phi_B = 0$, and $\phi_d = 0$.

FIG. 12: Spin relaxation as a function of detuning ($B = 5$ T). Multiple peaks are due to multiple crossings of orbital states with opposite spin orientation. Spin relaxation dip at certain detuning is due to the destructive interference of two possible paths of spin relaxation.

FIG. 13: Energy diagram as a function of detuning when magnetic field $B = 5$ T. The ground orbital spin-up state crosses three times with excited orbital spin-down states, which is responsible for the spin relaxation hot-spots in Fig. 12. At spin relaxation cool-spot, a schematic diagram shows two possible spin relaxation paths (dashed and dotted lines), whose interference leads to the cancellation of spin relaxation.
cited orbital spin-down states, which is responsible for the spin relaxation hot-spots in Fig. 12. At the spin relaxation cool-spot, a schematic diagram shows two possible spin relaxation paths (dashed and dotted lines), whose interference leads to the cancellation of spin relaxation. The interference dip can dramatically reduce the spin relaxation rate and may be utilized for coherent spin qubit transfer; for example, by staying at the particular detuning to transfer spin qubit with minimum spin relaxation rate for the protection of spin qubit information.

Since detuning \( \epsilon \) can be controlled electrically the spin relaxation hot-spots can be used as a way to fast initialize spin state in experiments and reduce the spin initialization error. The multiple hot-spots can also be used to study valley physics, such as valley splitting in QDs. The qubit operation near a spin relaxation cool-spot could be of particular interest as a way to preserve quantum information during coherent transfer of spin information between donor atoms via interface states.

VI. COMPARISON WITH SPIN RELAXATION IN A BULK DONOR IN SILICON

The spin relaxation in a bulk P donor in silicon is dominated by Zeeman interaction, which hybridizes the donor ground spin-up state with the excited valley states of a single donor.\(^{29}\)\(^{30}\) The spin relaxation shows the \( B^2 \) dependence without peak or dip structures since the excited states of a bulk donor are at least 10 meV higher than the donor ground state, and the energy scale is much larger than the range of magnetic fields in experiment. The angular dependence of spin relaxation on the orientation of the applied magnetic field is given by \( |\Delta_{XZ}^{(15)}|^2 + |\Delta_{XZ}^{(16)}|^2 + |\Delta_{YZ}^{(15)}|^2 + |\Delta_{YZ}^{(16)}|^2 \propto \sin^2 \theta_B (4 \cos^2 \theta_B + \sin^2 \theta_B \sin^2 2\phi_B) \) (see Appendix E and reference [30]). The magnitude of the spin relaxation is on the order of \( 10^{-2} \) s\(^{-1} \) for 1 T magnetic field along the [111] direction.\(^{30}\)

In comparison, the spin relaxation in a P donor coupled to interface states in silicon can be a result of Zeeman interaction or SOI. Typically, the spin relaxation due to Zeeman interaction is still more important although it could be dominated by SOI in certain circumstances. When Zeeman interaction dominates the spin relaxation, the spin relaxation shows the same \( B^2 \) dependence when detuning \( \epsilon \) is much smaller than the range of magnetic fields in experiment. The angular dependence of spin relaxation on the orientation of the applied magnetic field is given by \( |\Delta_{XZ}|^2 \propto \sin^2 (2\theta_B) \).

We should mention that if the donor system is close to the metallic gates, where electrical noise such as Johnson noise could have a significant effect, then, the spin relaxation rate could show \( B^3 \) dependence with magnetic field because of the linear \( \omega \) dependence of spectral density for Johnson noise.\(^{20}\)\(^{48}\)\(^{51}\) Finally, we should mention that most of our analysis in this paper is also applicable when the donor is laterally coupled to a gate-defined QD, although the relative magnitude of spin relaxation rates due to Zeeman interaction and SOI could be modified; And the physics of spin relaxation hot-spot and cool-spot should also apply for an electron in a DQD.

VII. CONCLUSION

In conclusion, we have studied the spin relaxation of a donor coupled to QD-like interface states, we find both g-factor anisotropy and SOI can couple the donor ground state and QD states with opposite spin states, and together with phonon emission will lead to additional spin relaxation mechanisms. We find that both spin relaxation mechanisms shows \( B^5 \) dependence with the applied magnetic field when \( B \) is much smaller than the \( B \)-field of hot-spots. The spin relaxation mechanisms show different angular dependencies with the orientation of the applied magnetic field. Spin relaxation hot-spots are found due to crossings of orbital states with opposite spin orientations. The electrically tunable spin relaxation hot-spots can be used to fast initialize spin state and to study valley physics in silicon QDs. We also find spin relaxation dips due to the interference of spin relaxation paths, which may be used for quantum information transfer among spin qubits in different donor atoms. The orientation of the donor/QD geometry can be further used to suppress or enhance spin relaxation for the purpose of qubit initialization and information protection.

