Coherent electron transport in silicon quantum dots

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In this paper, we study electron transport in a silicon double quantum dot. First, in the valley-orbital dynamics, we discuss several practical schemes to detect the valley phase difference, with particular methods based on transport through the double dot and the Landau-Zener-Stückelburg interference. We also discuss the feasibility of implementing these schemes with current experimental technologies. Second, taking spin degree of freedom into consideration, we show the inhomogeneous magnetic field and the spin-orbit coupling can cause considerable spin flip errors. We analyze the spectrum of the double dot and how valley splittings in the two dots affect the formation of spin-valley anti-crossings. At last, we discuss a mechanism for spin fidelity loss in silicon quantum dots caused by the mixing between spin and valley states, with an example where the classical information (spin population) is faithfully transported but the quantum information (coherence) is lost.

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I. INTRODUCTION

Spin qubits in silicon quantum dots (SiQD) have intriguing potentials for quantum information processing due to their long coherence time, helped by isotopic purification that could efficiently reduce nuclei spin noises [1–8]. Spin relaxation is also extremely slow in Si because of the relatively weak spin-orbit coupling (SOC) [9]. The powerful silicon industry could be another important factor in the scale-up of quantum qubit architectures [1, 4, 10, 11]. For example, the current commercial 14nm/10nm process technology [12, 13] is already at the level of feature sizes required for gated Si quantum dots. These advantages make SiQD a promising candidate as a building block for future semiconductor quantum computers [6, 8, 14].

However, SiQD system does have its own challenges, especially in a conduction band that has multiple minima (valleys) [11, 12, 28]. A small energy splitting between valley eigenstates can introduce unwanted orbital dynamics to a spin qubit, and spin-valley coupling can lead to mixture with spin degree of freedom and cause significant spin relaxation (spin hot spots) [24]. In other words, a quantum information processor based on spin qubits in Si still requires more explorations in terms of high-fidelity coherent manipulations in SiQDs [25]. In this context, coherent electron transport over multiple QDs is one of the fundamental operations to manipulate quantum states of spin qubits [2, 18, 19, 29–32]. It aims at transporting the information carrier (electron) over a finite distance without disturbing the spin state in which quantum information is encoded [20, 31, 34–39], which is particularly important in a scaled-up computer [2, 40, 43]. Other important tasks such as quantum error correction and quantum measurement may also involve electron tunneling between quantum dots [31, 34, 44–51]. Beyond applications in conventional qubit control, transport between quantum dots and nanowires help to characterize electronic states and properties of a semiconductor nanostructure, and could have wide ranging applications, such as in the search and control of possible Majorana excitations in hybrid structures [52, 53]. We are thus motivated to make a thorough examination of coherent electron transport in SiQDs.

In this paper, we study electron transport in a silicon double quantum dot (DQD). We first consider charge dynamics (coupled valley and orbital dynamics) and study possible Landau-Zener-Stückelburg (LZS) interference [54, 55] in the transport because of the multiple valleys and level crossings. In a SiQD, valley-orbit coupling is in general a complex parameter. While its magnitude, which determines the size of the valley splitting, has been widely studied [15, 60–62], in a single dot its phase is generally not important. However, in the case of a double dot, the phase of the valley-orbit coupling, particularly the phase difference between the two dots, is of great importance in determining interdot tunneling and exchange coupling [61]. Here we propose several schemes to detect this valley phase difference in a Si DQD, ranging from conventional tunneling current measurement for an open DQD to schemes that take advantage of Landau-Zener transitions and interferences in the multiple level anti-crossings of the DQD. All these schemes are based on charge dynamics and measurements. We also discuss their feasibility within the current experimental technologies.

In addition to charge dynamics in SiQD, we also investigate spin dynamics in the tunneling process. This is an important problem in the context of spin qubit transport and communication [63]. We first investigate spin flip caused by SOC [64, 65]. In SiQD, spin flip is usually slow due to the weak SOC. However, the presence of valleys gives rise to an anti-crossing that is particularly broad in the interdot detuning, such that considerable spin flip can occur when the double dot is swept through such an anti-crossing. We identify four regions in the valley-splitting-Zeeman-splitting parameter space, and examine the anti-crossings and the resultant spin flip
in these regions. Furthermore, we investigate the loss of spin purity in the transport caused by mixing between the spin states and the valley states as the electron passes through various level anti-crossings. Specifically, we calculate the purity and coherence of the spin state after the transport, and show an example where classical information (spin population) is preserved while quantum information (quantum phase or superposition) is lost in the transport.

The rest of paper is organized as follows: In Sec. II, we describe the double quantum dot model and our protocol for electron transport. In Sec. III, we consider the electron charge dynamics involving the orbital and valley degrees of freedom. We first clarify the low-energy spectrum of a single electron in the double dot, and propose several schemes to detect the valley phase difference between two dots, ranging from conventional DC transport through a double dot, to Landau-Zener-Stückelburg interference in sweeping the interdot detuning. We also discuss the experimental feasibility of these schemes. In Sec. IV, we include the spin degree of freedom into consideration and investigate three topics: (a) spin flip error caused by SOC near zero detuning, (b) several types of spin-valley anti-crossings and the resultant spin flip errors enhanced by an inhomogeneous magnetic field, and (c) loss of fidelity caused by spin-valley mixing. At last, we conclude in Sec. V.

II. THE DOUBLE QUANTUM DOT

In this work, we study electron transport by considering a single electron tunneling in a Si double quantum dot (DQD). The scheme is described in Fig. 1. A single electron is confined in a biased double potential well, with a tunable detuning \( \epsilon \), controlled by gate voltage between the two dots. A tunnel barrier \( E_t \) is controlled by additional top gates between two dots. The external magnetic field provided by nano-magnet is homogeneous in \( z \)-direction and inhomogeneous in \( x \)-direction. By tuning \( \epsilon \) slowly from \(-\epsilon_0\) to \(+\epsilon_0\), the electron is transported from one dot to the other.

The electron in such a DQD system has three degrees of freedom. First, the tunneling of the electron between the two dots connects two local charge (orbital) states \(|(1, 0)\) and \(|(0, 1)\), which are labeled by the basis \(|L\) and \(|R\) respectively. Second, At the interface, the confinement along the growth direction couples the two lowest-energy valley states \(|z\) and \(|\bar{z}\) from the other four branches of higher-energy states. Third, the spin of the electron along \(z\)-direction also has two possible states \(|\downarrow\) and \(|\uparrow\). Therefore, the tensor of all three degrees of freedom gives the basis in the total Hilbert space \(|\{D, \xi, \sigma\}\rangle\), where \(D = L, R, \xi = z, \bar{z}\), and \(\sigma = \downarrow, \uparrow\). In this basis, the total Hamiltonian of the DQD can be written as

\[
H = E_0 + \begin{pmatrix}
\epsilon + E_z & S_1 + E_x & \Delta_L & 0 & E_t & S_2 & 0 & 0 \\
S_1 + E_x & \epsilon - E_z & 0 & \Delta_L & -S_2 & E_t & 0 & 0 \\
\Delta_L & 0 & \epsilon + E_z & S_1 + E_x & \Delta_R & 0 & 0 & 0 \\
E_t & -S_2 & 0 & 0 & -S_2 & E_t & 0 & 0 \\
S_2 & E_t & 0 & 0 & -S_2 & E_t & 0 & 0 \\
0 & 0 & E_t & -S_2 & 0 & \Delta_R & 0 & 0 \\
0 & 0 & S_2 & E_t & 0 & 0 & -\epsilon + E_z & -S_1 - E_z \\
0 & 0 & 0 & \Delta_R & 0 & 0 & -\epsilon + E_z & -S_1 - E_z \\
\end{pmatrix}.
\]

