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Impact of valley phase and splitting on readout of silicon spin qubits

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We investigate the effect of the valley degree of freedom on Pauli-spin blockade readout of spin qubits in silicon. The valley splitting energy sets the singlet-triplet splitting and thereby constrains the detuning range. The valley phase difference controls the relative strength of the intra- and intervaley tunnel couplings, which, in the proposed Pauli-spin blockade readout scheme, couple singlets and polarized triplets, respectively. We find that high conversion fidelity is possible for a wide range of phase differences, while taking into account experimentally observed valley splittings and tunnel couplings. We also show that the control of the valley splitting together with the optimization of the readout detuning can compensate the effect of the valley phase difference. To increase the measurement fidelity and extend the relaxation time we propose a latching protocol that requires a triple quantum dot and exploits weak long-range tunnel coupling. These opportunities are promising for scaling spin qubit systems and improving qubit readout fidelity.

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I. INTRODUCTION

The experimental demonstration of high-fidelity quantum dot qubits with long coherence [1,2] that can be coupled to perform two-qubit logic gates [3,4] and used to execute small quantum algorithms [5] has positioned silicon as a promising platform for large-scale quantum computation. Building upon these advances, exciting new directions forward have been proposed [6–13] that exploit uniformity [14], robustness against thermal noise [15], or semiconductor manufacturing [16], and aim for operation of quantum error correction codes [17] on qubit arrays.

Despite its promises, silicon poses specific challenges due to the sixfold degeneracy of its conduction band minimum in bulk. This degeneracy is lifted close to an interface, and a gap opens between perpendicular and in-plane valley doublets. Interfaces and gate electric fields cause coupling either in the same or different orbital levels. The same-doublet same-orbital coupling is the so-called valley mixing, while the others are same or different orbital levels. The same-doublet same-orbital interfaces and gate electric fields cause coupling either in the gap opens between perpendicular and in-plane valley doublets. This degeneracy is lifted close to an interface, and a gap opens between perpendicular and in-plane valley doublets.

In Sec.II, we investigate how the valley phase difference and splitting impact Pauli-spin blockade readout of silicon spin qubits. Here, we investigate its effect on readout, now one of the most challenging operations for spin qubits. We concentrate on Pauli-spin blockade readout and show that high spin-to-charge conversion fidelity is achievable in a wide parameter range. This readout technique is considered in large-scale quantum computation proposals [14–16] since it requires few electron reservoirs and is compatible with moderate magnetic fields [33,34]. However, in standard Pauli-spin blockade schemes the readout time is limited due to spin relaxation [35–37]. Moreover, usually two spin states are projected on charge states with different electric dipoles, leading to a readout fidelity smaller than the conversion fidelity [38,39]. A possible solution is to exploit latching mechanisms in the pulsing scheme, locking the charge in a long-lived metastable state [40–42]. The final states now have a different number of electrons, improving the readout fidelity [39]. Here we overcome these limitations and propose a protocol based on a triple quantum dot, removing the need of an external reservoir.

We investigate the effect of the valley degree of freedom on Pauli-spin blockade readout of spin qubits in silicon. The valley splitting energy sets the singlet-triplet splitting and thereby constrains the detuning range. The valley phase difference controls the relative strength of the intra- and intervaley tunnel couplings, which, in the proposed Pauli-spin blockade readout scheme, couple singlets and polarized triplets, respectively. We find that high conversion fidelity is possible for a wide range of phase differences, while taking into account experimentally observed valley splittings and tunnel couplings. We also show that the control of the valley splitting together with the optimization of the readout detuning can compensate the effect of the valley phase difference. To increase the measurement fidelity and extend the relaxation time we propose a latching protocol that requires a triple quantum dot and exploits weak long-range tunnel coupling. These opportunities are promising for scaling spin qubit systems and improving qubit readout fidelity.

II. MODEL AND PROCEDURE

a. Model

The model describing a multivalley two-electron double quantum dot and discuss Pauli-spin blockade readout. In Sec. III, we investigate how the valley phase difference and
FIG. 1. (a) Spin-valley single-particle energy levels of a silicon double quantum dot. The valley ground states are shown in red, while the excited valley states, separated by the dot-dependent valley splitting $E_{v}^{L,R}$, are in blue. A dot- and valley-dependent Zeeman energy (e.g., $E_{Z}^{L,R}$) splits the spin states. The constant-color arrows represent the intravalley tunnel coupling $t_{±}$, while intervalley coupling $t_{±}$, arrows have a color gradient. (b) Top: Cross section of a schematic device. The confinement gate (C) defines the dots, plunger gates (G) accumulate the electrons and control the out-of-plane electric field, while the barrier gates (B) tune the tunnel coupling $t$. Bottom: Schematic stability diagram of a double quantum dot. Green and orange lines mark the dot-lead transitions. Intersdot intervalley tunneling occurs along the dashed line, separated from the ground state line by the right dot valley splitting $E_{v}^{R}$.

splitting energy impact the spin-to-charge conversion fidelity. We identify the conditions that enable conversion fidelities beyond 99.9%. A triple quantum dot scheme combining Pauli-spin blockade with long-lived charge states is proposed and studied in Sec. IV. We discuss the conclusions and opportunities in Sec. V.