Appendix A: Effective mass approximation and orbital basis

In this appendix, we review the effective mass theory for silicon and give explicitly the orbital eigenstates in terms of envelope function and Bloch function. We study cases when an electric potential is from a donor atom or a gate-defined QD. We also give the connection of the basis states used in main text and the eigenstates of a single donor and the eigenstates of a QD.

In the absence of the spin degree of freedom, the Schrödinger equation is given by \( (H_{Si} + V_e)\Phi_n(\vec{r}) = E_n\Phi_n(\vec{r}) \), where \( H_{Si} \) is the unperturbed Hamiltonian of an electron near the conduction band minimum in a silicon crystal, \( V_e(\vec{r}) \) is the electrical potential from donor atom, interface and metallic gates, and \( \Phi_n(\vec{r}) \) is an eigenstate of the Hamiltonian. In a pure silicon crystal, the conduction band minima occur near the X symmetry points with six-fold degeneracy, normally referred to as valley degeneracy. In the presence of the potential \( V_e(\vec{r}) \), the valley degeneracy is lifted. The wavefunction can be
written as

$$\Phi_n(\vec{r}) = \sum_{j=1}^{6} a_n^{(j)} F_n^{(j)}(\vec{r}) \psi_j(\vec{r}), \quad (A1)$$

where $j$ is the valley index, $\psi_j(\vec{r}) = e^{i\vec{k}_j \cdot \vec{r}} u_j(\vec{r})$ is a Bloch function, $\vec{k}_j$ is one of the six minima $\pm k_0 \hat{x}, \pm k_0 \hat{y}$ or $\pm k_0 \hat{z}$ ($k_0 = 0.85 \cdot 2\pi/a_0$ and $a_0$ is the lattice constant), and $u_j(\vec{r})$ is the periodic function (Bloch’s theorem). $F_n^{(j)}(\vec{r})$ is the slowly varying envelope function, and $a_n^{(j)}$ is the probability amplitude of $j$th valley state due to valley coupling in the presence of a sharp potential.

Within the effective mass approximation, $F_n^{(j)}(\vec{r})$ satisfies a Schrödinger-like equation for the $j$-th valley. For example, $F_n^{(\pm)}(\vec{r})$ satisfies

$$\left[-\frac{\hbar^2}{2m_\parallel} \frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{2m_\perp} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V_c(\vec{r}) \right] F_n^{(\pm)}(\vec{r}) = (E_n^{(\pm)} - E_n^{(\Delta)}) F_n^{(\pm)}(\vec{r}), \quad (A2)$$

where $m_\parallel$ and $m_\perp$ are the longitudinal and transverse mass, $E_n^{(\Delta)}$ is the energy of band minimum at $\vec{k} = \pm k_0 \hat{z}$, $E_n^{(\pm)}$ is the eigenenergy. Similar equations can be obtained for the envelope functions $F_n^{(x)}(\vec{r})$ and $F_n^{(y)}(\vec{r})$ at $\vec{k} = \pm k_0 \hat{x}$ and $\pm k_0 \hat{y}$ minima. A sharp potential can further couple different valley states of $F_n^{(j)}(\vec{r}) \psi_j(\vec{r})$. By solving the coupled multi-valley Schrödinger equation, the eigenstates $\Phi_n(\vec{r})$ in Eq. (A1) can be obtained, and valley degeneracy can be lifted due to the broken of symmetry in presence of potential $V_c(\vec{r})$.

According to the symmetry, when $V_c(\vec{r})$ is the potential of a single $P$ donor in silicon, the coefficients of the six lowest eigenstates as given by Kohl and Luttinger, and modified to be orthogonal are,[22, 53]

$$
ap_{P,1} = 1/\sqrt{[1,1,1,1,1,1]}, 
ap_{P,2} = 1/\sqrt{[1,-1,0,0,0,0]}, 
ap_{P,3} = 1/\sqrt{[0,0,1,-1,0,0]}, 
ap_{P,4} = 1/\sqrt{[0,0,0,1,-1,0]}, 
ap_{P,5} = 1/\sqrt{[0,-1,1,-1,0,0]}, 
ap_{P,6} = 1/\sqrt{[1,1,1,1,1,0]},$$

where the basis used is $\{F_P^{(x)} \psi_x, F_P^{(y)} \psi_y, F_P^{(z)} \psi_z\}$ and $F_P^{(j)}(\vec{r} - \vec{R}_P)$ is the ground state envelope function satisfies the Schrödinger-like equation with $V_c(\vec{r})$ a single donor potential.