Here \(E_0\) is the confinement energy for either of the DQD with zero detuning (setting a reference energy). The interdot tunnel coupling between the two orbital states \(|L\) and \(|R\) is labeled by \(E_t\), and the detuning between the two dots is given by \(\epsilon\). The off-diagonal elements \(\Delta_D = |\Delta_D|e^{i\phi_D}\) \((D = L, R)\) is the valley-orbit coupling connecting the two valleys in each of the two dots with corresponding valley phase \(\phi_D\). The Zeeman splitting in \(z\)-direction is described by \(E_z = \frac{g\mu_B}{2}B_z\) and the inhomogeneous magnetic field in \(x\)-direction causes a splitting \(\pm E_x = \pm \frac{g\mu_B}{2}B_x\) governing the spin rotation. Here, we consider a magnetic field provided by...
a micromagnet which causes a homogeneous field in z-direction and an inhomogeneous field in x-direction $(\pm B_x$ in left/right dot), so that the matrix element such as $\langle L, \xi, \uparrow | H_Z | L, \xi, \downarrow \rangle = E_x$ and $\langle R, \xi, \uparrow | H_Z | R, \xi, \downarrow \rangle = -E_x$ $(\xi = z$ or $\bar{z}$, $H_Z = \frac{1}{2} g \mu_B B \cdot \sigma$) are different. At last, the spin-orbit coupling matrix elements are $S_1 = \langle L, \xi, \uparrow | H_{SO} | L, \xi, \downarrow \rangle$ and $S_2 = \langle L, \xi, \uparrow | H_{SO} | R, \xi, \downarrow \rangle$, where $H_{SO}$ is the spin-orbit coupling Hamiltonian $H_{SO}$. 

Among all the parameters in Hamiltonian $H$, $E_t$, $E_z$, $E_x$, and $E_z$ are tunable (or at least adjustable between different devices) experimentally: A top gate between the two dots can modify the tunnel barrier and effectively control $E_t$; The bias voltage between two dots can control the detuning $\epsilon$; and lastly, the position and strength of the micromagnet can change $E_z$ and $E_x$. In comparison, $\Delta_{E}$, $\phi_D$, $S_1$, and $S_2$ are typically harder to modify/control if not impossible, although some recent studies show the possibility of tuning the valley splitting $\Delta_{E}$ and $E_z$. In the following discussion, we simply assume $\Delta_{E}$, $\phi_D$, $S_1$, and $S_2$ are fixed for a particular DQD.

The transport protocol we consider is driven by changing the detuning $\epsilon$ [20, 73, 74]. Specifically, here we consider an increasing detuning from $-\epsilon_0$ to $\epsilon_0$. Initially, the detuning is negative, resulting in a lower energy for state $|L\rangle$, therefore the electron is trapped in the left dot. As the detuning gradually increases to a positive value, $|R\rangle$ will eventually have lower energy and the electron would tunnel to the right dot.

The electron evolution is governed by the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle.$$  

In our study, we numerically solve the time-dependent Schrödinger equation to obtain the dynamics of the electron. In the meantime, we also diagonalize the Hamiltonian at each time point with detuning $\epsilon(t)$ to obtain the instantaneous eigen-energies $E_i(\epsilon)$ and corresponding eigen-states $|\psi_i(\epsilon)\rangle$. These instantaneous eigen-states are helpful in the study of Landau-Zener (LZ) transitions at level anti-crossings, which will be investigated in the following sections.

At large detunings and without spin-valley mixing, the instantaneous eigen-states of Hamiltonian $H$ can be approximately expressed as

$$|\psi_i(\epsilon \gg E_t)\rangle \approx |D, \pm, \sigma\rangle,$$

$$|D, \pm, \sigma\rangle = \frac{1}{\sqrt{2}} (|D, z, \sigma\rangle \pm e^{i\phi_D} |D, \bar{z}, \sigma\rangle).$$

Here $|D, \pm, \sigma\rangle$ is obtained by partially diagonalizing the valley part in the left or right dot, respectively. A specific example is given in the following section. Indeed, in most situations, tunneling can be treated as a perturbation, so that the orbital eigenstates are approximately $\{|L\rangle, -|R\rangle\}$. Similarly, for the spin part, $E_z$ is typically much larger than $E_x$, $S_1$, and $S_2$, so that the diagonalized eigen-states are still Zeeman eigenstates $\{|\downarrow\rangle, -|\uparrow\rangle\}$ approximately. In more special situations when close to level anti-crossings, the DQD eigenstates are more mixed. For example, when $\epsilon \approx 0$, $|L\rangle$ and $|R\rangle$ would mix with each other; when spin-valley mixing (near particular anti-crossings) is present, the instantaneous eigenstates will be a mixture of $|\downarrow\rangle$ and $|\uparrow\rangle$. These special cases will be studied in detail in the following sections.

### III. VALEY-ORBIT DYNAMICS: MEASUREMENT OF VALEY PHASE DIFFERENCE

In this Section we focus on the valley-orbit dynamics in a Si DQD. We first solve for the low-energy spectrum of the one-electron DQD as a function of interdot detuning. As we discussed in Sec. I, valley phase difference is an important yet hard to control property of a Si DQD. The knowledge acquired in the spectral calculation further confirms the importance of this phase difference, and prompts us to examine in detail how we can determine the valley phase difference between the two dots. In the rest of the Section we propose several schemes to measure the valley phase difference based on DC transport, Landau-Zener transitions, and Landau-Zener-Stückelburg interference in a charge-sensing experiment. We believe that our study here may open a path toward a quantitative experimental investigation of the valley phase difference.