II. MODEL

A. Silicon double quantum dot Hamiltonian

The model developed in this section can be generalized to other doubly occupied multivalley double quantum dots, but here we restrict the discussion to quantum dots at the Si/SiO$_2$ interface. We define the left and right quantum dots as target and ancilla qubits, respectively. We consider ten single-particle spin-valley states: the four lowest orbital spin-valley states of the valley spectrum of the dot, $|0\rangle$, $|1\rangle$, $|2\rangle$, $|3\rangle$, and the four lowest orbital spin-valley states of the four lowest orbital spin-valley states of the valley spectrum of the dot, $|4\rangle$, $|5\rangle$, $|6\rangle$, $|7\rangle$, and the four lowest orbital spin-valley states of the valley spectrum of the dot, $|8\rangle$, $|9\rangle$, $|10\rangle$, and the four lowest orbital spin-valley states of the valley spectrum of the dot, $|11\rangle$, $|12\rangle$, $|13\rangle$, $|14\rangle$. The valley ground states are shown in red, while the excited valley states, separated by the dot-dependent valley splitting $E_{v}^{L,R}$, are in blue. A dot- and valley-dependent Zeeman energy (e.g., $E_{Z}^{L,R}$) splits the spin states. The constant-color arrows represent the intravalley tunnel coupling $t_{±}$, while intervalley coupling $t_{±}$, arrows have a color gradient. (b) Top: Cross section of a schematic device. The confinement gate (C) defines the dots, plunger gates (G) accumulate the electrons and control the out-of-plane electric field, while the barrier gates (B) tune the tunnel coupling $t$. Bottom: Schematic stability diagram of a double quantum dot. Green and orange lines mark the dot-lead transitions. Intersdot intervalley tunneling occurs along the dashed line, separated from the ground state line by the right dot valley splitting $E_{v}^{R}$.

H^R_{o}$ the orbital levels of the right dot ($\delta_{d,R}$ is the Kronecker delta). In particular,

$$H^d_{o} = E^d_{o} \sum_{x=-,+,+} \delta_{x,+} + \sum_{x=0,1,1,\uparrow} \hat{c}^\dagger_{d,x,\sigma} \hat{c}_{d,x,\sigma},$$

$$H^Z_{o} = \frac{1}{2} \sum_{x=0,1} E^d_{Z}(\hat{c}^\dagger_{d,x,\uparrow} \hat{c}_{d,x,\downarrow} - \hat{c}^\dagger_{d,x,\downarrow} \hat{c}_{d,x,\uparrow}),$$

$$H^R_{o} = E^R_{o} \sum_{x=0,1} \delta_{x,0} + \sum_{x=0,1,\uparrow,\downarrow} \hat{c}^\dagger_{x,\sigma} \hat{c}_{x,\sigma},$$

where $o, v,$ and $\sigma$ are the orbital, valley, and spin labels, respectively. The Zeeman splitting is defined as $E^d_{Z} = g_{d,v} \mu_{BB} B_{d,v}$. In general the $g$ factor is valley and dot dependent due to spin-orbit coupling [43,44]. Here we assume a vanishingly small spin-orbit coupling [45-47] arising from a magnetic field applied along one of the minimizing directions. This assumption is further warranted by the possibility of low magnetic field operation when using Pauli-spin blockade readout (low-field operation has several other advantages; see Refs. [14,15]). In this range, finite $\delta E_{Z} = E^d_{Z} - E^R_{Z}$ can be realized via nanomagnets, and we restrict ourselves to the case $E^R_{Z} > E^L_{Z}$. $H_o$ describes the splitting between the valley eigenstates due to the mixing of the $k_{±}$ bulk valleys induced by the Si/SiO$_2$ interface and the electric field [23,48,49] (see Appendix A). We consider dot-dependent valley splittings [50] due to interface effects and local variations in electric field [19]. The valley coupling is $\Delta_{o} \equiv E_{o} e^{i\phi_{o}}$, whose modulus is the valley splitting energy and whose phase is the valley phase (i.e., the phase of the fast Bloch oscillations of the wave function) [50,51]. The valley eigenstates are of the form $|D_{k} \rangle = (1/\sqrt{2})(D_{±} \pm e^{i\phi_{o}} D_{±})$, where $D_{±} = L_{±}, R_{±}$ are the bulk $±z$ valleys wave functions of the quantum dots [23,49].