When $V_c(\vec{r})$ is the potential of a single QD at a z interface, the coefficients of the two lowest eigenstates are

$$a_{QD,1} = 1/\sqrt{[1,0,0,0,0,0],} \quad a_{QD,2} = 1/\sqrt{[0,0,0,0,0,0],}$$

where the basis is $\{F_{QD}^{(x)} \psi_x, F_{QD}^{(y)} \psi_y, F_{QD}^{(z)} \psi_z\}$ and $F_{QD}^{(j)}(\vec{r} - \vec{R}_{QD})$ is the ground state envelope function satisfies the Schrödinger-like equation with $V_c(\vec{r})$ the QD potential, $\phi_0$ is the valley phase difference between $+z$ and $-z$ valleys.[52]

In the main text, we use basis state $|n\rangle$ of a donor ground state and two lowest QD states, which can be expressed in terms of envelope and Bloch functions

$$\langle r | n \rangle = \sum_{j=1}^{6} a_n^{(j)} F_n^{(j)}(\vec{r}) \psi_j(\vec{r}), \quad (A2)$$

where the coefficients $a_n$ is related to $a_P$ and $a_{QD}$; $a_0 = a_{P,1}, a_1 = a_{QD,1}, a_2 = a_{QD,2}$; The envelope functions $F_0^{(j)}$ and $F_1^{(j)} = F_2^{(j)}$ are the orthornormalized states of $F_P^{(j)}$ and $F_{QD}^{(j)}$.

Appendix B: Zeeman interaction when $g^{(j)}$ is different for donor and QD

In this appendix, a general form of the Zeeman interaction is studied when the g-factor is different for donor and QD. Based on the general form of Zeeman interaction, we study the spin-orbit hybridization due to the Zeeman interaction. We find that the hybridization exhibits a similar form as in the main text. The only difference is that the hybridization is proportional to the g-factor anisotropy $g_{QD,ani}$ in a QD instead of $g_{ani}$.

In the presence of an external magnetic field, the Zeeman interaction is given by

$$H_Z = \frac{1}{2} \mu_B \sum_{nj} \left| F_n^{(j)} \psi_j \right\rangle \left\langle F_n^{(j)} \psi_j \right| \vec{\sigma} \cdot \vec{g}^{(n,j)} \cdot \vec{B}, \quad (B1)$$

where $\vec{g}^{(n,j)}$ are the g-factor tensor when an electron is in $j$th valley with envelope function $F_n^{(j)}$. g-factor tensor $\vec{g}^{(n,j)}$ is anisotropic (which is also a result of SOI that hybridizes spin and electronic bands),

$$\vec{g}^{(n,j)} = g_{n,\parallel} \vec{U}^{(j)} + g_{n,\perp} \left( \vec{1} - \vec{U}^{(j)} \right), \quad (B2)$$

where $j$ is the index for six valley states in silicon, $g_{n,\parallel}$ ($g_{n,\perp}$) is the g-factors along (perpendicular to) the valley ellipsoid for an electron in the n-th orbital state. $\vec{U}^{(j)}$ is the projection operator in the 3-dimensional coordinate space, for example, when $j = z$, we have

$$\vec{U}^{(z)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \vec{1} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Alternatively, g-factor tensor can be written as

$$\vec{g}^{(n,j)} = g_{n,\perp} \vec{1} + g_{n,ani} \vec{U}^{(j)}, \quad (B4)$$

where $g_{n,\perp} = g_{n,avg} - 1/3 g_{n,ani}, g_{n,avg} = (g_{n,\parallel} + 2g_{n,\perp})/3$, and $g_{n,ani} = g_{n,\parallel} - g_{n,\perp}$. Thus, one can see that the g-factor anisotropy $g_{n,ani}$ causes the hybridization of spin
and valley states within the donor eigenstates. This is known for an electron binding to a donor atom, where g-factor anisotropy will couple the ground state and excited donor orbital states with opposite spin orientation.

We express the Zeeman interaction in the basis of donor ground state $|0\rangle$ and QD ground states $|1\rangle$ and $|2\rangle$:

$$H_{Z,nn'} = \frac{1}{2} \mu_B \vec{\sigma} \cdot \vec{g}(nn') \cdot \vec{B},$$

where

$$\vec{g}(nn') = \left(g_{\parallel} \hat{\mathbf{1}} + g_{\perp} \alpha_{n,n'} \hat{D}(nn')\right) \delta_{nn'}.$$  

If $n \neq n'$, one can find that $H_{Z,nn'} = 0$. Therefore, we have

$$\vec{g}(nn') = \left(g_{\parallel} \hat{\mathbf{1}} + g_{\perp} \alpha_{n,n'} \hat{D}(nn')\right) \delta_{nn'},$$

