Spin Relaxation in a Si Quantum Dot due to Spin-Valley Mixing

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We study the relaxation of an electron spin qubit in a Si quantum dot due to electrical noise. In particular, we clarify how the presence of the conduction band valleys influences the spin relaxation. In single-valley semiconductor quantum dots, spin relaxation is through the mixing of spin and envelope orbital states via spin-orbit interaction. In Si, the relaxation could also be through the mixing of spin and valley states. We find that the additional spin relaxation channel, via spin-valley mixing and electrical noise, is indeed important for an electron spin in a Si quantum dot. By considering both spin-valley and intra-valley spin-orbit mixings and the Johnson noise in a Si device, we find that spin relaxation rate peaks at the hot spot, where the Zeeman splitting matches the valley splitting. Furthermore, because of a weaker field-dependence, the spin relaxation rate due to Johnson noise could dominate over phonon noise at low magnetic fields, which fits well with recent experiments.

I. INTRODUCTION

Spin qubit is a promising candidate as an information carrier for quantum information processing and silicon is one of the best host materials for a spin qubit. Specifically, the low abundance of isotopes with finite nuclear spins (29Si) in natural Si significantly reduces hyperfine interaction strength and the induced spin dephasing. Isotopic purification further suppresses this decoherence channel, so that Si behaves as if it is a “semiconductor vacuum” for a spin qubit. Spin-orbit (SO) interaction in Si is also weak because of the lighter mass of Si atoms and the lattice inversion symmetry in bulk Si. Therefore, as has been calculated theoretically and measured experimentally, (donor-confined) spin dephasing and relaxation times are extremely long in bulk Si.

But Si is not perfect. The existence of multiple conduction band valleys gives additional phase factors to the electron wave function, so that interaction between donor electron spins becomes sensitively dependent on the donor positions. While interface confinement and scattering can lift this degeneracy, details at the interface, whether it is surface roughness or steps, play important roles in determining the magnitude of the valley splitting. Experimentally measured $E_{VS}$ ranges from vanishingly small, to several hundreds of $\mu$eV, to possibly a few meV. Furthermore, to achieve controllability, spin qubits are generally located near or at the interface between the host and the barrier materials. Dangling bonds, charge traps, and other defects are inevitably present at the many interfaces of a semiconductor heterostructure, and the coherence properties of a spin qubit in a nanostructure is not as clearly understood and measured as in bulk Si.

With pure dephasing strongly suppressed in Si, spin relaxation becomes an important indicator of decoherence for a spin qubit. Spin relaxation could come directly from magnetic noise in the environment, or from electrical noise via spin-orbit or exchange interaction. Indeed, for a single spin in a quantum dot, we have shown that electrical noise from the circuits or surrounding traps could be an important cause for spin relaxation, particularly at a smaller qubit energy splitting. In this previous study, however, we only considered intra-valley orbital dynamics for an electron in Si. On the other hand, it has been shown experimentally and theoretically that the presence of valleys in Si can be significantly modify spin relaxation through spin-valley mixing, and a relaxation hot spot appears at the degeneracy point where the Zeeman splitting matches the valley splitting.

In this paper, we study spin relaxation of a single QD-confined electron in Si due to the presence of electrical noise (including Johnson noise, phonon noise, and the 1/f charge noise) and the spin-valley mixing. We find that this relaxation channel is indeed important for an electron spin in a Si quantum dot. We find that spin relaxation rate peaks at the hot spot where the Zeeman splitting matches the valley splitting. Furthermore, because of a weaker field-dependence, the spin relaxation rate due to Johnson noise through spin-valley mixing could dominate over phonon noise and intra-valley scattering at low magnetic fields, which fits well with recent experiments.

The rest of the paper is organized as follows. In Sec. II we set up the system Hamiltonian and describe the mechanism of spin valley mixing. In Sec. III we derive the spin relaxation rate due to spin valley mixing and electrical noise. In Sec. IV we evaluate the spin relaxation rates due to Johnson and phonon noises, and compare the different spin relaxation mechanisms. Finally, conclusions are drawn in Sec. V. In the Appendices we discuss the field dependence of the spin relaxation, effects of the 1/f noise, and phonon noise spectrum in more details.

II. SYSTEM HAMILTONIAN

We consider an electron in a gate-defined quantum dot in a Si heterostructure (whether a Si/SiO$_2$ or a Si/SiGe structure). The growth-direction ([001]-direction in this
paper) confinement is taken to be very strong, so that we focus on the in-plane dynamics of the confined electron. The strong field and strain at the interface lower the degeneracy of the Si conduction band by raising the energy of four of the valleys relative to the other two (in this case $z$ and $-z$ valleys). Moreover, scattering off the smooth interface further mix and split the two low-energy valleys. We label the two valleys as $+$ and $-$, with valley splitting $E_{VS}$. At this smooth-interface limit, and without considering the spin-orbit interaction, the valley degrees of freedom and the intra-valley effective-mass dynamics can be separated, so that the electron wave function can be written as $|v, i, \alpha\rangle$, where $v = \pm$ is the index for the two lowest-energy eigen-valleys, $i$ is the orbital excitation index within an eigen-valley, and $\alpha = \uparrow$ or $\downarrow$ is the spin index.