The two-electron double-dot Hamiltonian reads

$$H_{2e} = H_{0} + H_{e} + H_{C} + H_{t}.$$  

Here $H_{0}$ describes two noninteracting quantum dots. $H_{e}$ is the detuning term, describing the gate-controlled shift $\epsilon$ of the ancilla qubit energy levels with respect to those of the target qubit. Referring to Fig. 1(b), this corresponds to increasing the voltage on G3. The third term $H_{C}$ accounts for the effect of the Coulomb potential $V_{ee}$. For the system considered here and within the Hund-Mulliken approximation, the Coulomb exchange integral $J = (L_{o} R_{o}) | V_{ee} | R_{±} L_{±}$ and the valley exchange integral $j_{o} = (D_{±} D_{±}| V_{ee} | D_{±} D_{±})$ are negligible [22,52,53]. Theoretical works have estimated $J \approx 1 \mu eV$ for 30 nm separated dots [54] and $j_{o} \ll 1 \mu eV$ [22]. The on-site re-pulsion in the ancilla (right) dot $U_{o} = (R_{o} R_{o}) V_{ee} | R_{o} R_{o} \rangle$, or charging energy, is assumed to be a few tens of meV [26,27]. In the Pauli-spin blockade readout scheme only the ancilla qubit can be doubly occupied; thus the (2,0) states are neglected and hence terms of the form $|LL \rangle V_{ee} | LL \rangle$ do not appear in $H_{C}$. The remaining two Coulomb integrals do not appear explicitly in $H_{t}$ since the direct Coulomb interaction $k = (L_{o} R_{o}) | V_{ee} | L_{±} R_{±}$ is an offset, while the Coulomb interaction enhancement terms $s = (R_{±} R_{±}) V_{ee} | L_{±} R_{±} \rangle$ are part of the tunnel coupling $t$. It holds that $t = t_{0} + s$, where $t_{0} = \langle R_{o} | H_{0} | L_{±} \rangle$. The last term in $H_{2e}$ is the tunnel Hamiltonian [26,27].
expressing the hopping of one electron between the two dots. The different terms of the Hamiltonian are

\[ H_0 = \sum_{d=L,R} H_0^d, \]

\[ H_e = -\epsilon \sum_{\sigma = 0,1} \sum_{v,v',\sigma} c_{R,\sigma}^\dagger c_{R,\sigma} |_{v,\sigma} c_{R,\sigma} |_{v',\sigma} \]

\[ H_C = \sum_{r=0,1} \sum_{\sigma,\sigma'} n_{R,\sigma} n_{R,\sigma'}, \]

\[ H_t = \sum_{v,v',\sigma,\sigma'} t_{v,v'} c_{v,\sigma}^\dagger c_{v',\sigma'} \prod_{r=R,L,O} (-1)^{\delta_{r,0}} \delta_{r,0} + H_c, \]

where \( n \) is the number operator, \( \sigma_R, v_R, \) and \( o_R \) are the spin, valley, and orbital indexes of the right electron, and \( S, V, O \) are the spin, valley, and orbital numbers of the two-electron state. The label \( ES \) stands for the excited state of the quantum number expressed by \( r \). The condition \( S(V,O) = 0 \) means that the spin (valley or orbital) part of the 2-electron wave function is a spin singlet (valley or orbital) built from the single-particle states. \( I_{L,0} \) and \( I_{L,0} \) are the intravalley and intervalley tunnel couplings, respectively [22,55,56]. The first(second) coupling allows for tunneling between valley eigenstates of the same(valley) form. We note that both terms prevent tunneling between states that have a different bulk valley index [49]. It allows for tunneling between valley eigenstates of the same valley number, while in the middle branch they are opposite (±π). The (1,1) same-valley branches consist of four states each, while in the (0,2) configuration these same states include only the spin singlet state, because of the Pauli exclusion principle. The different-valley branch includes eight levels when in the (1,1) and four states in the (0,2) charge states. The difference in Zeeman energy sets the energy splitting between the antiparallel spin states in the three branches. A small difference in valley splitting energy splits the (+−) and (−−) states, as shown in Fig. 2(a). The control of \( \Delta \phi \) allows to select the nature of interdot tunneling, ranging from intra- to intervalley-only tunneling, as shown in Fig. 2(b). In particular, for \( \Delta \phi = 0 \) the \( |↓, ↓⟩ \) states are uncoupled from the (0,2) charge states in the lowest orbital and the blocked region extends to the orbital spacing energy.

C. Two-dot Pauli-spin blockade readout

At negative detuning (i.e., \( \epsilon < U_R^R \)), the two lowest eigenstates can be approximated with the basis states \( |↓, ↓⟩, |↑, ↓⟩ \) and \( |↑, ↑⟩ \). Differing only in the spin orientation of the target qubit, these states are hereafter used as initial states of the Pauli-spin blockade readout protocol and their valley label is dropped.

As shown in Fig. 2(c), Pauli-spin blockade readout consists of a spin-to-charge conversion. At the beginning of the readout protocol, the ancilla qubit is in the ground state while the target qubit can be either spin up or spin down. The readout pulse detunes the double quantum dot beyond the intravalley anticrossing and inside the blocked region \( U^R < \epsilon < U^R + E_R^R - E_R^L \), the brown region in Fig. 2(c). As shown in Fig. 2(d), if the two spins are initially antiparallel [blue level in Fig. 2(c)] the final state will be the singlet \( S_{0,0}^\dagger \) (green level); otherwise, the system will remain blocked in \( |↓, ↓⟩ \) (red level) until it relaxes via a spin flip. Experimentally, the final state can be probed either by charge sensing [33,34] or by gate-based dispersive rf readout [58]. However, these techniques require slightly different pulses. The former detects differences in the electric field due to a difference in the charge configuration, while the latter probes the level mixing via the quantum capacitance [59]. The highest fidelities are obtained far from or close to the intravalley anticrossing [60], respectively.