If $n = n'$, then, $\hat{D}(00) = \frac{1}{3} \sum_j \hat{U}(j)$. Thus,

$$\vec{g}(00) = g_p \hat{\mathbf{1}} + \frac{1}{3} g_{\perp} \alpha_{nn'} \hat{U}(j),$$

$$H_{Z,00} = \frac{1}{2} \mu_B \vec{g}_{avg} \mu_B \vec{\sigma} \cdot \vec{B},$$

where $g_{avg} = g_p \parallel + g_{\perp} / 3$. If $n = n' = 1$ or 2, then,

$$\vec{g}(11) = \hat{D}(22) = \hat{U}(z).$$

$$H_{Z,11} = \frac{1}{2} \mu_B \left( g_{QD,\perp} \hat{\mathbf{1}} + g_{QD} \alpha_{nn'} \hat{U}(z) \right),$$

Then, we can express Zeeman interaction in the basis of orbital eigenstates $|n\rangle$. Since

$$|\bar{n}\rangle = \sum_n C_{\bar{n}n} |n\rangle = \sum_n C_{\bar{n}n} \alpha_{nj} \left| F_n^{(j)} \psi_j \right>,$$

we have

$$(H_{Z})_{\bar{n}n} = \sum_n C_{\bar{n}n}^* C_{nn'} H_{Z,nn'},$$

Therefore, the Zeeman interaction in the basis of orbital eigenstates is

$$(H_{Z})_{\bar{n}n} = \frac{1}{2} \mu_B \hat{\mathbf{1}} \cdot \hat{g}(\bar{n}n) \cdot \vec{B},$$

$$(\hat{g}(\bar{n}n)) = |C_{00}^*| g_{(00)} \delta_{\bar{n}n} + C_{0n}^* C_{n0} (g_{(00)} - g(11)),$$
where 
\[ g_X = \frac{G_{xx}}{2} \sin \theta_B \cos \theta_s - G_{zz} \frac{G_{xz}}{2} \cos \theta_B \sin \theta_s, \] (B25) 
\[ g_Z = \frac{G_{xx}}{2} \sin \theta_B \sin \theta_s + G_{zz} \frac{G_{xz}}{2} \cos \theta_B \cos \theta_s. \] (B26) 

Note that, for the spin flip process, only the term \( \frac{1}{2} \mu_B B g^X \sigma_X \) is relevant, where

\[ g_X = \frac{1}{2} \frac{G_{xx}}{2} (G_{xx} - G_{zz}) \sin(\theta_B + \theta_s) \]
\[ + \frac{1}{2} \frac{G_{xx}}{2} (G_{xx} + G_{zz}) \sin(\theta_B - \theta_s) \]
\[ \approx \frac{1}{2} \frac{G_{xx}}{2} (G_{xx} - G_{zz}) \sin(2\theta_B) \]
\[ = \frac{1}{2} g_{D,B} a_{D,ani} C_{00} C_{00} \sin(2\theta_B). \] (B27)

Thus, the only difference in comparison with the results in the main text is that the hybridization is proportional to \( g_{D,B,ani} \) in stead of \( g_{ani} \).

### Appendix C: Electron-phonon interaction

In this appendix, we derive the Hamiltonian \( H_{EP} \) and obtain the explicit coefficients of \( \Pi^{(j)}_{\beta \lambda} \) for the electron-phonon interaction in silicon.

An electron in a semiconductor conduction band interacts with phonon (lattice vibration) because band energy shifts under elastic strain. The electron-phonon interaction is

\[ H_{EP} = \sum_{\alpha \beta} \sum_j P_j \sum_{\hat{q} \lambda} \Pi^{(j)}_{\alpha \beta} \tilde{\gamma}_{\beta \lambda} \tilde{e}_{\alpha \lambda} \tilde{q}, \]  

where \( \Pi^{(j)}_{\alpha \beta} \) is the deformation potential tensor and \( \tilde{\gamma}_{\beta \lambda} \) is the strain tensor \((\alpha, \beta = x, y, z)\).

In silicon, there are six valley states, and the electron-phonon deformation potential (without umklapp process) can be expressed as

\[ \tilde{\gamma}_{\alpha \beta} = \sum_j P_j \tilde{\gamma}_{\beta \lambda}^{(j)}, \] (C1)

where \( \tilde{\gamma}_{\beta \lambda}^{(j)} = \sum \alpha \beta \sum_j P_j \tilde{\gamma}_{\beta \lambda}^{(j)} \),

\[ \tilde{\gamma}_{\beta \lambda}^{(j)} = \Xi_{d} \tilde{\gamma}^{(j)}_{d} + \Xi_{u} \tilde{\gamma}^{(j)}_{u}, \] (C2)

where \( P_j = |\psi_j \rangle \langle \psi_j| \) is the projection operator that selects the \( j \)-th valley, \( \Xi_{d} \) and \( \Xi_{u} \) are the dilatation and uniaxial shear deformation potential constants.