### A. Orbital spectrum of a Si DQD

Without considering the spin degree of freedom and spin-orbit coupling, and focusing on the low-energy charge dynamics of the DQD, the full Hamiltonian in Eq. (1) can be reduced to a single-electron valley-orbit Hamiltonian

$$H_{VO} = \begin{pmatrix} E_0 & \Delta_L & 0 & E_t \\ \Delta^*_L & E_0 + \epsilon & 0 & E_t \\ 0 & E_t & E_0 - \epsilon & \Delta_R \\ 0 & E_t & \Delta^*_R & E_0 - \epsilon \end{pmatrix}.$$  

In general each single quantum dot in Si has its own complex valley-orbit coupling $\Delta$. Thus from an experimental perspective it is helpful to project Hamiltonian $H_{VO}$ onto the single-dot eigenbasis. Specially, the eigenstates of a single dot Hamiltonian (for instance, the left dot) $H_L = \begin{pmatrix} E_0 + \epsilon & \Delta_L \\ \Delta^*_L & E_0 + \epsilon \end{pmatrix}$ are $|L, \pm\rangle \equiv \frac{1}{\sqrt{2}} (|L, z\rangle \pm e^{i\phi_L} |L, \bar{z}\rangle)$ [20, 21]. Using the set of new basis $\{|L, +\rangle, |L, -\rangle, |R, +\rangle, |R, -\rangle\}$, the valley-orbit Hamiltonian [15] takes the form

$$H_{VO} = \begin{pmatrix} E_0 + \epsilon + |\Delta_L| & 0 & E_{t, +} & E_{t, -} \\ 0 & -\epsilon - |\Delta_L| & E_{t, -} & E_{t, +} \\ E_{t, +} & E_{t, -} & -\epsilon + |\Delta_R| & 0 \\ E_{t, -} & E_{t, +} & 0 & -\epsilon - |\Delta_R| \end{pmatrix},$$  

(6)
The general non-vanishing intra- and inter-valley tunnelings \( E_{t,-} \) and \( E_{t,+} \) produce four anti-crossings, labeled as “A”, “B”, “C”, and “D”. If we sweep the inter-dot detuning through any of these anti-crossings, the probability of a diabatic or an adiabatic transition is determined by the tunnel coupling \( E_{t,-} \) or \( E_{t,+} \) as compared to the sweeping speed.

Noticing that both tunnel couplings \( E_{t,-} \) and \( E_{t,+} \) are sensitively dependent on the valley phase difference \( \delta \phi \equiv \phi_L - \phi_R \) between the two dots, and they in turn determine the eigenstates and energies of the DQD. Beyond charge dynamics, valley properties are also essential to spin-based quantum information processing in Si quantum dots \cite{15, 60–62}, and valley phase properties are of particular importance there, too \cite{71}. One example is discussed later in this manuscript in Sec. IV C. Therefore, in the current study of charge dynamics in a Si DQD, one of our major goals is to identify possible ways to measure \( \delta \phi \).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2}
\caption{(color online) (a) Energy levels as a function of detuning \( \epsilon \). (b) Applied pulses of \( \epsilon \) as functions of time. The parameters are chosen as \( |\Delta_L| = 40 \mu eV, |\Delta_L| = 60 \mu eV, E_0 = 8 \mu eV, |E_{t,-}| = 40 \mu eV, \delta \phi = 0.3 \pi \).}
\end{figure}

\begin{equation}
\frac{|E_{t,-}|}{|E_{t,+}|} = \tan \frac{\delta \phi}{2}.
\end{equation}

Therefore, the ratio \( \frac{|E_{t,-}|}{|E_{t,+}|} \) extracted from the experiment in Ref. \cite{75} directly gives the valley phase difference \( \delta \phi \).

C. Measuring valley phase difference \( \delta \phi \) by transport

In the absence of a cavity, the valley phase difference \( \delta \phi \) can also be studied in a conventional transport experiment. In a GaAs DQD, tunnel coupling can be measured by detecting equilibrium charge distribution dependence on interdot detuning \cite{76}. In Si, however, the presence of two valleys means that a complete description of the low energy dynamics requires knowledge of two tunnel couplings, \( |E_{t,-}| \) and \( |E_{t,+}| \). Such an evaluation can be done in a DC transport experiment where the DQD is coupled to a source and drain lead. One can measure the current through the DQD as a function of the inter-dot detuning. The resonant tunnel current at the anti-crossings “A” and “B” should then give a good estimate of the tunnel couplings and therefore the valley phase difference between the two dots:

\begin{equation}
\frac{I_A}{I_B} = \frac{|E_{t,-}|^2}{|E_{t,+}|^2} = \tan^2 \frac{\delta \phi}{2}.
\end{equation}

The setup here is that of a conventional transport experiment, and should be relatively straightforward to realize. It does require that the double dot couples to the source and drain leads. For an electron spin or charge qubit this may not be the optimal arrangement unless the coupling to the leads can be cut off almost completely.

D. Measuring valley phase difference \( \delta \phi \) by charge sensing

For a closed double dot without close-by leads, a dynamic method that can access the excited states is needed to measure the tunnel couplings and the valley phase difference. One dynamical approach is based on Landau-Zener transitions across the energy-level anti-crossings for the Si DQD. When sweeping the inter-dot detuning through an anti-crossing, the probability of the confined electron following a diabatic path can be roughly predicted by the general Landau-Zener (LZ) formula \cite{54},

\begin{equation}
P_D = \exp\left(-\frac{2 \pi a^2 / h}{|dE_m - E_n|/dt}\right),
\end{equation}

where \( a \) is the off-diagonal element coupling the two involved energy levels \( E_m \) and \( E_n \), which is also the half
energy gap at the anti-crossing. In a transport experiment, the output state is mainly determined by the LZ velocity \(v_{LZ} = \frac{\partial}{\partial t}(E_m - E_n)\), which can be controlled by the detuning pulse.

Let us first consider a pulse “\(\alpha\)” depicted by the magenta-dotted line in Fig. 2 (b), where the interdot detuning is swept through anti-crossing “\(A\)” relatively slowly, then through anti-crossing “\(C\)” quickly. The system is initially prepared in the ground state at a large negative detuning (left end of the figure). At the anti-crossing “\(A\)”, the LZ velocity is designed to be comparable to the energy gap \(|E_{t,-}|/2\). This would split the evolution into two paths and the probability of the electron getting excited into the first excited state (solid green line) is given by Eq. (9). As the detuning \(\epsilon\) is quickly swept past the anti-crossing “\(C\)”, at a speed much faster than the energy gap \(|E_{t,+}|/2\), the probability for the electron in the first excited state to be excited into the second excited state (solid blue line) after anti-crossing “\(C\)” is almost 100%. Eventually, the total probability of finding the electron in the left dot at large positive detuning (blue line, state \(|L\rangle\) ) is

\[
P_{L\alpha} = \exp \left(-\frac{\pi |E_{t,-}|^2}{2\hbar v_{LZ}^\alpha} \right),
\]

which can be easily monitored by a charge sensor. We can revert the pulse sequence, and design it like the cyan-dotted line in Fig. 2 (b), labeled as pulse “\(\beta\)”. Now the interdot detuning is swept through anti-crossing “\(A\)” quickly, so that the electron ends up in the first excited state after the first pulse. Then the second pulse goes through anti-crossing “\(C\)” more slowly, at a speed comparable to \(|E_{t,+}|\), so that the electron has a certain probability to jump into the second excited state. The final charge distribution after the pulses is

\[
P_{L\beta} = \exp \left(-\frac{\pi |E_{t,+}|^2}{2\hbar v_{LZ}^\beta} \right).
\]

If the valley phase difference between the two dots is not very small or close to \(\pi\), the two tunnel coupling matrix elements \(E_{t,-}\) and \(E_{t,+}\) would have similar magnitudes. We can thus choose the same LZ velocities for the front and back half of the \(\alpha\) and \(\beta\) pulse sequences, respectively, as shown in Fig. 2 (b), so that \(v_{LZ}^\alpha = v_{LZ}^\beta = v_{LZ}\). The ratio of charge distribution for the two pulses is then

\[
\frac{P_{L\alpha}}{P_{L\beta}} = \exp \left[\frac{-\pi}{2\hbar v_{LZ}} (|E_{t,-}|^2 - |E_{t,+}|^2) \right].
\]

The ratio now is directly related to the valley phase difference, and is independent of both \(E_t\) and \(v_{LZ}\). One can thus perform multiple experiments with different combinations of \(E_t\) (by tuning the tunnel barrier between the dots) and \(v_{LZ}\) to increase the accuracy of this estimate.