Here we consider 1 μs long linear adiabatic pulses conceived for charge sensing. (See Appendix B for details on pulse adiabaticity.) We note that shaped pulses could improve speed and performance (see Ref. [14] and therein references), although in arrays operated by shared control linear pulses could be required [14]. The duration is chosen as a trade-off between fast pulses and adiabaticity. The conversion fidelity \( F \) is defined as the probability that \( |↑, ↓⟩ \) evolves to a (0,2) state while \( |↓, ↓⟩ \) remains in a (1,1) state. Since at the beginning of the readout protocol the system is in either of the two lowest-lying eigenstates with the same probability, the conversion
fidelity is the weighted sum of $F^{(1,1)}_{\uparrow\downarrow}$ and $F^{(1,1)}_{\downarrow\uparrow}$:

$$F = \frac{F^{(1,1)}_{\uparrow\downarrow} + F^{(1,1)}_{\downarrow\uparrow}}{2}$$

$$= \frac{1}{2} \left[ \sum_{a \in (0,2)} |\langle a | f \rangle|^2 + \sum_{b \in (1,1)} |\langle b | f' \rangle|^2 \right], \quad (9)$$

where $f$ and $f'$ are the two final states calculated from the time evolution of the two lowest-lying eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively.

From Eq. (9) it can be seen that the ultimate limit to the readout fidelity is set by the final state composition, which depends on the valley phase difference. Even a perfectly adiabatic pulse results in $F < 1$ if the final state $f'$ has a non-negligible contribution from $T^+_{\uparrow,\downarrow}(0,2)$, [see Fig. 2(a)].

We recall that we have assumed negligible spin-orbit coupling. Contrarily to bulk silicon, in quantum dots defined at the Si/SiO$_2$ interface it can be non-negligible. The structural inversion asymmetry leads to a Rashba spin-orbit coupling, while the dominant Dresselhaus [47] arises from the interface inversion asymmetry [61–63]. The spin-orbit coupling strength depends, apart from the magnetic field orientation, on the vertical electric field, valley composition, and microscopic properties of the interface [44]. In actual devices it causes g-factor variability [45], valley dependency [43,46], and mixing between antiparallel and parallel spin states [64]. As a consequence, when including the spin-orbit Hamiltonian in $H_z$, anticrossings between $S_{\uparrow,\downarrow}(0,2)$ and the polarized triplets emerge [38,44]. Further, such mixing would reduce $F$ even for adiabatic pulses. The shape of the pulse used for Pauli-spin blockade readout has to be modified accordingly, i.e., a two-speed linear pulse, to allow for a diabatic crossing of the $S$-$T^-$ anticrossing [65]. Therefore our assumption of negligible spin-orbit coupling ensures that our results demonstrating the impact of the valley phase are not obscured by spin-orbit effects.

III. RESULTS

From previous considerations, it emerges that the larger $E^R_v$ the greater $F$. In general, $E^R_v$ can be tuned via a vertical electric field [1,19,48]. In the device shown in Fig. 1(b), valley splitting can be controlled via the combined tuning of G3 and confinement gate C.

In Fig. 3 we show how the phase difference impacts on $F$ for different valley splittings (here $E^R_v = E^L_v$). Whenever $E^R_v > E^R_z/2$, $F > 80\%$ can be reached; in general we find a fidelity higher than $90\%$ for $E_v \gtrsim 40eV$. For a fixed valley splitting, the phase dependence of $F$ is nonmonotonic, as visible for small splittings ($E_v < 30\mu eV$). At low $\Delta\phi$ the fidelity is high because the intervalley anticrossing is very narrow and the two final states have different charge configurations over a large detuning range. The minimum at $\Delta\phi \approx \pi/2$ arises from the opposite phase dependence of $t_{\uparrow,\downarrow}$ and $t_{\downarrow,\uparrow}$. Here a higher $E^R_v$ is needed to realize a large energy separation between the two anticrossings in order to reach the same fidelity (see 90% contour line in Fig. 3). For $\Delta\phi > \pi/2$ the fidelity increases with increasing phase, since the increasing intervalley coupling is compensated by the smaller detuning needed for the $|\uparrow\rangle, |\downarrow\rangle$ to evolve to $S_{\uparrow,\downarrow}(0,2)$ (see Fig. 4). The decrease in $F$ at high $\Delta\phi$ is due to the increase in the pulse diabaticity. The conversion fidelity in the adiabatic case shows that a fidelity higher than 90% can be reached even for $\Delta\phi \approx \pi$, as highlighted by the dotted red lines in Fig. 3, although it requires an impractical slow pulsing rate.
for $\Delta \Phi$ approaching $\pi$ (i.e., $t_{\pm} \to 0$) is caused by an increase in diabaticity, due to the constant pulse duration, absent in adiabatic evolution (red). For each point of the map, we have plotted the maximum achievable fidelity by taking the optimal detuning.