The strain \( \tilde{\gamma}_{\alpha \beta} \) is \((\alpha, \beta = x, y, z)\). 

\[ \tilde{\gamma}_{\alpha \beta} = \frac{1}{2} \left( \frac{\partial u_{\alpha}}{\partial r_{\beta}} + \frac{\partial u_{\beta}}{\partial r_{\alpha}} \right), \] (C3)

Based on the coefficients in Table I, the averaged value for donor ground and QD ground states

\[ \Pi^{(j)}_{\beta \lambda} \] (C10)
can be obtained as shown in table III. Then,

$$\Pi_{\lambda} = \Pi_{\lambda,00} - \Pi_{\lambda,11} = \Xi_u \delta_{\lambda,0} \cdot \Delta \cdot \hat{q}, \quad (C11)$$

is also obtained (see Table III).

| $\Pi_{\lambda,n}$ | $\lambda = l$ | $\lambda = t_1$ | $\lambda = t_2$ |
|------------------|----------------|----------------|----------------|
| $n = 0$ (P)      | $\Xi_d + \Xi_u/3$ | 0              | 0              |
| $n = 1, 2$ (QD)  | $\Xi_d + \Xi_u \cos^2 \vartheta$ | $-\Xi_u \sin \vartheta \cos \vartheta$ | 0              |
| $\Pi_{\lambda}$  | $\Xi_u(1/3 - \cos^2 \vartheta)$ | $\Xi_u \sin \vartheta \cos \vartheta$ | 0              |

TABLE III: Averaged coefficients $\Pi_{\lambda,n}$ for donor ground and QD ground states as well as the coefficient $\Pi_{\lambda} = \Pi_{\lambda,00} - \Pi_{\lambda,11}$ for the $\lambda$th branch of phonons.

Appendix D: Commutation relation

In this appendix we study the commutation property of $[x, H_O]$ in silicon for the evaluation of $(p_x)_{\bar{\theta}x \bar{\vartheta}}$ within the multivalley effective mass approximation. To evaluate the matrix element $(p_x)_{\bar{\theta}x \bar{\vartheta}}$, it is convenient if we have $[x, H_O] = i\hbar p_x/m^*$, which is valid in the case of single valley physics. Since the effective mass is different for different valleys, we need to re-derive a new commutation relation.

We consider the orbital Hamiltonian

$$H_O = H_K + V = \sum_j \sum_{i,j} \frac{(p_{ij}^j)^2}{2m_{ij}^j} \langle j | \langle j | V | \bar{r} \rangle$$

$$= \sum_j \left[ \sum_i \frac{(p_{ij}^j)^2}{2m_{ij}^j} + V_{jj'} | j \rangle \langle j | + \sum_{jj'} V_{jj'} | j \rangle \langle j' | \right],$$

where $i = x, y, z$, and $j$ is the valley index. In the kinetic term $H_K$, we have $m^{(\pm z)} = (m_x^{(\pm z)}, m_y^{(\pm z)}, m_z^{(\pm z)}) = (m_t, m_z, m_t)$, where $m_t$ and $m_z$ are the transverse and longitudinal effective mass in silicon; similarly, we have $m^{(\pm x)} = (m_t, m_x, m_t)$ and $m^{(\pm y)} = (m_t, m_y, m_t)$. We have assumed that the kinetic term $H_K$ does not mix different valley states. However, the potential term can couple different valley states, when the electrical potential varies abruptly. For example, when an electron is in a donor potential, or an electron is near a rough interface.

We can separate the contribution from donor potential into two terms $V_{jj'}$ and $V_{j'j}$, where $V_{jj'}$ does not couple and $V_{j'j}$ couples different valley states.

With the knowledge of the orbital Hamiltonian $H_O$, we can evaluate the commutation relation $[r, H_O]$, we will take $[x, H_O]$ as an example. Consider $x \approx \sum_j x^{(j)} | j \rangle$, where $x^{(j)} = \langle j | x | j \rangle$ is a coordinate operator that does not couple different valley states, and it satisfies commutation relation $[x^{(j)}, p^{(j)}] = i\hbar$. Then,

$$[x, H_O] = [x, \sum_j \sum_i \frac{(p_{ij}^{(j)})^2}{2m_{ij}^{(j)}} | j \rangle \langle j | = i\hbar \sum_j \frac{(p_{ij}^{(j)})^2}{m_{ij}^{(j)}} | j \rangle \langle j |.$$  