When the lateral confinement of the QD is sufficiently strong ($> 1$ meV), the intra-valley orbital level spacing is larger than the valley splitting $E_{VS}$ (assuming it is up to a fraction of 1 meV). In this case we can neglect the intra-valley excitation, and focus on only the lowest four spin-valley states, all in the ground intra-valley orbital state. These four states (with an implicit common orbital index $i = 0$) are $|1\rangle = |-, \downarrow\rangle$, $|2\rangle = |-, \uparrow\rangle$, $|3\rangle = |+, \downarrow\rangle$ and $|4\rangle = |+, \uparrow\rangle$. Within the space spanned by these four lowest-energy spin valley product states, the total Hamiltonian for the QD-confined electron is given by

$$H = H_0 + H_{SV} + H_{\text{noise}}$$

where

$$H_0 = \sum_i \frac{\epsilon_i}{2} |i\rangle \langle i|$$

$$H_{SV} = \frac{\Delta_{23}}{2} |2\rangle \langle 3| + \frac{\Delta_{14}}{2} |1\rangle \langle 4|$$

$$H_{\text{noise}} = -e\vec{E} \cdot \left[ \vec{r}^{\pm} - \sum_{i=1,2} |i\rangle \langle i| + \vec{r}^{++} \sum_{i=3,4} |i\rangle \langle i| \right]$$

Here $H_0$ contains valley and Zeeman splitting, with $\epsilon_i/2$ being the energies of the product states in the absence of SO interaction and the environmental noise. Specifically, $\epsilon_4 = -\epsilon_1 = E_{VS} + g\mu_B B$, $\epsilon_3 = -\epsilon_2 = E_{VS} - g\mu_B B$. $H_{SV}$ represents spin-valley (SV) mixing due to the SO interaction, with $\Delta_{23}$ and $\Delta_{14}$ the mixing energy: $\Delta_{23} = \frac{2}{\hbar} \left( H_{SO} |3\rangle \langle 2| + H_{SO} |2\rangle \langle 3| \right)$ and $\Delta_{14} = \frac{2}{\hbar} \left( H_{SO} |4\rangle \langle 1| + H_{SO} |1\rangle \langle 4| \right)$. Here the SO interaction is $H_{SO} = -p_y \sigma_x + \alpha_p x \sigma_y$, with the interaction strength $\alpha_{\pm} \equiv (\alpha_D \pm \alpha_R)$, and the $x$ and $y$ axes along the $[110]$ and $[\bar{1}10]$ directions (which also define the plane of the quasi-2D quantum dot). Here $\alpha_D$ and $\alpha_R$ are the Dresselhaus and Rashba SO interaction constants. The Dresselhaus SO interaction arises from the bulk inversion asymmetry, which in a Si QD could be from the interface disorder; While Rashba SO interaction arises from the structure inversion asymmetry and is tunable through the electric field across the QD. Lastly, $H_{\text{noise}}$ contains the electrical noise from the environment, with $E(\vec{r})$ the noise electric field. It could come from Johnson noise, $1/f$ charge noise, phonon noise, etc. Here $\vec{r}^{\pm} = (-|\vec{r}|\pm)$ is the electric dipole matrix element between different valley states, which could arise from disorders at the interfaces of the QD.

We first find the eigenstates of the confined electron in the presence of spin-valley mixing but in the absence of the environmental noises. As indicated in Fig. 1, states $|1\rangle$ and $|4\rangle$ are always well separated energetically, by neglecting the mixing of states $|1\rangle$ and $|4\rangle$ by $\Delta_{14}$ in this study. On the other hand, near $g\mu_B B = E_{VS}$, states $|2\rangle$ and $|3\rangle$ are strongly mixed by the spin-valley coupling $\Delta_{23}$. This degeneracy point is the so-called spin relaxation hot spot. $\Delta_{23}$ is in general a complex number, and can be written as $\Delta_{23} = \Delta_1 - i\Delta_2$ and $\Delta = |\Delta_{23}|$. The electron eigenstates for $H_0 + H_{VS}$ are thus $|1\rangle$, $|2\rangle$, $|3\rangle$, $|4\rangle$, where

$$|3\rangle = \cos(\gamma/2)e^{-i\delta/2} |3\rangle + \sin(\gamma/2)e^{i\delta/2} |2\rangle,$$

$$|2\rangle = -\sin(\gamma/2)e^{-i\delta/2} |3\rangle + \cos(\gamma/2)e^{i\delta/2} |2\rangle. \tag{3}$$

Here $\gamma = \arctan(|\Delta_1/\Delta_3|)$ and $\delta = \arctan(\Delta_2/\Delta_1)$. The energy splitting between $|3\rangle$ and $|2\rangle$ is $\Delta_3 = \sqrt{\Delta_1^2 + |\Delta_2|^2}$. When the magnetic field is along $[110]$ axis as in Ref. 3, the spin-valley mixing matrix element $\Delta_{23}$ can be expressed as (see Appendix A)

$$\Delta_{23} = 2m^* E_{VS} \alpha_\sigma r_x^{-} / \hbar. \tag{4}$$

where the relationship $\vec{p}^{-} = (-\vec{p})^+ = im^* E_{VS} \vec{r}^{-}/\hbar$ has been employed.