The method proposed above involves relatively straightforward manipulations, though it also has its limitations. First, the LZ formula (9) is obtained from a two-level theoretical model. In general, if the valley splitting and tunnel couplings are of the same order of magnitude, a Si DQD is better described as a four-level system, and the impacts from excited levels can cause notable corrections. An example is discussed in the following subsection and in Appendix A. Second, when \(\delta \phi\) close to 0 or \(\pi\), one of the tunneling couplings \(E_{t,-}\) or \(E_{t,+}\) will be vanishing small. Adiabatic transition through such an anti-crossing would then require ultra-fast LZ velocity, which may not be feasible. Third, orbital relaxation would reduce the fidelity of the charge distribution measurement. Finally, the accuracy of \(\delta \phi\) relies on high-precision measurement of charge distribution and precise control of the sweeping speed. In the next subsection, we propose an alternative method to measure \(\delta \phi\) based on the LZS interference. These two methods can be complementary to each other.

### E. Measuring valley phase difference \(\delta \phi\) by Landau-Zener-Stückelburg interference

Here we propose another scheme to detect valley phase difference \(\delta \phi\) in a closed Si DQD using LZS interferences and charge sensing. In this scheme, instead of directly measuring \(|E_{t,+}|\), we propose to measure the energy gap \(\Delta E\) at zero detuning (shown in Fig. 2). The “zero detuning” here can be determined by shifting the detuning by the amount of \(\pm \frac{1}{2}(\Delta L - |\Delta R|)\) from the anti-crossing “\(A\)” or using the mean value \(\frac{1}{2}(\epsilon_B + \epsilon_C)\) for detuning. The eigen-energies of Hamiltonian (5) and (6) at zero detuning (shown in Fig. 2). The “zero detuning” in a closed Si DQD is better described as a four-level system, and tunnel couplings are of the same order of magnitude, a Si DQD is better described as a four-level system, and the impacts from excited levels can cause notable corrections. An example is discussed in the following subsection and in Appendix A. Second, when \(\delta \phi\) close to 0 or \(\pi\), one of the tunneling couplings \(E_{t,-}\) or \(E_{t,+}\) will be vanishing small. Adiabatic transition through such an anti-crossing would then require ultra-fast LZ velocity, which may not be feasible. Third, orbital relaxation would reduce the fidelity of the charge distribution measurement. Finally, the accuracy of \(\delta \phi\) relies on high-precision measurement of charge distribution and precise control of the sweeping speed. In the next subsection, we propose an alternative method to measure \(\delta \phi\) based on the LZS interference. These two methods can be complementary to each other.

\[
E_A = \frac{|\Delta L|^2 + |\Delta R|^2}{2} + E_t^2,
\]

\[
E_B = \frac{1}{4} \left(|\Delta L|^2 + |\Delta R|^2\right) + E_t^2 \left(|\Delta L|^2 + |\Delta R|^2 + 2|\Delta L|\Delta R|\cos(\delta \phi)\right).
\]
The relation between $\Delta E = (E_3 - E_2)|_{\epsilon=0}$ and $\delta\phi$ can then be obtained as

$$\frac{\Delta E^2}{4} = \frac{|\Delta L|^2}{2} + \frac{|\Delta R|^2}{2} + \left(\frac{E_{t,\epsilon}}{\cos\frac{\delta\phi}{2}}\right)^2 - \sqrt{\left|\frac{|\Delta L|^2}{2} - \frac{|\Delta R|^2}{2}\right|^2 + \frac{4|\Delta L||\Delta R|\cos^2\frac{\delta\phi}{2}}{4}}.$$

(17)

In any given Si DQD, the valley splittings ($|\Delta L|$, $|\Delta R|$) are fixed. If we also fix the intra-valley tunneling coupling $E_{t,\epsilon}$, the energy gap $\Delta E$ is then only determined by the valley phase difference $\delta\phi$. Therefore, $\delta\phi$ can be extracted from measurement of $\Delta E$ through the interference in the LZS process. Specifically, as shown in Fig. 2 two adjacent LZ processes “B” and “C” can form an LZS interferometer. Our designed pulse sequence “γ” has a plateau at $\epsilon = 0$ as shown in Fig. 2 (b), which leads to tuning of the charge distribution of the output state. In order for the electron to pass through both “B” and “C” anti-crossings, the system needs to be initially prepared in the second lowest energy state $|2\rangle \approx |L, +\rangle$ (green on the left side) at $\epsilon \ll -E_t$. After the pulse sequence, the probabilities of finding $|L, -\rangle$ (blue on the right side) and $|R, +\rangle$ (green on the right side) in the final state is then strongly dependent on the dynamical phase $\exp(-i\Delta E\tau/h)$ accumulated at $\epsilon = 0$, which can be tuned by $\tau$ and monitored by a charge sensor.

In Fig. 3 we plot the probability of finding the electron in the right dot $P_R$ in the final state as a function of the tunnel coupling between the lower valley eigenstates $E_{t,-}$ and pulse plateau duration $\tau$. As expected, the figure clearly shows the interference between the two LZ transitions at “B” and “C”. The period $\tau_p$ as shown in Fig. 4 corresponds to a total accumulated phase $2\pi$. The energy gap $\Delta E$ at $\epsilon = 0$ is then obtained as $\Delta E = E_3 - E_2|_{\epsilon=0} = 2\hbar\pi/\tau_p$. It is worth noting that a similar scheme using interference pattern to measure energy gap has been demonstrated in a recent experiment.

A necessary condition for this proposal to measure $\delta\phi$ successfully is that the values of tunnel coupling $|E_{t,-}|$, and single-dot valley splittings $|\Delta L|$ and $|\Delta R|$ are known. The single-dot valley splitting $|\Delta L|, |\Delta R|$ is controllable by both magnetic and electric field, and can be measured by detecting relaxation hot-spots. The intra-valley tunneling coupling $E_{t,-}$ can be controlled by the top gates, and is easily detected through charge sensing. With knowledge of $|\Delta L|$, $|\Delta R|$, and $|E_{t,-}|$, $\Delta E$ is a single-variable function of $\delta\phi$. One can then determine $\delta\phi$ by either solving Eq. (17) or directly fitting the original experimental data of $\Delta E$ and $E_{t,-}$.