Therefore,

$$\langle \bar{0} | [x, H_O] | \bar{r} \rangle = \langle \bar{0} | x H_O | \bar{r} \rangle - \langle \bar{0} | H_O x | \bar{r} \rangle = (E_{\bar{r}} - E_{\bar{0}}) \langle \bar{0} | x | \bar{r} \rangle = \hbar \sum_j \frac{(p_{ij}^{(j)})^2}{m_{ij}^{(j)}} \langle j | \langle j | \bar{r} \rangle$$

$$= \hbar \sum_n C_{\alpha_{\bar{0}}\bar{r}} \alpha_{\bar{r}} n \langle n | \sum_j \frac{(p_{ij}^{(j)})^2}{m_{ij}^{(j)}} | j \rangle (j | n') \rangle$$

$$= \hbar \sum_{n,n'} \sum_j C_{\alpha_{\bar{0}}\bar{r}} C_{\alpha_{\bar{r}}n'} \alpha_{\bar{r}} (j | n') \langle F_{nj} | \frac{p_{ij}^{(j)}}{m_{ij}^{(j)}} | F_{nj'} \rangle,$$

while what we need is

$$\langle \bar{0} | p_x | \bar{r} \rangle = \langle \bar{0} | \sum_j p_{ij}^{(j)} | j \rangle \langle j | \bar{r} \rangle$$

$$= \hbar \sum_{n,n'} \sum_j C_{\alpha_{\bar{0}}\bar{r}} C_{\alpha_{\bar{r}}n'} \alpha_{\bar{r}} (j | n') \langle F_{nj} | p_{ij}^{(j)} | F_{nj'} \rangle,$$

Thus, there is no direct connection between $(p_x)_{\bar{0}x \bar{0}} \equiv \langle \bar{0} | p_x | \bar{r} \rangle$ and $x_{\bar{0}0} \equiv \langle \bar{0} | x | \bar{r} \rangle$. However, we can estimate a value by using

$$(p_x)_{\bar{0}x \bar{0}} \approx m^* E_{\bar{r}0} x_{\bar{0}0}/(i\hbar),$$

where $E_{\bar{r}0} = E_{\bar{r}} - E_{\bar{0}}$ is the energy difference of the orbital eigenstates, and the effective mass $m^*$ can be chosen as $m^* = 2m_z m_t / (m_z + m_t) \approx 0.43 m_0$ or $m^* = 3(2m_z + m_t)^{-1} \approx 0.26 m_0$, or $m^* = 2(1 / m_t + 1 / m_z)^{-1} \approx 0.315 m_0$. We can also find out the upper and lower bound values of $\langle \bar{0} | p_x | \bar{r} \rangle$ by using $m^* = m_t = 0.92 m_0$ and $m^* = m_t = 0.19 m_0$. In our calculation, we choose $m^* = 0.315 m_0$. By using the single effective mass $m^*$, the estimated matrix element can be different from actual values by at most a factor of three.
Appendix E: comparison with bulk donor: Zeeman interaction

In this appendix, we compare the Zeeman interaction of an electron in a bulk P donor and the Zeeman interaction in a coupled donor-QD system.

In the case of a bulk P donor in silicon, we consider the lowest six valley states, i.e. ground state $|A\rangle$ ($n = 1$), three-fold degenerate states $|T\rangle$ ($n = 2, 3, 4$), and two-fold degenerate states $|E\rangle$ ($n = 5, 6$). The electron Zeeman interaction in a bulk P donor is given by ($r \neq 0$)

$$H_{Z1r}^{(p)} = \frac{1}{2} \mu_B \vec{\sigma} \cdot \vec{g}^{(p1,Pr)} \cdot \vec{B}, \quad (E1)$$

$$\vec{g}^{(p1,Pr)} = g_{ani} \vec{\Delta}^{(p1,Pr)}, \quad (E2)$$

$$\vec{\Delta}^{(p1,Pn)} = \sum_j a_j^{(p1)} a_j^{(p3)} \vec{U}(j). \quad (E3)$$

For an electron in the ground state $|A\rangle$, the Zeeman interaction only couples to states $|E\rangle$ with opposite spin.

$$\vec{\Delta}^{(p1,P5)} = \sum_j a_j^{(p1)} a_j^{(p3)} \vec{U}(j) = \frac{1}{\sqrt{3}} \left[ -\vec{U}(x) - \vec{U}(y) + 2\vec{U}(z) \right], \quad (E4)$$

$$\vec{\Delta}^{(p1,P6)} = \sum_j a_j^{(p1)} a_j^{(p6)} \vec{U}(j) = \frac{1}{\sqrt{6}} \left[ \vec{U}(x) - \vec{U}(y) \right] (E5)$$

whose matrix form is given explicitly in Table IV.

| $\Delta$ | $\Delta_{Z1}$ | $\Delta_{X1}$ | $\Delta_{Y1}$ |
|---------|---------------|---------------|---------------|
| bulk-P: $\sqrt{2}\Delta^{(p1,P5)}$ | $-1/3 + \cos^2 \theta$ | $\frac{1}{2} \sin 2\theta$ | 0 |
| bulk-P: $\sqrt{6}\Delta^{(p1,P6)}$ | $\sin^2 \theta \cos 2\phi$ | $\frac{1}{2} \sin 2\theta \cos 2\phi - \sin \theta \sin 2\phi$ | 0 |
| P-QD: $\Delta$ | $1/3 - \cos^2 \theta$ | $\frac{1}{2} \sin 2\theta$ | 0 |

TABLE IV: Expressions for the components of tensors $\vec{\Delta}$ in the Cartesian coordinate system, where $Z$-axis is along the applied magnetic field. The corresponding expressions can be obtained as shown in Table [V].