III. SPIN RELAXATION

With states $|2\rangle$ and $|3\rangle$ spin-valley mixed, and assuming that the electric dipole matrix element between the

FIG. 1: Inset (a) shows the relations between the product states $|3\rangle$ (or $|2\rangle$) and the eigenstate $|3\rangle$, $\gamma$ and $\delta$ are the polar and azimuthal angles of the orientation of the eigenstate $|3\rangle$ in the basis of product states. Inset (b): The level diagram of the system as a function of the applied magnetic field. States $|1\rangle$, $|2\rangle$, $|3\rangle$ and $|4\rangle$ are the product states, states $|2\rangle$ and $|3\rangle$ are the eigenstates after the SV mixing. $E_{VS}$ and $E_Z$ are the valley splitting and Zeeman splitting, respectively. The small arrows on the energy levels indicate the spin orientations.
two eigen-valleys is non-vanishing, any electrical noise, which couples only states with the same spin orientations, can induce transitions between them and the other two eigenstates. The transition rate is proportional to the spectrum of the noisy electric field $E(r) = \mathcal{V} U_{ph}(r)/\epsilon$, where $U_{\text{noise}}(r)$ captures the potential of the noise in the system, such as Johnson noise, 1/f charge noise or phonon noise, which will be discussed later.

Experimentally, in the preparation of a spin-up initial state, the electron orbital and valley states are generally kept in the lowest eigenstates in order to avoid the unnecessary mixing of the spin and orbital dynamics. Therefore the most spin relevant relaxation processes involve the relaxation of states $|2\rangle$ and $|3\rangle$. When $E_Z \ll E_{VS}$, a spin-up electron is mostly loaded into the energy eigenstate $|2\rangle$, while when $E_Z \gg E_{VS}$, it is mostly loaded into $|3\rangle$.

We first consider the relaxation of state $|2\rangle$ to the ground state $|1\rangle$. The relaxation rate $\Gamma_{21} = \frac{2\pi e^2}{\hbar^2} \int_{-\infty}^{\infty} \langle 1 | \hat{E} \cdot \mathbf{r}/2 \rangle \langle 2 | \hat{E} \cdot t \rangle \langle 1 | \mathbf{r} \rangle / \cos(\omega t) dt$, where $S_{ii}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau \langle 1 | E_i(0) E_i(\tau) \rangle \cos(\omega \tau)$ is the noise spectrum ($i = x, y, z$) and $\omega_Z = g\mu_B B_0/\hbar$ is the Zeeman frequency. We have also assumed that noise in different directions are not correlated. The relevant transition matrix element in this case is $\langle 1 | \mathbf{r} \rangle \mathbf{r} \rangle = -\mathbf{r}^+ \sin(\gamma/2)$, which is proportional to the transition matrix elements $\mathbf{r}^+ \sin(\gamma/2)$ between the $\pm$ valleys.

State $|3\rangle$ can relax to both $|2\rangle$ and $|1\rangle$ because of the spin-valley mixing and inter-valley transitions. The relaxation rates are

$$\Gamma_{31} = \frac{4\pi e^2}{\hbar^2} \sum_i \left| \langle 1 | r_i \rangle \langle 2 | r_i \rangle \right|^2 S_{ii}(\omega_Z),$$

$$\Gamma_{32} = \frac{4\pi e^2}{\hbar^2} \sum_i \left| \langle 2 | r_i \rangle \langle 3 | r_i \rangle \right|^2 S_{ii}(\omega_Z),$$

where the relevant matrix elements are $\langle 1 | r_i \rangle \langle 3 | r_i \rangle = \langle \mathbf{r}^+ \sin(\gamma/2) \rangle, \langle 2 | r_i \rangle \langle 3 | r_i \rangle = \langle \mathbf{r}^+ \sin(\gamma/2) \rangle$.

The spin-valley relaxation rates $\Gamma_{31}$ and $\Gamma_{21}$ take the same algebraic form, which we denote as $\Gamma_{SV}$,

$$\Gamma_{SV} = \frac{2\pi e^2}{\hbar^2} \sum_i \left| \langle r_i \rangle \frac{1}{2} S_{ii}(\omega_Z) F_{SV}(\omega_Z),$$

$$F_{SV}(\omega_Z) = 1 - \left[ 1 + \frac{\Delta^2}{(E_{VS} - \hbar \omega)^2} \right]^{-\frac{1}{2}}.$$
where \( \omega_d \) is the lateral confinement strength of the QD, \( \omega_z \) is the Zeeman frequency, and \( S_{\ell i}^E(\omega) \) is the Fourier spectrum of the correlation of in-plane electric field fluctuations (the in-plane electrical noise is assumed to be isotropic, and out of plane electrical noise is neglected because of the strong vertical confinement at the interface). \( F_{SO} \) contains the dependence on the SO interaction strength and the orientation of magnetic field. For a magnetic field along \([110]\) direction as in Ref. 9, we have \( F_{SO} = \alpha^2 \).

### IV. RESULTS

In this Section we present spin relaxation rates for different noises, and compare the spin relaxation channels due to SV mixing and intra-valley SO mixing. We mainly focus on the electrical noise from Johnson noise and phonon noise. Although 1/f charge noise is ubiquitous as well in semiconductor material, we do find that spin relaxation due to 1/f noise is much slower compared to that due to Johnson and phonon noise. Thus we only give a brief discussion on 1/f noise in Appendix B.

#### A. Johnson Noise

Johnson noise is the electromagnetic fluctuations in an electrical circuit. For a gate-defined QD, Johnson noise inside the metallic gates, such as the source and drain circuits, could give rise to strong electrical fluctuations acting on the QD, and could induce spin decoherence for the electron confined in the QD.