Properly tuning the readout position given a random phase difference is beneficial and enables reaching the 99% fidelity threshold in a very large range of valley splittings and phase differences. The optimal readout point shifts with threshold in a very large range of valley splittings and phase difference is beneficial and enables reaching the 99% fidelity ing the state composition. As shown by the dots in Fig. 4, for $99\%$ and $\Delta \Phi$ is strongly (e.g., $\epsilon \sim 0$ and $\Delta \Phi \sim 0$ or $\epsilon \sim \epsilon^{R}$ and $\Delta \Phi \sim \pi$), but there are two separate regions where $F > 99\%$, because $E^{R}/t \sim 50$.

However, when aiming at $F > 99\%$ or higher, the control of the ancilla qubit valley splitting enables overcoming the low-fidelity region at intermediate $\Delta \Phi$. The two $99.9\%$ regions merge for $E^{R}/t \sim 54$; e.g., when $t = 1.5$ GHz a valley splitting of at least $0.36$ meV is required. Figure 5 shows that for experimentally obtained valley splitting high fidelity can be achieved for a quite large range of tunnel coupling $t$. For a valley splitting of $0.1$ meV and considering perfect adiabatic pulses, a fidelity beyond $99.9\%$ can be reached for $t \leq 500$ MHz and $0 \leq \Delta \Phi \leq 0.7\pi$. When the valley splitting is slightly larger, i.e., $300$ $\mu$eV, the same fidelity can be achieved for $t < 1.5$ GHz. When the valley splitting is $700$ $\mu$eV, a fidelity of $99\%$ can be reached when $t < 5$ GHz and a fidelity of $99.9\%$ requires $t < 3$ GHz. Moreover, Fig. 5 shows that $t$ could be used as an additional knob to improve the fidelity, in the case of limited control of the valley splitting.

**IV. TRIPLE-DOT READOUT PROTOCOL**

Experimental works on Pauli-spin blockade in silicon quantum dots show readout fidelity significantly lower than the conversion fidelities reported here [38,39,42]. This reduction is

![FIG. 3. Fidelity obtained by pulsing from $\epsilon = U^{R} - 1$ meV to $U^{R} + E^{R}_{v}$ in $1$ $\mu$s with $\Delta t = 1$ $ps$, $t = 1.5$ GHz, and $\delta E^{R}_{v} = 5$ MHz, for a range of experimentally achieved valley splitting energies (here $E^{R}_{v} = E^{R}_{v}$). Contour lines are shown in white. The decrease in $F$ for $\Delta \Phi$ approaching $\pi$ (i.e., $t_{\pm} \to 0$) is caused by an increase in diabaticity, due to the constant pulse duration, absent in adiabatic evolution (red). For each point of the map, we have plotted the maximum achievable fidelity by taking the optimal detuning.](image)

![FIG. 4. Fidelity obtained by time evolution simulations (color map with white contour lines) and perfectly adiabatic pulses (red). The difference between the detuning position of maximum fidelity obtained from time evolution simulations (dots) and adiabatic pulses (dashed line) is due to the finite speed of the pulse. As a consequence of the chosen parameters (e.g., $\delta E^{I}_{v} = 5$ MHz, $E^{R}_{v} = 300$ $\mu$eV, $t = 1.5$ GHz, and pulsing from $U^{R} - 2E^{R}_{v}$ to $U^{R} + 2E^{R}_{v}$ a gap where $F < 99.9\%$ opens for intermediate $\Delta \Phi$. The maximum fidelity has a nonmonotonic dependence on $\Delta \Phi$, visualized here by the color map of the dots; a minimum is observed at $\pi/2$ (light green), a local maximum at $\pi$ (blue), and the maximum at $0$ (dark blue).](image)

![FIG. 5. Fidelity obtained by time evolution simulations (color map with white contour lines) and adiabatic pulses (red). A realistic value of $0.3$ meV enables reaching $F > 99\%$ for $t$ up to $4.5$ GHz in a wide range of phase differences (here up to $\Delta \Phi = 0.8\pi$). The reduction in fidelity at low $t$ is caused by higher diabaticity of the pulse. In the top right panel it prevents reaching $F > 99.9\%$. As in Fig. 4 $\delta E^{I}_{v} = 5$ MHz and the pulse extremes are $U^{R} \pm 2E^{R}_{v}$](image)
The actual readout process, which can be beneficial when the sensor signal induced by a different number of electrons consequently to a long charge relaxation time. The variation in the sensor signal induced by a different number of electrons predominantly due to the small sensitivity of the charge sensor to variations in the electric dipole caused by a difference in the charge position. Therefore protocols involving metastable states [38–40,42] have been proposed. Typically, after projecting the initial states onto a singlet (0,2) or a triplet (1,1), the system is pulsed deep in the (0,2) region, past an excited charge state. While the singlet (0,2) is still the ground state, the triplet (1,1) relaxes (i.e., an electron tunnels from or to an electron reservoir) to the excited charge state. Coulomb blockade leads consequently to a long charge relaxation time. The variation in the sensor signal induced by a different number of electrons trapped in the double quantum dot is typically larger by a factor 1.4–4 and fidelities approaching 99.9% have been reported [38,39]. Furthermore, such latching mechanisms allow for delayed readout, splitting the spin-to-charge conversion from the actual readout process, which can be beneficial when scaling to large qubit arrays [14,16].