The angular dependence of spin-orbit hybridization due to Zeeman interaction is determined by the $\vec{\Delta}$ and $\vec{\Delta}_{YZ}$ components of tensors $\vec{\Delta}$ in the $(X, Y, Z)$ coordinate system, where $Z$-axis is along the applied magnetic field (it is also the spin quantization axis in the lowest order approximation). The corresponding expressions can be obtained as shown in Table [V].

Appendix F: comparison with bulk donor: Electron-phonon interaction

In this appendix, we compare the electron-phonon interaction of an electron in a bulk P donor and electron-phonon interaction in a coupled donor-QD system.

In the case of a bulk donor in silicon, we consider again the lowest six valley states, i.e. $|A\rangle$ ($n = 1$), $|T\rangle$ ($n = 2, 3, 4$), $|E\rangle$ ($n = 5, 6$). Suppose there is an electron in the donor ground state $|A\rangle$, then, the electron-phonon interaction $H_{EP}$ could couple the ground orbital state $|A\rangle$ to states $|E\rangle$, and the electron-phonon interaction of an electron in a bulk donor in silicon is given by ($r \neq 0$)

$$H_{EP}^{(p)} = \sum_{\vec{q}, \lambda} M_{\vec{q}, \lambda, 1r}^{(p)} (b_{\vec{q} \lambda}^\dagger - q_{\lambda}) \equiv \sum_{\vec{q}, \lambda} M_{\vec{q}, \lambda, 1r}^{(p)} (b_{\vec{q} \lambda}^\dagger - b_{\vec{q} \lambda}), \quad (F1)$$

$$M_{\vec{q}, \lambda, 1r}^{(p)} = \sum_j a_j^{(p)} a_j^{(p)} f_{nr}^{(j)} (q_{\lambda}^j \Pi_{\vec{q}, \lambda, 1r}^{(p)}), \quad (F2)$$

where, in the limit of long wave phonons, we have $f_{nr}^{(j)}(q_{\lambda}) \approx \left| F_n^{(j)} \right| \left| F_n^{(j)} \right| \approx 1$. Therefore,

$$M_{\vec{q}, \lambda, 1r}^{(p)} = \sum_j a_j^{(p)} a_j^{(p)} M_{\vec{q}, \lambda}^{(p)} = i \sqrt{2 \rho_{\vec{q}, \lambda}} \Pi_{\vec{q}, \lambda, 1r}^{(p)}, \quad (F3)$$

$$\Pi_{\vec{q}, \lambda, 1r}^{(p)} = \Xi a_\lambda \vec{C}_{\vec{q}0}^{(j)} \cdot \vec{g}^{(p1,Pr)}, \quad (F4)$$

where the expressions for the tensors $\vec{\Delta}^{(p1,Pr)}$ are listed in Table IV.
In comparison, for an electron in the coupled donor-QD system, the electron-phonon interaction is

\[ (H_{EP})^{\dagger}_{k\lambda} = \sum_{\lambda} (M_{\lambda \lambda} b_{\lambda}^\dagger b_{\lambda} + \text{h.c.}), \]  

where \( M_{\lambda \lambda} = \Xi_{\lambda} (1 - \cos^2 \theta) \), \( \Pi_{q\lambda} = \Xi_{\lambda} \cos \theta \sin \theta \), and \( \Pi_{q\lambda} = 0 \).

The difference of electron-phonon interaction will modify the angular distribution of phonon emissions. Thus, it will modify the magnitude of spin relaxation after averaging phonon modes in all three dimensions.