The spectrum of Johnson noise \( S_V(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} \langle \delta V(0) \delta V(t) \rangle \cos(\omega t) dt \) is given by

\[
S_V(\omega) = 2\xi \omega \hbar f_c(\omega) \coth(\hbar \omega / 2k_B T),
\]

where \( \xi = R/R_k \) is a dimensionless constant, \( R_k = \hbar / e^2 = 26 \, k\Omega \) is the quantum resistance, and \( R \) is the resistance of the circuit. \( f_c(\omega) = 1/[1 + (\omega/\omega_R)^2] \) is a natural cutoff function for Johnson noise, where \( \omega_R = 1/R_C \) is the cutoff frequency, and \( C \) is capacitors in parallel with the resistance \( R \).

As shown in Fig. 2, the Johnson noise of the circuits outside the dilution refrigerator is generally well filtered. Thus we consider only Johnson noise of the low-temperature circuit inside dilution refrigerator. The corresponding spectrum of electric field is \( S_{\ell i}^E(\omega) = S_V(\omega)/(\varepsilon_0 l_0)^2 \), where \( l_0 \) is the length scale between the source and drain. Accordingly, the spin relaxation rate due to SV mixing and Johnson noise is

\[
\Gamma_{SV} = \frac{2\pi}{\hbar^2} \sum_i |r_i^{+\dagger}|^2 S_V(\omega) F_{SV}(\omega)/l_0^2,
\]

where \( F_{SV}(\omega) \) is given by Eq. 9. The small capacitance of source and drain leads means that cutoff frequency \( \omega_R \) satisfies \( \omega_R \gg \omega_z \), so that the cutoff function \( f_c(\omega) \approx 1 \). The low temperature environment ensures \( \coth(\hbar \omega / 2k_B T) \approx 1 \). Therefore, the \( \omega_z \) dependence of \( \Gamma_{SV} \) is determined by \( \omega_z F_{SV}(\omega_z) \).

Compared with the intra-valley SO mixing mechanism, where \( \Gamma_{SO} \) shows an \( \omega_z^2 \) dependence, \( \Gamma_{SV} \) is linearly dependent on \( \omega_z \) at low fields, when \( |E_{VS} | \gg \hbar \omega_z \) so that \( F_{SV}(\omega_z) \sim \Delta^2/2E_{VS}^2 \). Because of this weaker field dependence, the spin relaxation rate \( \Gamma_{SV} \) would dominate over \( \Gamma_{SO} \) at very low magnetic fields. On the other hand, at high fields, when \( \hbar \omega_z \gg E_{VS} \), \( F_{SV}(\omega_z) \sim \Delta^2/2\omega_z^2 \), so that \( \Gamma_{SV} \propto 1/\omega_z \): the relaxation rate is slower as the external field increases. Thus at high fields the intra-valley spin relaxation should dominate over inter-valley spin relaxation.

Below we carry out numerical calculations of spin relaxation rate in a small Si/SiO\(_2\) QD. Based on the parameters of Ref. 3, the valley splitting here is set as \( E_{VS} = 0.33 \, \text{meV} \), the dot confinement energy is \( \hbar \omega_d = 8 \, \text{meV} \), and the electric dipole matrix elements for the valley states are set as \( r_{i-\rightarrow} = r_{i+\rightarrow} = 0 \) and \( r_{x-\rightarrow} = r_{y-\rightarrow} = 1.1 \, \text{nm} \). The magnetic field is along the \( z \) direction, and the SO interaction strength for Si is set as \( \alpha_R = 45 \, \text{m/s} \) and \( \alpha_D = 0 \, \text{m/s}^2 \). We use the bulk g-factor \( g = 2 \), and the electron effective mass is \( m^* = 0.19 m_0 \), where \( m_0 \) is the free electron rest mass. For the Johnson noise parameters, we choose the resistance \( R = 2 \, \text{k}\Omega \), length scale \( l_0 = 100 \, \text{nm} \) and temperature \( T = 0.15 \, \text{K} \).

Figure 3 shows the spin relaxation rates \( \Gamma_{SV} \) through SV mixing (red dashed line), \( \Gamma_{SO} \) through SO mixing (blue dash-dotted line) and the total spin relaxation rate \( \Gamma_{SV} + \Gamma_{SO} \) (black solid line) as a function of the applied
magnetic field \(B_0\) due to Johnson noise. As shown in Fig. 3, the relaxation rate through the intra-valley SO mixing is dominant in the high-field regime, showing a \(B_0^3\) dependence. The relaxation due to SV mixing peaks at the degenerate point \((q\mu_B B_0 = E_{VS})\), and dominates in the low magnetic field regime due to a linear \(\omega_Z\) dependence. The relaxation time due to the Johnson noise is about 10 s when \(B_0 = 1\) T, and about 0.01 s when \(B_0 = 10\) T.

### B. Phonon Noise

Phonon noise is the most studied spin relaxation source, and is usually the dominant source of spin relaxation in the strong-magnetic-field regime because of the higher phonon density of states at high frequency.\(^{2,4,5,39,45}\) Although results for spin relaxation due to SV mixing and phonon noise have been obtained in Ref. \(^{4}\), we include this spin relaxation channel here for completeness. Furthermore, a unified treatment is given here for both phonon and Johnson noise, and the phonon bottleneck effect is taken into account in a simplified manner.\(^{34}\)

To obtain the results for phonon noise, we need the correlation of the electric field \(E(\vec{r}) = \nabla U_{ph}(\vec{r})/e\), which can be derived based on the electron-phonon interaction potential \(U_{ph}(\vec{r})\).\(^{24,35}\)

\[
U_{ph}(\vec{r}, t) = \sum_{qj} \frac{f(q_2)}{\sqrt{2\rho_c \omega_{qj}}} \frac{q_1}{\hbar} (-iq\Xi_{qj})(b_{-qj}^\dagger + b_{qj}),
\]

where \(b_{qj}^\dagger\) (\(b_{qj}\)) creates (annihilates) an acoustic phonon with wave vector \(q = (q_1, q_2)\), branch index \(j\), and dispersion \(\omega_{qj}\); \(\rho_c\) is the sample density (volume is set to unity).