FIG. 6. (a) Schematic of a triple-dot device with negligibly weak long-range coupling. (b) Left panel: Hysteresis stabiity diagram of a tripled quantum dot with the readout pulse scheme. The first step [from (I) to (II)] is a standard double-quantum-dot Pauli-spin blockade readout pulse. In the second step [from (II) to (III)], charge moves from the target to the left ancilla qubit only if the target qubit is initially spin blocked (III′). Transitions between nearest-neighboring dots are denoted by two-color interdot transition lines. The edges of the hysteresis regions are marked by three-color lines. The line color reflects the involved dots. Right panels: Energy level diagrams showing the triple-dot occupation at (I), (II), (III), and (III′) positions depending on the initial spin state. (c) Left panel: The readout is performed by oscillating the middle and left dot energy levels forcing the system to oscillates between the (1,0,1) and (0,1,1) charge states. Right panel: The charge state mixing leads to a capacitive term in the sensor signal induced by a different number of electrons, which can be beneficial when scaling to large qubit arrays [14,16].

Here we replace the reservoir used in recent experimental works [38–40,42] with a third dot (L′) added to the left side of the double dot considered in the previous sections, providing clear benefits in scalability. In the following we consider that the triple dot is loaded with two electrons at the beginning of the protocol and then the coupling to the electron reservoir is switched off. The triple dot is controlled by two “virtual” gates GL and GR, which are linear combinations of the B and G gates shown in Fig. 6(a). In particular, defining \( \mu_d \) the chemical potential of the dot \( d \), we assume that \( \mu_L \) is kept to a reference level and that \( G_L \) shifts only \( \mu_L \). On the other hand, \( G_R \) is mainly coupled to \( \mu_R \), but controls also \( \mu_L \). The interdot transition lines with a positive (negative) slope in Fig. 6(b) correspond to \( \mu_{L(R)} = \mu_R \). We assume negligible long-range tunnel coupling \( t^{RL}_k \) between the two outer ancilla qubits [see Fig. 6(a), right panel]. This condition results in a stability diagram similar to the case of hysteretic double quantum dots [66]. The transition lines arising from direct tunneling between the ancilla qubits R and L′ [e.g., the one between (1,0,1) and (0,0,2)] are hysteretic and depend on the sweeping direction of the gate \( G_R \). When \( t^{RL} \neq 0 \) the condition \( \mu_L = \mu_R \) leads to electron transfer. The corresponding transition lines appear vertical in a stability diagram and are independent from \( G_L \). However, when \( t^{RL} = 0 \), tunneling can only occur when \( \mu_{L(R)} > \mu_L \geq \mu_{R(L)} \) [39,66]. For increasing voltage \( G_R \) an electron can be transferred to R from \( L' \) when \( \mu_{L(R)} = \mu_R \). Consequently, the lines have a negative slope. For decreasing \( G_R \), transfer occurs when \( \mu_R = \mu_L \geq \mu_{L(R)} \) and the slopes have positive slope, as in Fig. 6(b).

The pulse protocol starts in a (0,1,1) charge configuration, position (I) in Fig. 6(b). Here \( \mu_{L(1)} > \mu_{L(2)} \). The system is detuned inside the (0,0,2) spin-blocked window to position (II) where \( \mu_{L(1)} > \mu_{R(2)} \). Transitions between the two states \( \mu_{L(1)} > \mu_{R(2)} \) are optimized accordingly to the previous sections to allow for high conversion fidelity. The initial state (0,1,1) is then converted to a (0,0,2) charge state, while (0,1,1) remains blocked in a (0,1,1) configuration. \( G_L \) and \( G_R \) are then lowered together, raising the chemical potentials \( \mu_R \) and \( \mu_L \).

The detuning direction is parallel to the (0,1,1) ↔ (0,0,2) charge transition line so that \( \mu_R(2) > \mu_{L(2)} \) and their relative offset is kept constant. The pulse ends in the hysteretic (0,0,2) region at position (III) where \( \mu_{L(1)} > \mu_{R(2)} \), past the extension of the (0,1,1) transition line. The short-range coupling enables spin-to-charge conversion and charge shelving. If the separated spins were antiparallel, the \( S_{0,0,2} \) would remain in the same charge configuration. This holds even for \( \mu_{L(1)} < \mu_{R(2)} \), since no electrons can tunnel when \( t^{RL} = 0 \). Parallel spins, however, remain in the (0,1,1) charge configuration. In that case, when \( \mu_{L(1)} = \mu_{L(1)} \) an electron is transferred between \( L \) and \( L' \). As a consequence, (0,1,1) evolves to (1,0,1) and (0,0,2), respectively. The negligible long-range tunnel coupling extends the spin flip relaxation time to a charge relaxation time, determined by cotunneling.