Figure 4 shows a numerical example to determine $\delta\phi$ from curve fitting. Suppose a DQD sample has valley splittings $|\Delta L| = 60\mu eV$, $|\Delta R| = 40\mu eV$, and an unknown valley phase difference $\delta\phi$. Charge sensing in an LZS experiment should lead to the interference pattern as in Fig. 3 (obtained here numerically). For a particular $E_{t,-}$ set by bias voltage, the period $\tau_p$ can be measured, and the energy gap at $\epsilon = 0$ can be computed as $\Delta E = 2\hbar\pi/\tau_p$. The curves “$\Delta E$ vs. $|E_{t,-}|$” is then dependent on the values of $\delta\phi$ as shown in Fig. 4.

Below we clarify another few technical details in our proposed scheme of measuring the valley phase difference $\delta\phi$.

(a) Measuring $\Delta E$ accurately is the cornerstone of the proposal, and it seems that the anti-crossing “A” in Fig. 2 may negatively impact the LZS interference by diverting the electron into an irrelevant state (the ground state). However, $\Delta E$ is measured from the accumulated phase, instead of directly measuring charge distribution $P_R$. Therefore, even if there is a probability leakage at “A”, it only lowers the contrast of the interference pattern without changing $\tau_p$. Furthermore, at the high-energy end there is also the anti-crossing “D”, which symmetrically compensates the effect of “A”. Our numerical simulation confirms the discussion here. In Fig. 3 $\tau_p$ can be measured as $\tau_p \approx 0.71$ ns. The calculated energy gap is $\Delta E = 2\hbar\pi/\tau_p \approx 58.4\mu eV$, which is

Figure 3. (color online) Probability of finding the electron in the right dot after the LZS process ($P_R = \langle |R|\psi_{\text{final}}\rangle^2$) as a function of the tunneling energy $E_{t,-}$ and the waiting time $\tau$. The lower panel is a cross-section of the 3-d contour plot at $|E_{t,-}| = 35\mu eV$. The parameters are chosen as $|\Delta L| = 60\mu eV$, $|\Delta L| = 40\mu eV$, $\delta\phi = 0.3\pi$. $\epsilon(t)$ is changing from $-0.2$ meV to $0.2$ meV in an operation time (excluding $\tau$) $T - \tau = 1$ ms.
gests examples indicated by black circles, the best curve fitting suggests \( \delta \phi = 0.4 \pi \).

consistent with the theoretical values from Eq. (14) and numerical results obtained in Fig. 2(a).

(b) Since the accumulated phase is sensitively dependent on the energy gap, one may worry about the charge noise which can affect the energy gap [79, 80]. However, at zero detuning (where the extra phase is accumulated), the first order derivative of the energy gap with respect to detuning is zero, namely \( \frac{d\Delta E}{d\epsilon} = 0 \) at \( \epsilon = 0 \). This can be verified either from Eq. (14) or from Fig. 2(a). Therefore, the scheme we proposed is robust against charge noise, at least in the leading order.

(c) The conventional method of measuring tunneling rate \( |E_{t,-}| \) is based on a GaAs DQD model, where valley degeneracy is absent. However, the low-energy spectrum of a Si DQD is actually a four level system with valley states. The traditional two-level theory used in Refs. [28, 76, 77] may no longer predict the results accurately. As a by-product of the research on charge dynamics of a Si DQD, we quantitatively study the measurement of tunnel coupling in a Si DQD through static charge detection. The details are shown in Appendix A.

We show that when \( \delta \phi \) is very small, the conventional method used in GaAs DQD is almost a perfect approximation. When \( \delta \phi \) is large, particularly \( \delta \phi \rightarrow \pi \), one need to consider the contributions from nearby LZ transitions. A new formula to evaluate \( |E_{t,-}| \) in Si DQD is given in Appendix A.

In short, in this section we have discussed several possible schemes to measure the valley phase difference of a Si DQD. These proposals should open new paths toward understanding of the valley properties of Si DQD samples. We also discuss the feasibility of the schemes with current experimental technologies.

In this subsection, we investigate the impact of spin-orbit coupling on spin flip without considering the effect of inhomogeneous magnetic field, by assuming \( E_z = 0 \). In a sweep of interdot detuning, transitions to unwanted states mainly arise from the LZ transitions at the anti-crossings, which enables spin flip. The probability for the non-adiabatic transition at the anti-crossings can be roughly determined by the LZ formula (9).

IV. SPIN-V ALLEY-ORBIT DYNAMICS: TRANSFER FIDELITY IN A DOUBLE QUANTUM DOT

In this section we focus on spin dynamics for a single electron in a Si double dot. In the task of transporting an electron spin qubit from one dot to the other, it is crucial to maintain the spin state in which quantum information is encoded. For a Si DQD, the extra valley degree of freedom can cause additional anti-crossings of the energy levels, potentially leading to spin flip errors. Besides, these anti-crossings could also cause entanglement between spin states and valley states. This again could cause loss of coherence for the spin state when tracing over the valley degree of freedom. In this section, we will study the anti-crossings induced by spin-valley mixing and investigate the resulting impact on spin transport.

A. spin orbit coupling induced spin flip error

In this subsection, we investigate the impact of spin-orbit coupling on spin flip without considering the effect of inhomogeneous magnetic field, by assuming \( E_z = 0 \). In a sweep of interdot detuning, transitions to unwanted states mainly arise from the LZ transitions at the anti-crossings, which enables spin flip. The probability for the non-adiabatic transition at the anti-crossings can be roughly determined by the LZ formula (9).
Typically, the SOC in silicon is weak, so that the energy gaps at spin-flip anti-crossings are small. According to the LZ formula (9), the probability of adiabatic transition should be close to 0 in most cases and almost all anti-crossings are approximately reduced to crossings. However, our study shows a special case where, because of the presence of the valleys, the LZ transition can cause significant spin flip error in the transport.

Figure 5 (a) shows a typical energy diagram of a DQD. Two types of anti-crossings are marked with red and blue rectangular box. In the blue box, which is enlarged in subplot (b), the anti-crossing occurs away from zero detuning. Since the anti-crossing is between states that have different locations (left and right here), the energy gap changes fast near the anti-crossing. This is the most common anti-crossings caused by SOC. Typically, $a^2/h$ is much smaller than $|dE_m - E_n|/dt$, so that $P_D \approx 1$ and the anti-crossings are roughly crossings. In contrast, in the red box, which is enlarged in subplot (c), the anti-crossing occurs near zero detuning, and is between different valley states in the same dot. Here the energy levels change slowly relative to each other, which allows the possibility that $a^2/h$ is comparable to $|dE_m - E_n|/dt$. Consequently, such anti-crossings can cause considerable spin flip during spin transport.

To confirm this qualitative analysis, we perform a series of numerical simulations with the same set of parameters except the initial states. For an initial state prepared in the 4th lowest energy level (approximately $|L+, \uparrow \rangle$ initially), it passes through two anti-crossings away from zero detuning as $\epsilon$ is swept from negative to positive. Numerical results show that the probability of keeping spin up is about 98.5%. In comparison, for an initial state in the 2nd lowest energy level (approximately $|L, -\downarrow \rangle$ initially), it passes through two anti-crossings near zero detuning as $\epsilon$ is swept. The probability of keeping spin up is sharply decreased to 86.6%.