The factor \(f(q_2)\) equals unity for \(|q_2| \ll d^{-1}\) and vanishes for \(|q_2| \gg d^{-1}\), where \(d\) is the characteristic size of the quantum well along the \(z\)-axis. Here we consider deformation potential electron-phonon interaction, with \(\Xi_{qj}\) being the deformation potential constants (piezo-electric interaction vanishes in Si due to the non-polar nature of the lattice). In Si, the deformation potential strength for different branches are \(\Xi_1 = \Xi_3 = \Xi_d = 5\) eV, \(\Xi_2 = 0\) (TA) and \(\Xi_3 = \Xi_u = 8.77\) eV (TA), where \(\Xi_d\) and \(\Xi_u\) are the dilation and uniaxial shear deformation potential constants.

To calculate spin relaxation due to the phonon noise, we first need to obtain the phonon correlation functions, which are discussed in detail in Appendix C. Substituting the correlation functions into Eq. (8), we find that the dependence of \(\Gamma_{SV}\) on the applied magnetic field is determined by the factor \(\omega_Z^2 F_{SV}(\omega_Z)\). \(\Gamma_{SO}\), on the other hand, is proportional to \(\omega_Z^2\). Both rates are proportional to the deformation potential strength \(\Xi_j\) and inversely proportional to the seventh power of phonon velocity \(v_j\).

Figure 4 shows the spin relaxation rates \(\Gamma_{SV}\) through SV mixing (red dashed line), \(\Gamma_{SO}\) through SO mixing (blue dash-dotted line) and the total spin relaxation \(\Gamma_{SV} + \Gamma_{SO}\) (black solid line) as a function of the applied magnetic field \(B_0\) due to phonon noise. The parameters are \(\rho_c = 2200\) kg/m\(^3\), \(v_1 = 5900\) m/s, \(v_2 = v_3 = 3750\) m/s (data for SiO\(_2\)), \(\Xi_d = 5\) eV, \(\Xi_u = 8.77\) eV, \(T = 0.15\) K, and the other parameters are the same as before. Similar to Johnson noise, the relaxation through the SV mixing dominates in the low magnetic field regime, and peaks at the degeneracy point. The relaxation rate through the intra-valley SO mixing is dominant in the high-magnetic-field regime, which shows \(B_0^3\) dependence before the phonon bottleneck takes effect and the curves bend downward from the \(B_0^3\) line.\(^{34,35}\) The phonon bott-
Figure 5 shows the spin relaxation due to phonon noise and Johnson noise as a function of the applied magnetic field. The total spin relaxation is plotted as black solid line, and the experimental results (red dots) are from Ref. 9. For comparison, the result (black dotted thin line) of phonon induced relaxation without considering the phonon bottleneck effect (without the cutoff function) is also presented, which reproduces the original fitting in Ref. 9. This discrepancy could be due to another level crossing (and the associated spin hot spot) at a higher field that is not taken into consideration in the current study.

Figure 6 shows the spin relaxation rate due to phonon noise and Johnson noise as a function of the applied magnetic field. The total spin relaxation is plotted as black solid line, and the experimental results (red dots) are from Ref. 9. For comparison, the result (black dotted thin line) of phonon induced relaxation without considering the phonon bottleneck effect (without the cutoff function) is also presented, which reproduces the original fitting in Ref. 9. There are three interesting features to this figure: the spin hot spot, which we have discussed extensively in previous subsections, the high-field trend, and the low-field trend. Below we examine the later two features in more detail.

In figure 4, the curve without phonon bottleneck effect is more consistent with the experimental data. This somewhat unexpected discrepancy is probably due to the over estimation of the phonon bottleneck effect. In our calculation, we use an isotropic two-dimensional Gaussian envelope function for the electron ground state, which in reality could be modified due to the irregular shape and the anharmonicity of the QD confinement potential. We also note that the measured relaxation rate seems to increase faster at the very high fields (> 4 T) than both theoretical calculations, with or without the phonon bottleneck effect. This discrepancy could be due to another level crossing (and the associated spin hot spot) at a higher field that is not taken into consideration in the current study.

At low magnetic fields, the dominant spin relaxation channel crosses over from phonon noise to Johnson noise (around 2 T). As discussed in subsection IV A, the dominant relaxation mechanism at low magnetic field is due to Johnson noise and SV mixing. By considering the Johnson noise, the theoretical results of total spin relaxation (black solid line) is now more consistent with the experimental measurements in Ref. 9, where the relaxation rate at $B = 1$ T is around 0.1 s$^{-1}$.

Figure 6 shows the spin relaxation rate due to phonon noise and Johnson noise as a function of the applied magnetic field at a valley splitting of $E_{VS} = 0.75$ meV. The other parameters are the same as in Fig. 5 except the dipole matrix elements are a bit larger at $r_x^+ = r_y^+ = 1.1$ nm. In essence, throughout the whole field range in this figure, the system is on the low-energy side of the degeneracy point or the spin hot spot. As shown in Fig. 5 (a), at higher magnetic fields, the dominant relaxation source is phonon noise and SV mixing. For lower fields, the dominant relaxation channel changes over to Johnson noise and SV mixing. Figure 6 (b) shows that, similar to Fig. 5 after including the effects of Johnson noise, the theoretical results of total spin relaxation (black solid line) is now more consistent with the experimental measurements (green triangles) at lower magnetic fields, where the relaxation rate at $B = 1$ T is around 0.3 s$^{-1}$.