The next step of the protocol is the actual readout [Fig. 6(c)]. First the tunnel coupling \( t^{LR} \) is completely switched off. The two possible final states of the \( L'L' \) double dot are (0,0) and (1,0), if at the beginning of the pulse the two spins were, respectively, antiparallel or parallel. Now rf gate-based dispersive readout can be used. The presence or absence of an electron in the \( L'L' \) double dot can be translated with high fidelity to the spin state of the target qubit. We note that in the case of limited control of \( t^{LR} \) this scheme can still be implemented, since the rf tone is applied such that the system oscillates between (1,0,1) and (0,1,1). Importantly, the possibility to doubly occupy the left ancilla qubit softens the experimentally demanding requirements of the triple donor scheme of Ref. [67].
V. CONCLUSIONS

In summary, we have investigated the impact of an uncontrolled valley phase difference on the conversion fidelity of Pauli-spin blockade readout. The damping effect of the phase can be mitigated by the control of the valley splitting of the ancilla qubit. In particular, we have shown that the control of the valley splitting energy together with the optimization of the readout position is sufficient to overcome randomness of the valley phase difference, even when the control of the tunnel coupling is limited and \( t \) assumes realistic values. For \( E_v > 0.3 \text{ meV} \) a fidelity higher than 99.9\% can be reached for \( t < 2 \text{ GHz} \), as long as evolution is adiabatic with respect to the intravalley anticrossing. In addition, we have proposed a protocol based on an isolated triple quantum dot to extend the Pauli-spin blockade readout measurement time by orders of magnitude, significantly improving readout fidelity.

Our results show that the randomness of the valley phase difference can potentially lower the readout fidelity. However, the experimentally demonstrated control of valley splitting and fine tuning of the detuning can overcome such variability. The extended relaxation time obtainable in a triple-dot protocol makes Pauli spin blockade thereby an excellent method to be integrated in large-scale spin qubit systems.

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APPENDIX A: VALLEY MIXING HAMILTONIAN

Although the valley degree of freedom can be regarded as a pseudospin, there are some differences between the case of silicon bulk valleys and a single spin in a magnetic field. The general Hamiltonian of a spin-1/2 in a magnetic field has three parameters, i.e., the three components of the magnetic fields, and the mixing perturbation is fully described by two angles and the magnitude. The particular case of the silicon \( z \) bulk valleys can be derived from the general case by setting the \( z \) component of the (effective) magnetic field (diagonal terms of the Hamiltonian) to zero. As demonstrated by early works on valley physics in silicon [21–23], the sixfold degeneracy of the conduction band is first split by confinement, which lifts the \( x \) and \( y \) valleys leaving the degeneracy between the \( z \) and \(-z\) bulk (or bare) valleys. The remaining degeneracy is lifted by the electric field in the \( z \) direction and the interface (and a small contribution from the magnetic field). This perturbation (\( V_z \)) has the same effect on the two \( \pm z \) valleys. The valley mixing Hamiltonian written in the basis spanned by the bulk valley states has equal diagonal terms, i.e., \( (D_z|V_z|D_z) = (D_{-z}|V_z|D_{-z}) = \Lambda \). The effective valley Hamiltonian thus reads

\[
H_v = \begin{bmatrix}
\Lambda & \Delta_v & 0 \\
\Delta_v^* & \Delta_v^* & 0 \\
0 & 0 & \Lambda
\end{bmatrix}.
\]  

As a result, the offset \( \Lambda \) can be extracted and included in the orbital energy and the mixing of the bulk valleys is fully described by the complex number \( \Delta_v \) [32]. By rewriting \( H_c \) in the eigenstate basis \( (D_{\pm}) \) Eq. (1) of the main text is obtained.

APPENDIX B: ADIABATICITY THRESHOLD

In this Appendix we discuss the adiabatic condition for a linear pulse. For two-level systems a detailed theory has been developed and the Landau-Zener formula [68,69] \( p = \exp(-4\pi^2 t^2/\hbar v) \) links the speed \( v \) of a linear pulse to the probability \( p \) of a diabatic transition between the eigenstates of the system. In the case of a multilevel system an analytical equation exists for the simple case of three-state ladder systems [70,71], where two states are differently coupled to a third state and which successfully describes coherent adiabatic passage [72] or stimulated Raman adiabatic passage [73].