In short, most anti-crossings cannot cause significant spin flip during spin transport through a DQD, because SOC in silicon is too weak to produce a large energy gap at the anti-crossings. The only case that deserves special attention is the anti-crossings near zero detuning. In that region, all the energy levels change slowly, which enables much larger probabilities of spin flip. It is worth noting that the region where energy gap changes slowly (typically called sweet-spot) is also often a working region to manipulate the spin qubit. Our results suggest a possible source of error due to non-adiabatic LZ transitions.

### B. Inhomogeneous magnetic field induced spin flip error

While SOC usually has a weak impact on spin flip in a Si DQD, the inhomogeneous magnetic field from a micro-magnet can connect different spin states strongly. Here we focus on an inhomogeneous field in the $x$-direction (interdot axial direction). Comparing to the strength of SOC ($S_i \sim 0.2 \mu eV$ $^{51}$), the coupling between spin states caused by $\pm B_z$ could be tuned to larger than 1 $\mu eV$ $^{68}$. As a result, most anti-crossings caused by an inhomogeneous field can induce relatively fast spin flips. Here, the main issues are the conditions for the formation of such anti-crossings, and the types of anti-crossings that lead to fastest spin flips.

Here we show the overall numerical result first, then analyze individual cases. Figure 6 shows spin infidelity $1 - F_{\text{spin}} = |P_{\sigma,\text{fin}} - P_{\sigma,\text{ini}}|$ after the transport in a parameter space, where $P_{\sigma,\text{ini}}$ and $P_{\sigma,\text{fin}}$ indicate the spin population for initial state and final state respectively (can be measured from spin readout $^{82, 83}$). We choose a particular Zeeman splitting $E_z = 40 \mu eV$, then change the valley splittings in left and right dots. The initial state is always chosen as the second lowest energy state at $\epsilon \ll -E_z$. The relations of three important energy scales $|\Delta_L|$, $|\Delta_R|$, and $E_z$ can cast the whole parameter space into four regions as we marked in Fig. 6. The spin dynamics is dramatically different in each of these four regions. The detailed energy diagrams for these four cases are plotted in Appendix B.

In region “A”, both $|\Delta_L|$ and $|\Delta_R|$ are smaller than the Zeeman energy $E_z$, therefore spin orientation is the most important factor in determining the total energy. In both left and right dot, state $-\downarrow \downarrow$ always has a larger energy than $+\downarrow \downarrow$, so that there will be no crossings or anti-crossings in the energy diagram when changing $\epsilon$ from negative to positive. Consequently, no obvious spin flip happens in region “A” for $|\Delta_L| < E_z$ and $|\Delta_R| < E_z$.

In region “B” and “C”, one of the valley splittings is smaller than $E_z$, while the other is larger than $E_z$. As a result, an anti-crossing appears in the energy diagram. For example, in region “B”, $|\Delta_L| > E_z > |\Delta_R|$, the val-
ley state determines the total energy in left dot, while in the right dot spin state is dominant. When $\epsilon$ is negative, the state $|L, -, \uparrow\rangle$ has lower energy than $|L, +, \downarrow\rangle$ in the left dot. When $\epsilon$ is positive, on the other hand, $|R, -, \uparrow\rangle$ has higher energy than $|R, +, \downarrow\rangle$ in the right dot. Therefore, near $\epsilon = 0$, the two energy levels must cross, which becomes an anti-crossing due to $E_x$ and/or SOC. These anti-crossings are reflected in the numerical results in Fig. 6, which show that there is a small but notable anti-crossings in the energy diagram between $|-, \uparrow\rangle$ and $|+, \downarrow\rangle$.

Lastly, region "D" is the low-field regime, where $|\Delta_L| > E_z$ and $|\Delta_R| > E_z$. Here it is possible to form two anti-crossings in the energy diagram between $|-, \uparrow\rangle$ and $|+, \downarrow\rangle$ (See the energy diagram Appendix [B]). The interference between the two anti-crossings can either enhance or weaken spin flip, as is shown in Fig. 6 in the interfer-ence pattern. Given different $\delta\phi$, which becomes an anti-crossing due to $\delta\phi$. The two energy levels must cross, which becomes an anti-crossing due to $E_x$ and/or SOC. These anti-crossings are reflected in the numerical results in Fig. 6, which show that there is a small but notable anti-crossings in the energy diagram between $|-, \uparrow\rangle$ and $|+, \downarrow\rangle$ (See the energy diagram Appendix [B]). The interference between the two anti-crossings can either enhance or weaken spin flip, as is shown in Fig. 6 in the interference pattern. Given different $|\Delta_L|$ and $|\Delta_R|$, the two anti-crossings would form at different detunings, so that the dynamical phase accumulated between the two anti-crossings would be different, leading to varying period widths of the interference pattern in the figure. Spin flip error in this region can be large because the unwanted transitions can be amplified by interference.

In summary, in this subsection we have studied the conditions under which the anti-crossings would form. We identified four regions based on the relations among the valley splittings $|\Delta_L|$ and $|\Delta_R|$, and the Zeeman splitting $E_z$. In the high field region, when $|\Delta_L| < E_z$ and $|\Delta_R| < E_z$, no anti-crossing forms, so that spin flip probability is minimized. In the region of intermediate field, when $|\Delta_L| > E_z > |\Delta_R|$ or $|\Delta_R| > E_z > |\Delta_L|$, one anti-crossing appears, which may cause spin flip. In the low field region, when $|\Delta_L| > E_z$ and $|\Delta_R| > E_z$, two anti-crossings form, and spin flip could be significantly enhanced by interference between the two anti-crossings.

C. Spin-valley mixing and valley-induced spin decoherence

Besides spin flip without orbital loss (i.e. the electron is always transferred properly), loss of spin purity could also be an important issue in high-fidelity quantum information transfer. In a Si DQD, under certain conditions, the valley states could mix with the spin states in which the quantum information is stored [17]. Consequently, tracing over the valley degree of freedom could cause spin state to become mixed.

Let us consider spin evolution in our DQD protocol. Assume that after the transport, the orbital state is localized in the right dot at a large final detuning $\epsilon \gg E_z$. Without loss of generality, the final state can be written as $|\psi_{fin}\rangle = |R\rangle \otimes |\psi_S\rangle$, where

$$|\psi_S\rangle = a|+, \uparrow\rangle + b|+, \downarrow\rangle + c|-\rangle + d|\downarrow\rangle.$$  \hspace{1cm} (18)

After tracing over the valley degree of freedom, the spin density matrix becomes

$$\rho_{spin} = \text{Tr}_V (|\psi_S\rangle\langle \psi_S|) = \begin{bmatrix} |a|^2 + |c|^2 & ab^* + cd^* \\ ab^* + cd^* & |b|^2 + |d|^2 \end{bmatrix}.$$  \hspace{1cm} (19)

If $|\psi_S\rangle$ cannot be factorized into a tensor product of a spin state and a valley state, $\rho_{spin}$ would become a mixed state and whatever superposition is lost. For example, if $a = d = 0$ and $b = c = 1/\sqrt{2}$, $\rho_{spin}$ is a completely mixed state without any quantum superposition. The off-diagonal elements of $\rho_{spin}$ would be all zero and the state becomes a classical mixture of $|\uparrow\rangle$ and $|\downarrow\rangle$.