Figure 6 is essentially the low-energy side of Fig. 5 with a shift in the peak position and a slight increase in the peak width. The enlarged plot does reveal more
FIG. 6: Spin relaxation rate as a function of magnetic field in Si QD with valley splitting $E_{vs} = 0.75$ meV for phonon and Johnson noises. In panel (a), we compare the spin relaxation rates for phonon noise with SO mixing (black solid line) and SV mixing (red dashed line), and Johnson noise with SO mixing (blue dash-dotted line) and SV mixing (magenta dash-double-dotted line). In panel (b), the total spin relaxation rate is plotted as a black solid line, and the total phonon contribution (red dashed line) and the total Johnson noise contribution (blue dot-dashed line) are also included. The experimental results (green triangles) are taken from Ref. 9. For comparison, the result (black dotted thin line) of phonon induced relaxation without considering the phonon bottleneck effect (i.e. no cutoff function) is also presented, which reproduces the original fitting in Ref. 9.

clearly one important fact: with the given Si parameters the phonons provide a more important relaxation channel compared to Johnson noise at the spin hot spot. The transition of the dominant relaxation channel happens at a field significantly below the degeneracy point, at just below 2 T. Again the no-cut-off results seem to fit the experimental data better than results with phonon bottleneck effect, probably with a similar reason as we discussed above.

V. CONCLUSION

In conclusion, we have studied spin relaxation of an electron due to Johnson noise and phonon noise in a Si QD with valley splitting. In particular, we clarify how the presence of the conduction band valleys influences the spin relaxation. By considering both mechanisms of SV mixing and intra-valley SO mixing in a Si QD, we find that spin relaxation rate due to Johnson noise and SV mixing peaks when the Zeeman splitting matches the valley splitting. Because of a weaker field-dependence, the spin relaxation rate due to Johnson noise dominates over phonon noise at low magnetic fields, which is consistent with recent experiments.

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Appendix A: Effects of the magnetic field orientation

The spin relaxation mechanism we study in this paper involves the spin-orbit interaction. When both Dresselhaus and Rashba SO coupling are present in a system, such as in a Si heterostructure, the orientation of the applied magnetic field plays an important role in determining the amount of transverse magnetic noise and thus the relaxation rate. Here we discuss this field orientation dependence in detail.

Consider a magnetic field in an arbitrary direction $B_0 = B_0 (\text{sin} \theta \text{cos} \phi, \text{sin} \theta \text{sin} \phi, \text{cos} \theta)$, where $\theta$ and $\phi$ are the polar and azimuthal angles of the magnetic field in the (xyz) coordinate system. By using the relationship $\vec{p} = (-|\vec{p}|+) = i\hbar E_{\text{VZ}} r^{-1/2}/\hbar$, the spin-valley mixing matrix element $\Delta_{23}$ can be expressed in terms of the electric dipole matrix element $\Delta_{23, m}$

$$\Delta_{23} = \frac{2im^* E_{\text{VZ}}}{\hbar} \left[ \alpha_r r_y^+ \sigma_x^i + \alpha_\perp r_z^- \sigma_y^i \right], \quad (A1)$$

where $\sigma^i_{\perp} = (\uparrow | \sigma \downarrow)$ is the spin flip matrix elements, and $\alpha_{\perp}$ are the spin-orbit coupling constants.

In order to calculate the spin flip matrix elements $\sigma^i_{\perp}$, it is convenient for us to express the spin state $|\psi_{\mu}\rangle$ ($|\psi_{\mu}\rangle = |\uparrow\rangle$ or $|\downarrow\rangle$), which are the eigenfunctions of $\sigma_z^i$ (z’ axis along the magnetic field), in terms of the eigenstates $|\chi_{m}\rangle$ of $\sigma_z^i$: $|\psi_{\mu}\rangle = \sum_{m=\pm 1/2} D^{(1/2)*}_{\mu \gamma} (\phi, \theta, 0) |\chi_m\rangle$, where $D^{(1/2)}$ is the finite rotation matrix.$^2$

$$|\psi_{\uparrow}\rangle = e^{-i\phi/2} \text{cos} \theta/2 |\chi_{\uparrow}\rangle + e^{i\phi/2} \sin \theta/2 |\chi_{\downarrow}\rangle, \quad (A2)$$

$$|\psi_{\downarrow}\rangle = -e^{-i\phi/2} \sin \theta/2 |\chi_{\uparrow}\rangle + e^{i\phi/2} \cos \theta/2 |\chi_{\downarrow}\rangle \quad (A3)$$

Therefore, spin flip matrix elements are $\sigma^i_{\perp} = \cos \theta \cos \phi + i \sin \phi$ and $\sigma^i_{\parallel} = \cos \theta \sin \phi - i \cos \phi$, and the square of the magnitude of the SV mixing matrix

\[ \]
element is
\[
\begin{align*}
|\Delta_{23}|^2 &= (2m^*E_{VS}/\hbar)^2 \left\{ \alpha_\pm |r_{y+}^-|^2 (\cos^2 \theta \cos^2 \phi + \sin^2 \phi) \\
&+ \alpha_+^2 |r_{x+}^-|^2 (\cos^2 \theta \sin^2 \phi + \cos^2 \phi) + 2\alpha_- \alpha_+ \text{Re}[r_{y+}^- r_{x+}^-] \\
&\times (-\sin^2 \theta \cos \phi \sin \phi + i \cos \theta) \right\}.
\end{align*}
\] (A4)