Here we consider the three-level system described by the Hamiltonian

\[
H_{3L} = \begin{bmatrix}
-\Delta E_z/2 & 0 & t_- \\
0 & -\Delta E_z/2 & -t_- \\
\alpha_{ij} & -\alpha_{ij} & V_o^R - \epsilon
\end{bmatrix}
\]  

written on the basis \( |\uparrow, \downarrow, \rangle, |\downarrow, \uparrow, \rangle, S_{0,2,3} \rangle \). It approximates the 26-level system considered in the main text close to the lowest valley branch intravalley anticrossing (\( \epsilon \sim U^R \)). Each of the three eigenstates \( \Psi_{1,2,3} \) of \( H_{3L} \) undergoes an adiabatic evolution when the criterion [74]

\[
|\alpha_i^\text{max} / \alpha_i^\text{min}|^2 \ll 1
\]  

is satisfied. Here \( \alpha_i^\text{min} \) is the minimum energy difference between the \( i \)th eigenstate and the closest neighbor, while \( \alpha_i^\text{max} \) can be seen as the maximum “angular velocity” [74] of the state \( \Psi_i \) since it is defined as

\[
|\alpha_i(t)|^2 = \sum_{j \neq i} |\alpha_{ij}(t)|^2 = \sum_{j \neq i} \langle \Psi_i(t)|\Psi_j(t) \rangle ^2.
\]  

It has been shown (Ref. [74] for more details) that the total diabatic probability \( p_i \) during the time evolution of the \( i \)th eigenstate satisfies

\[
p_i \lesssim \max \left( \sum_{j \neq i} |\alpha_{ij}(t)|^2 \right) < p_i^\text{max} = \left| \alpha_i^\text{max} / \alpha_i^\text{min} \right|^2.
\]  

From Eq. (B4) the dependency of \( p_i \) on the pulse speed can be obtained. Since for a linear pulse the speed \( v = \dot{\epsilon} \) is constant we can rewrite \( \Psi_i(t) \) as \( \Psi_i(t) = \frac{\alpha_i(t)}{\alpha_i^\text{max}} v \). An upper bound to the diabaticity probability is obtained by converting the inequality in Eq. (B4) to

\[
p_i = v^2 \max \left( \sum_{j \neq i} |\tilde{\alpha}_{ij}(t)|^2 \right),
\]  

where \( \tilde{\alpha}_{ij}(t) \) is the speed-normalized “angular velocity”. Equation (B5) can be used as a lower bound for the speed to obtain a defined \( p_i \).

In Fig. 7(a) \( \tilde{\alpha}_1 \) is plotted, as well as the two contributions \( \tilde{\alpha}_{12} \) and \( \tilde{\alpha}_{13} \), as a function of the detuning. At negative detuning
the dominant term is $\tilde{\alpha}_{12}$ meaning that the Zeeman energy difference sets the adiabaticity condition, while $\tilde{\alpha}_{13}$ better describes the system around zero detuning. For the particular case shown in Fig. 7 of $t_{\pm} = 1.5$ GHz and $\delta E_Z = 10$ MHz the peak at zero detuning is lower than the one related to the Zeeman energy difference. In such a scenario, it is possible to adiabatically pulse from $S_{0,2}$ to $|\uparrow, \downarrow\rangle$, defining the adiabaticity with respect to the tunnel coupling only, given a large detuning range and a small $p_i$. For higher tunnel coupling the zero-detuning peak becomes dominant and the two-level approximation becomes more accurate.

Equation (B5) can be used to set the speed of a Pauli-spin blockade pulse in such a way that pulses with different $t$ satisfy the same adiabaticity condition. The function to be maximized on the right-hand side of Eq. (B5) can be viewed as a “local” speed since it is a function of time and thus detuning. As shown in Fig. 7(b), it has the same trend as $\tilde{\alpha}$ and can be analogously split into two contributions. While the speed obtained from Eq. (B5) corresponds to the global minimum of the “local” speed, the global speed calculated from $p_i^{\text{max}}$ is orders of magnitude smaller. Since $p_i^{\text{max}}$ is an upper bound, using this definition will make the pulses much slower than what is required, and the use of $p_i$ allows for faster pulses. The fidelity of a $|\uparrow, \downarrow\rangle \rightarrow S_{0,2}$ pulse is limited by the adiabaticity of the charge transition; therefore the higher the adiabaticity the higher the fidelity. In general, the global speed derived using the Landau-Zener formula for $p = 0.1\%$ would result in a fidelity approaching 99.9%, while setting $p_i = 0.2$ in Eq. (B5) or replacing $t$ with $t/2$ in the Landau-Zener formula allows for fidelity higher than 99.9%.

In the time evolution shown in Fig. 2(d) a linear pulse from $\epsilon = 0$ to $\epsilon = U_R + 2E_v^R$, with the $p_i = 0.2$ approximation, was used.

![FIG. 7. (a) The speed-normalized “angular velocity” $\tilde{\alpha}_i$ of the ground state as a function of the detuning. At negative detuning it reduces to $\tilde{\alpha}_{12}$, while at positive to $\tilde{\alpha}_{13}$. Here $t = 1.5$ GHz, $\delta E_Z = 10$ MHz, and $\Delta \Phi = 0$. The peak at the anticrossing corresponds to the contribution of a pure two-level system, while the broad peak is due to the fact that $|\uparrow, \downarrow\rangle$ and $|\downarrow, \uparrow\rangle$ are coupled to each other only via the singlet (0,2). (b) The “99.9% adiabatic probability” local speed as a function of detuning. The lower and upper horizontal lines are the global speed obtained using Eq. (B2) and the Landau-Zener formula, respectively. The middle one stems from the global 99.8% probability speed.](image-url)