In order to evaluate the information lost, we use purity to measure the mixture of the final state, which is defined as $P = \text{Tr}_V (\rho_{spin}^2) \ (0 \leq P \leq 1)$. When $P = 1$, the state is still a pure state with the largest capacity to carry quantum information, while at $P = 0$, the state is completely mixed with no quantum information stored. For $\rho_{spin}$ in Eq. (19), we can compute $P$ as

$$P = 1 - |ab - c^* d^*|^2.$$  \hspace{1cm} (20)

Several other quantities can be also used to measure the spin fidelity loss, we list a couple of them and compare them in the Appendix [C].

In Fig. 7 (a), we plot spin purity as a function of the inter-dot valley phase difference $\delta\phi$. The initial state is a superposition of the two lowest-energy states at $\epsilon = -0.2 \text{ meV}$, namely $|\psi_{ini}\rangle \approx |L\rangle \otimes (-) \otimes \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle)$. The strong $\delta\phi$ dependence in Fig. 7(a) is a good example to demonstrate the importance of the phase difference $\delta\phi$ to the properties of a Si DQD.
We now focus on the two low-fidelity points, which represent two mechanisms that mix spin state with other degrees of freedom. At the first point, $\delta \phi / \pi = 0.132$, we plot the energy diagram in Fig. 7 (b). There is only one anti-crossing between states $| -, \uparrow \rangle$ and $|+, \downarrow \rangle$. Due to this anti-crossing, the state $|+, \downarrow \rangle$ splits into $|-, \uparrow \rangle$ and $|+, \downarrow \rangle$ with the probabilities $P_{D1}$ and $P_{A1}$, which can be roughly predicted by the LZ formula (9). Eventually, the final state approximately evolves into

$$\psi_{fin} \approx |R\rangle \otimes \left( \sqrt{\frac{P_{D1}}{2}} |-, \uparrow \rangle + \frac{1}{\sqrt{2}} |+, \downarrow \rangle \right).$$

(21)

According to Eq. (20), the final state $|\psi_{ini}\rangle$ corresponds to the case $a = 0$, therefore $P$ is reduced to $1 - \left|bc\right|^2$. Meanwhile, the spin population has changed because $|-, \uparrow \rangle$ has partially evolved into $|+, \downarrow \rangle$ at the spin-valley anti-crossing. This explains why there is a purity loss at $\delta \phi / \pi = 0.132$ in combination with a $P_{up}$ change. The final state (21) is just a rough estimate because the phase is not considered. But the numerical results in Fig. 7 is accurate, and show that spin purity is indeed lost.

At the second low fidelity point, $\delta \phi / \pi = 0.964$. The corresponding energy diagram is plotted in Fig. 7 (c). There are three anti-crossings, with one being a spin-valley anti-crossing at $\epsilon < 0$, and the other two valley anti-crossings at $\epsilon > 0$. Our numerical calculation shows that the spin-valley anti-crossing does not cause any significant transition, so that change to the spin population is minimal. This observation is also reflected in the dotted curve in Fig. 7 (a), where the probability of spin up is still close to the value of the initial state, $P_{up} \approx 0.5$, at $\delta \phi / \pi = 0.964$. On the other hand, the two valley anti-crossings in Fig. 7 (c) do lead to significant mixing between the spin state and the valley state of the electron. As a result, purity is partially lost for the spin state.

The low-fidelity point has a rather sharp dependence on the valley phase difference because the branching ratio of adiabatic versus non-adiabatic transition is sensitive to the energy gap. The gap must be compatible with the sweeping speed of detuning to ensure the state is split into two branches with similar weight at the anti-crossing. For example, when the inter-dot valley phase difference $\delta \phi$ is changed only slightly, from $\delta \phi / \pi = 0.964$ to $\delta \phi = \pi$, the gap disappears and the anti-crossing becomes a crossing, and $P = 1$ at $\delta \phi = \pi$ since the state will not be split at any crossing.

The low spin fidelity here is a good example that spin population is not a complete indicator for a perfect electron transport. Even when spin population is preserved in a process, spin coherence (superposition) could be lost due to the mixing between the spin state and the valley state. In this case, the classical information (population or probability) is faithfully transported, but a large part of the quantum information (coherence or superposition) is completely lost.

V. CONCLUSION

In this paper, we have studied the spectrum and dynamics of a single electron in a silicon double quantum dot. We first clarify the spectrum of the electron charge motion, and investigate the charge dynamics (valley and orbital) as the electron is driven between the two dots. We identify the phase difference of the valley-orbit coupling matrix elements in the two dots as a key parameter in determining the tunnel coupling between the two dots, and propose several schemes to detect this phase difference via transport through the DQD, or via charge sensing after pulsing the DQD through the anti-crossings near zero detuning. The Landau-Zener transitions or even Landau-Zener-Stückelburg interference during the detuning sweep lead to different charge distribution between the two dots as we change the pulse sequence, which allows us to calculate the valley phase difference. We derive expressions for the valley phase difference under different conditions and discuss feasibility of these schemes within the current experimental technologies.

Another key objective of the current study is to investigate spin dynamics during electron transport. In most cases, spin-orbit coupling caused spin flip remains minimal due to the small SOC in silicon. However, we identify a special type of anti-crossing near zero detuning, which contains a wide region (in detuning) where state mixing is significant, so that considerable spin flip can occur as a result. Recognizing the importance of the various types of anti-crossings to spin and charge transfer fidelity, we identify four different regions in the parameter space defined by valley splitting and Zeeman splitting, in which spin transfer fidelity has distinct dependences on the parameters and the resulting anti-crossings. Lastly, we investigate the relationship between spin transfer fidelity and the valley phase difference, and analyze loss of spin purity caused by spin-valley mixing. We show an example where the purity of the spin state is lost even though the spin population is faithfully transported.