When \(B_0\) is along the z-direction (\(\theta = 0\), \(\phi = 0\)),
\[
|\Delta_{23}|^2 = (2m^*E_{VS}/\hbar)^2 \left\{ \alpha_\pm |r_{y+}^-|^2 + \alpha_+^2 |r_{x+}^-|^2 \cos^2 \phi - \alpha_- \alpha_+ \text{Re}[r_{y+}^- r_{x+}^- \sin 2\phi] \right\}.
\] (A5)

When \(B_0\) is in the plane of 2DEG (\(\theta = \pi/2\)),
\[
|\Delta_{23}|^2 = (2m^*E_{VS}/\hbar)^2 \left\{ \alpha_\pm |r_{y+}^-|^2 \sin^2 \phi + \alpha_+^2 |r_{x+}^-|^2 \cos^2 \phi - \alpha_- \alpha_+ \text{Re}[r_{y+}^- r_{x+}^- \sin 2\phi] \right\}.
\] (A6)

Therefore, the magnetic field orientation dependence of \(\Delta\) (or \(\Gamma_{SV}\)) depends on the values of \(\alpha_-\), \(\alpha_+\), \(r_{y+}^-\) and \(r_{x+}^-\), which is material and device specific. In particular, if the magnetic field is along [110] crystal axis \(\phi = 0\), as the case in Ref. 36, \(\sigma_\pm^i = 0\), \(\sigma_\pm^i = -i\), and \(\Delta_{23} = 2m^*E_{VS}\alpha_R r_{x+}^-/2\hbar\). In our calculation, we used \(\Delta_{23} = m^*E_{VS}\alpha_R r_{x+}^-/2\hbar\) to reproduce the results of Ref. 36.

**Appendix B: 1/f charge noise and spin relaxation**

The 1/f charge noise is quite common in semiconductor devices, and is often believed to be an important decoherence source for charge qubits. Here we explore how much it affects a spin qubit.

The 1/f charge noise is often measured via the fluctuations it causes in the energy levels in a quantum dot or a quantum point contact (QPC).\(^{48–51}\) Consider the current through a QPC connected to two leads. The current is sensitively dependent on the gate voltage applied to the QPC. By measuring the electric current fluctuations, the overall effect of the 1/f charge noise on the QPC can be measured. Normally, such an experiment has a finite frequency range, e.g. from a few Hz to hundreds of Hz. The measured energy level fluctuations actually depend on the frequency range of the measurement, and is thus dependent on the specific experiment. Thus here we first try to extract a quantity that is independent of the frequency range in these experiments.

We assume the current fluctuation spectral density due to the 1/f charge noise in a QPC to be \(S_I(\omega) = A_I/\omega\). An integration of the spectrum yields
\[
\int_{\omega_0}^{\omega_c} d\omega S_I(\omega) = A_I \ln \frac{\omega_c}{\omega_0}.
\] (B1)

Phenomenologically, the current fluctuation can be represented by an effective gate voltage fluctuation\(^{48–51}\)
\[
\Delta V_{EG} = \sqrt{2 \int_{\omega_0}^{\omega_c} d\omega S_I(\omega) / \frac{dI_{QPC}}{dV_G}},
\] (B2)

where \(\omega_0\) and \(\omega_c\) are the lower and upper cutoff frequency (response frequency) in the experiment. \(dI_{QPC}/dV_G\) is the effective differential conductivity, which represents the variation of the electric current through QPC due to the gate voltage difference. Therefore, the quantity \(\Delta V_{EG}\) represents the effective gate voltage fluctuation due to charge noise in the system. In order to get the effective electric field on the electron in the QD, we should also consider the screening effect of the gate voltage.

The quantity \(\Delta V_{EG}\) defined here is dependent on the frequency range of the measurement in the experiments,
\[
\Delta V_{EG} = \sqrt{2A_I \ln \left( \frac{\omega_c}{2\omega_0} \right)} \frac{dI_{QPC}}{dV_G}.
\] (B3)

We define a quantity \(\tilde{\Delta}V_{EG} = \Delta V_{EG}/(\sqrt{2\ln(\omega_c/2\omega_0)})\) as the effective gate voltage fluctuation, which is independent of the frequency range. Take Ref. 51 as an example for the 1/f charge noise in Si/SiGe, where \(\Delta V_{EG} = 0.1\) meV, \(\omega_0 = 0.01\) Hz, \(\omega_c = 49\) Hz, and \(\sqrt{2\ln(\omega_c/2\omega_0)} = 11.03\). Therefore, the effective gate voltage fluctuation due to charge noise is \(\Delta V_{EG} \approx 10\) \(\mu\)eV. Due to the screening of the gate voltage, the effective voltage fluctuation sensed by the electron in the QD is around 1 \(\mu\)eV.

With the knowledge of the magnitude of 1/f charge noise, we can calculate the corresponding spin relaxation. The spin relaxation due to the SV mixing and 1/f charge noise is given by
\[
\Gamma_{SV} = \frac{2\pi}{\hbar} \sum_i |r_i^-|^2 e^{2A_0^2} F_{SV}(\omega_Z),
\] (B4)

where \(r_i^-\) are the transition matrix elements between the two lowest valley states, \(A\) is the charge noise amplitude, \(\omega_Z\) is the Zeeman frequency. The dependence of \(1/T_1\) on the applied magnetic field is \(1/T_1 \propto B_0^{-1} F_{SV}(\mu B B_0/\hbar)\), and the function \(F_{SV}(\omega_Z)\) is given by Eq. 4.