[1] D. Loss and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998), URL http://link.aps.org/doi/10.1103/PhysRevA.57.120
[2] B. E. Kane, Nature 393, 133 (1998), ISSN 0028-0836, URL http://www.nature.com/nature/journal/v393/n6681/full/393133a0.html
[3] R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, Rev. Mod. Phys. 79, 1217 (2007), URL http://link.aps.org/doi/10.1103/RevModPhys.79.1217
[4] F. A. Zwanenburg, A. S. Dzurak, A. Morello, M. Y. Simmons, L. C. L. Hollenberg, G. Klimeck, S. Rogge, S. N. Coppersmith, and M. A. Eriksson, Rev. Mod. Phys. 85, 961 (2013), URL http://link.aps.org/doi/10.1103/RevModPhys.85.961
[5] A. M. Tyryshkin, A. V. Lyon, A. V. Astashkin, and A. M. Raitisimring, Phys. Rev. B 68, 193207 (2003), URL http://link.aps.org/doi/10.1103/PhysRevB.68.193207
[6] J. J. L. Morton, A. M. Tyryshkin, R. M. Brown, S. Shankar, B. W. Lovett, A. Ardavan, T. Schenkel, E. E. Haller, J. W. Ager, and S. A. Lyon, Nature 455, 1085 (2008), ISSN 0028-0836, URL http://www.nature.com/nature/journal/v455/n7216/full/nature07295.html
[7] A. M. Tyryshkin, S. Tojo, J. J. L. Morton, H. Riemann, N. V. Abrosimov, P. Becker, H.-J. Pohl, T. Schenkel, M. L. W. Thewalt, K. M. Itoh, et al., Nat Mater 11, 143 (2012), ISSN 1476-1122, URL http://www.nature.com/nmat/journal/v11/n6/abs/nmat3582.html
[8] J. T. Muhonen, J. P. Dehollain, A. Laucht, F. E. Hudson, R. Kalra, T. Sekiguchi, K. M. Itoh, D. N. Jamieson, J. C. McCallum, A. S. Dzurak, et al., Nat Nano 9, 986 (2014), ISSN 1748-3387, URL http://www.nature.com/nnano/journal/v9/n12/abs/nnano.2014.211.html
[9] B. Weber, Y. H. M. Tan, S. Mahapatra, T. F. Watson, H. Ryu, R. Rahman, L. C. L. Hollenberg, G. Klimeck, and M. Y. Simmons, Nat Nano 9, 430 (2014), ISSN 1748-3387, URL http://www.nature.com/nnano/journal/v9/n6/full/nnano.2014.63.html
[10] A. Morello, J. J. Pla, F. A. Zwanenburg, K. W. Chan, K. Y. Tan, H. Huebl, M. Mttinen, C. D. Nguroho, C. Yang, J. A. van Donkelaar, et al., Nature 467, 687 (2010), ISSN 0028-0836, URL http://www.nature.com/nature/journal/v467/n7316/full/nature09392.html
[11] M. Singh, J. L. Pacheco, D. Perry, E. Garratt, G. T. Eyck, N. C. Bishop, J. R. Wendt, R. P. Manginell, J. Dominguez, T. Plyum, et al., Applied Physics Letters (2016), URL http://aip.scitation.org/doi/full/10.1063/1.4940421
[12] M. J. Caldern, B. Koiller, X. Hu, and S. Das Sarma, Phys. Rev. Lett. 96, 096802 (2006), URL http://link.aps.org/doi/10.1103/PhysRevLett.96.096802
[13] G. P. Lansbergen, R. Rahman, C. J. Wellard, I. Woo, J. Caro, N. Collaert, S. Biesemans, G. Klimeck, L. C. L. Hollenberg, and S. Rogge, Nat Phys 4, 656 (2008), ISSN 1745-2473, URL http://www.nature.com/nphys/journal/v4/n8/abs/nphys994.html
[14] F. A. Mohiyaddin, R. Kalra, A. Laucht, R. Rahman, G. Klimeck, and A. Morello, Phys. Rev. B 94, 045314 (2016), URL http://link.aps.org/doi/10.1103/PhysRevB.94.045314
[15] J. Salfi, B. Voisin, A. Tankasala, J. Bocquel, M. Usman, M. Y. Simmons, L. C. L. Hollenberg, R. Rahman, and S. Rogge, arXiv:1706.09261 [cond-mat] (2017), arXiv:1706.09261, URL http://arxiv.org/abs/1706.09261
[16] G. Feher and E. A. Gere, Phys. Rev. 114, 1245 (1959), URL http://link.aps.org/doi/10.1103/PhysRev.114.1245
[17] H. Bch, S. Mahapatra, R. Rahman, A. Morello, and M. Y. Simmons, Nature Communications 4, 2013, ISSN 2041-1723, URL http://www.nature.com/ncomms/2013/130618/ncomms3017/full/ncomms3017.html
[18] J. P. Dehollain, J. T. Muhonen, K. Y. Tan, A. Saraiva, D. N. Jamieson, A. S. Dzurak, and A. Morello, Phys. Rev. Lett. 112, 236801 (2014), URL http://link.aps.org/doi/10.1103/PhysRevLett.112.236801
[19] S. Kolkowitz, A. Safira, A. A. High, R. C. Devlin, J.-S. Moon, R. S. Ross, et al., arXiv:0908.0173 [cond-mat] (2009), arXiv:0908.0173, URL http://arxiv.org/abs/0908.0173
[20] S. Amasha, K. MacLean, I. P. Radu, D. M. Zumbhl, Croke III, P. W. Deelman, B. M. Maune, I. Milosavljevic, J.-S. Moon, R. S. Ross, et al., arXiv:0908.0173 [cond-mat] (2009), arXiv:0908.0173, URL http://arxiv.org/abs/0908.0173