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Appendix A: Tunneling coupling measurement in Silicon DQD

In a GaAs DQD there is a well established procedure for measuring tunneling rate in the conventional transport experiment [76], and it has also been extended to a Si DQD system as well [77]. There is no valley degeneracy in a GaAs DQD, and the low-energy dynamics of a single electron in the DQD can be described as a two-level system. Similarly, in a Si DQD with sufficiently large valley splitting, or if the valley phase are the same...
for the two dots, the electron dynamics is also well described by a two-level model. This can be easily seen in our model. Assuming \( \delta \phi = 0 \), anti-crossings “B” and “C” in Fig. 2 become crossings, and the charge properties near “A” can be modeled accurately using just \(|L, \)− and \(|R, \)− states. Therefore, the probabilities of finding the electron in the left/right dot (state \(|L, \)− and \(|R, \)−) are then

\[
P_{L}^{(1)} = \frac{1}{2} \left( 1 - \frac{\epsilon - \epsilon_A}{\Omega_A} \right), \quad P_{R}^{(1)} = \frac{1}{2} \left( 1 - \frac{\epsilon - \epsilon_A}{\Omega_A} \right),
\]

(A1)

where \( \epsilon_A = \frac{1}{2}(\Delta_L - |\Delta_R|) \) is the detuning at anti-crossing “A”, and \( \Omega_A = \sqrt{(\epsilon - \epsilon_A)^2 + |E_{L,-}|^2} \) is the energy splitting. The superscript “(1)” indicates that these are first-order results in a Si DQD, neglecting the two excited valley states in Fig. 2. Equations (A1) are identical to the formula in Ref. [76] for a GaAs DQD. When a detuning \( \epsilon \) is chosen and fixed, charge distribution in the DQD is determined, which can be experimentally detected by a nearby charge sensor such as a quantum point contact. \(|E_{L,-}\rangle\) can then be obtained through data fitting since it affects the charge distribution. In the analysis here we have assumed zero temperature for the electron. A finite temperature can be straightforwardly accounted for by adding a thermal broadening factor of \( \tanh \left( \frac{\hbar \omega}{2k_B T} \right) \) [76].

Generally \( \delta \phi \neq 0 \) in a Si DQD, and the valley splittings in the two dots may not be much larger than tunnel couplings, so that the charge distribution near the anti-crossing “A” cannot simply be modeled as a two-level system because the lowest-energy states would in general be superpositions of all four states \(|L, \)±, \(|R, \)±). The anti-crossings at “B” and “C” may also affect the charge distribution. The states become particularly mixed when \(|\Delta_L|\) and \(|\Delta_R|\) are small (in the same order as the tunnel couplings or smaller), so that the anti-crossings “B” and “C” are located near “A”. The corrections from all these couplings have to be taken into consideration in order to obtain an accurate assessment of the charge distribution. For example, in the region \( \epsilon_B < \epsilon < \epsilon_A \), if the probability of \(|R, \)−) is nonzero due to anti-crossing “A”, there has to also be a probability of finding \(|L, \)+) due to anti-crossing “B”. If we treat the energy diagram near “B” and “C” approximately as two-level systems, the second order corrections to the probability of \(|L, \)+) can be expressed as

\[
P_{L}^{(2)} = \frac{1}{2} P_{R}^{(1)} \left( 1 - \frac{\epsilon - \epsilon_B}{\Omega_B} \right), \quad P_{R}^{(2)} = \frac{1}{2} P_{R}^{(1)} \left( 1 + \frac{\epsilon - \epsilon_B}{\Omega_B} \right), \quad P_{R}^{(2)} = \frac{1}{2} P_{L}^{(1)} \left( 1 + \frac{\epsilon - \epsilon_C}{\Omega_C} \right).
\]

(A2)

Similarly, we have

\[
P_{L}^{(2)} = \frac{1}{2} P_{R}^{(1)} \left( 1 + \frac{\epsilon - \epsilon_B}{\Omega_B} \right), \quad P_{R}^{(2)} = \frac{1}{2} P_{L}^{(1)} \left( 1 + \frac{\epsilon - \epsilon_C}{\Omega_C} \right).
\]

(A3)

Taking these second order corrections into consideration, the final charge distribution can be obtained as, for example,

\[
P_{L}^{(2)} = P_{L}^{(1)} + P_{L}^{(2)} + P_{R}^{(2)}.
\]

When \( \delta \phi \approx 0 \) or \(|\Delta_L, \Delta_R| \gg E_z \), the first order approximation in Eq. (A1) should be sufficiently accurate. Furthermore, our numerical results in Fig. 8 indicate that even when \( \delta \phi \approx \pi \), the first order estimate in Eq. (A1) is still a decent approximation, while adding the corrections from “B” and “C” in the form of the second order results \( P_{L}^{(2)} \) leads to almost perfect match between numerical and perturbative results. Thus there is no need to consider higher order corrections from anti-crossing “D”.

The charge sensing method discussed here can be used to determine the tunnel coupling that leads to the Anti-crossing “A”, in other words \( E_{L,-} \). Unfortunately, such a static charge sensing scheme cannot be used to determine the tunneling rate at anti-crossings “B” and “C”, i.e. \( E_{L,+} \). As shown in the energy diagram of Fig. 2 tuning \( \epsilon \) near “B” simply does not affect the equilibrium charge distribution much, because the ground state at “B”-detuning is still \(|L, \)−). Instead, a dynamic/pulsed method is needed to access the excited states and their properties.

Appendix B: Energy diagrams for different valley splitting configuration

Here we plot the energy diagrams for the four cases identified in Fig. 3 with the four panels corresponding to the four regions marked in Fig. 6. The energy diagrams give clear indications on how many anti-crossings occur for a certain configuration of parameters \(|\Delta_L|, |\Delta_R|, \) and \( E_z \) (the valley splitting in the left and right dot, and the Zeeman splitting).
Figure 9. (color online) Energy diagrams for different valley splittings: (a) $|\Delta L| = |\Delta R| = 30 \, \mu eV$, (b) $|\Delta L| = 30 \, \mu eV$, $|\Delta R| = 60 \, \mu eV$, (c) $|\Delta L| = 60 \, \mu eV$, $|\Delta R| = 30 \, \mu eV$, (d) $|\Delta L| = |\Delta R| = 60 \, \mu eV$. All the other parameters are the same as in Fig. 6.

Appendix C: Measures of coherence loss

Figure 10. (color online) Several quantities to measure spin fidelity loss.

Besides the purity that we used in the main text, there are several other quantities that can measure coherence loss for a qubit. The off-diagonal element of the reduced density matrix $\rho_{\text{spin}}$ itself is a good measure for the superposition of the spin state. The entanglement between the spin state and the valleys is another indicator. By entanglement we mean the coupling of different degrees of freedom for the same electron. If the electron state cannot be written as a product of its spin and valley states, we call them entangled. If this entanglement is present, spin coherence must be partially lost when we trace out the valley degree of freedom (for example, if our charge sensing mechanism is not sensitive to the valley composition, but only to whether the electron is in the left or right dot).

In Fig. 10 we plot four quantities that characterize spin fidelity after transport. These include $2|\rho_{\text{spin}}(1,2)|$, $1 - C(|\psi_{VS}\rangle\langle\psi_{VS}|)$ (entanglement between spin and valley states), $P$ (purity), and $2P_{\text{up}}$ (probability of spin up). Here, spin-valley entanglement is measured by the “concurrence” described by “C”. With necessary normalization, all four quantities are in the range of 0 to 1, and their initial values before the transport are all set at 1, signifying a completely coherent initial state. After the transport, they all drop below 1, depending on $\delta \phi$. Interestingly and as expected, the results in Fig. 10 clearly show that all four quantities reflect coherence loss caused by anti-crossings due to spin-valley mixing. However, for anti-crossings due to valley mixing, the spin population $P_{\text{up}}$ fails to account for the coherence loss while the other three quantities still work fine.

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