Figure 7 shows the spin relaxation rates \(\Gamma_{SV}\) through SV mixing (red dashed line), \(\Gamma_{SO}\) through SO mixing (blue dash-dotted line) and the total spin relaxation \(\Gamma_{SV} + \Gamma_{SO}\) (black solid line) as a function of the applied magnetic field \(B_0\) due to 1/f charge noise. The results of spin relaxation rate \(\Gamma_{SO}\) due to charge noise and intra-valley SO mixing is from Ref. 52. As shown in the figure, the relaxation through the mechanism of SV mixing dominates in the low magnetic field regime, and peaks at the degenerate point \((\mu B B_0 = E_{VS})\). The relaxation rate through the intra-valley SO mixing is dominating in the high magnetic field regime. The relaxation time due to the 1/f charge noise is about \(10^4\) s for a Si QD, when the Zeeman energy is away from the valley splitting.

**Appendix C: Spectrum of Phonon Noise**

The electron phonon interaction \(U_{ph}(\vec{r})\) is given by Eq. 13. In the interaction picture, the electron phonon
Then, we simplify the exponential terms $e^{i\omega_q \cdot \vec{r}}$, and $e^{i\omega_q \cdot t}$. The correlation of the electric force due to phonons, $-eE(\vec{r}) = -\nabla U_{ph}(\vec{r})$, is thus given by (x component),

$$e^2 \langle E_x(0)E_x(t) \rangle = \sum_{q_j} \frac{|f(q_j)|^2}{2\rho_\omega q_j} \frac{\hbar^2 e^{i\vec{q}_j \cdot \vec{r}}}{4\pi^2} \times |\bar{\Xi}_{q_j}|^2 \left( b_{q_j}^\dagger b_{q_j} e^{i\omega_q t} + b_{q_j}^\dagger b_{-q_j} e^{-i\omega_q t} \right). \quad (C1)$$

We consider the adiabatic condition, where the energy scale of the noise is much less than dot confinement energy $E_d = \hbar \omega_d$ and the valley splitting, so that the electron orbital state stays in the instantaneous ground state $\psi(\vec{r}) = \exp\left(-\frac{\vec{r}^2}{2\lambda^2}\right)/\sqrt{\lambda^2/2\pi}$, where $\lambda^{-2} = h^{-1}\sqrt{(m^* \omega_d^2 + (eB_z/2c)^2)}$ is the effective radius. Then, we simplify the exponential terms $e^{i\vec{q}_j \cdot \vec{r}}$ by its mean-field value $e^{-q_j^2 \lambda^2/4}$.

The summation in Eq. (C1) for all possible $q$ in the momentum space can be expressed as integrals

$$\sum_j \int d\omega d\theta d\phi D_j(\omega,\theta) g_j(\omega,\theta,\varphi), \quad (C2)$$

where $D_j(\omega,\theta) = \frac{\hbar^2}{(2\pi)^2} \sin^2 \theta$ is the density of states for phonons, and

$$g_j(\omega,\theta,\varphi,t) = \frac{\hbar^2 \bar{\Xi}_{q_j}^2}{2\rho_\omega v_j^4} \sin^2 \theta \cos^2 \varphi$$

$$\times \omega^3 \left[ (N_\omega + 1) e^{i\omega t} + N_\omega e^{-i\omega t} \right] f_j(\omega,\theta). \quad (C3)$$

In Eq. (C3), $N_\omega = (\exp(\hbar\omega/k_B T) - 1)^{-1}$ is the phonon excitation number and the cutoff function $f_j(\omega,\theta) = \left| f(\omega \cos \theta / v_j) \right|^2 e^{-\omega^2 \lambda^2 \sin^2 \theta / 2v_j^2}$ is due to the suppression of the matrix element for the electron-phonon interaction in a large QD.

The spectrum of the phonon noise in the $x$-direction is therefore ($f_0^{2\pi} d\varphi \cos^2 \phi = \pi$)

$$S_{xx}^E(w) = \text{Re} \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \langle E_x E_x(t) \rangle \cos(wt)$$

$$= \sum_j \frac{\hbar w^5(2N_w + 1)}{16\pi^2 e^2 \rho_\omega v_j^4} \int_0^{\pi/2} d\theta \Xi_{q_j}^2 \sin^3 \theta f_j(w,\theta).$$

Similarly, $S_{yy}^E(w) = S_{xx}^E(w)$ and

$$S_{zz}^E(w) = \sum_j \frac{\hbar w^5(2N_w + 1)}{8\pi^2 e^2 \rho_\omega v_j^4} \int_0^{\pi/2} d\theta \Xi_{q_j}^2 \sin \theta \cos^2 \theta f_j(w,\theta).$$

If the dipole approximation $e^{i\vec{q}_j \cdot \vec{r}} \approx 1 + i\vec{q}_j \cdot \vec{r}$ is employed (for most spin qubit applications, the dipole approximation should be valid), so that $f_j(w,\theta) = 1$, the relaxation rate would have taken the form given in Ref. [34]. Furthermore, the temperature $T$ of the lattice vibration is normally very low ($T < 1 \text{ k}$), so that $2N_w + 1 = \cosh(\hbar w / 2k_B T) \approx 1$, in which case the spectrum of phonon noise shows a nice $w^0$ dependence.

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