

Micromagnet-free operation of electron spin qubits in Si/Si_{1-x}Ge_x vertical double quantum dots

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We study a vertical double quantum dot (DQD) in a Si/Si_{1-x}Ge_x/Si double-well heterostructure for full electrical control of electron Loss-DiVincenzo (LD) spin qubits, using realistic device modeling and numerical simulations. Due to the emerging spin-orbit interaction in the DQD, as well as strain from the gate electrodes, small (percentage range) but finite g -tensor variations emerge. In addition, we find a large valley splitting, on the order of $E_v \sim 250 \mu\text{eV}$. As a result, multiple avenues for fast electrical single-qubit rotations emerge. An ac electric field gives rise to electric dipole spin resonance, while electron spin resonance in the presence of an ac magnetic field can be electrically controlled by local gates due to varying g factors in DQDs. We also show that shuttling between neighboring dots, in vertical and horizontal directions, results in ultrafast single-qubit gates of less than a nanosecond. Remarkably, this DQD architecture completely eliminates the need for micromagnets, significantly facilitating the scalability of LD spin qubits in semiconductor foundries.

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I. INTRODUCTION

Spin qubits in silicon are deemed highly coherent and scalable [1–5] as well as the most integrable with existing semiconductor foundry processes [6,7]. Additional advantages of Si spin qubits include possible hyperfine-free isotopes [8] and the absence of piezoelectric coupling to phonons [9]. Several Si architectures have been successfully implemented in the few-dot regime [10–23]. Among these, Si/Si_{1-x}Ge_x heterostructures are particularly attractive due to the achievement of a very high mobility two-dimensional electron gas (2DEG) in almost nuclear spin-free ²⁸Si hosts [24–26]. Epitaxially grown strained silicon quantum wells in Si/Si_{1-x}Ge_x heterostructures offer a suitable platform for scalable quantum computation with electron spins [27–29]. These systems have been shown to host coherent electron spin qubits featuring high-fidelity one- and two-qubit gates [28,30–39].

However, there are two major challenges. First, for electron Loss-DiVincenzo (LD) spin qubits in silicon, micromagnets are required to perform single-qubit gates [30,40,41] because the intrinsic spin-orbit interaction (SOI) in pure Si is weak. This creates several issues, such as magnetic noise, crosstalk, and scalability [42–45]. It would thus be highly desirable to eliminate the need for micromagnets in LD qubit architectures. Second, the conduction band of bulk silicon has six degenerate minima close to the X point at $|\mathbf{k}_0| =$

$0.85 \frac{2\pi}{a_{\text{Si}}}$, known as valleys. For a heterostructure grown with Si/Si_{1-x}Ge_x, the tensile strain ($\epsilon_{xx} = \epsilon_{yy} \approx 0.42\%$) in the silicon layer partially lifts the sixfold valley degeneracy by inducing an energy gap between the $\pm z$ and $\pm x, \pm y$ valleys. However, the valley splitting between the lowest lying $\pm z$ states is highly device dependent, spanning from negligibly small values to several hundred μeV , reflecting a strong sensitivity to local electrostatics and interface disorder [46–48]. Extensive theoretical modeling has been conducted to study the multivalley physics of Si conduction bands [49–59], producing useful systematic strategies to lift valley degeneracy in practice [60–65]. In experiments, several valley-splitting enhancement strategies have been implemented, e.g., interface engineering [66–69], periodic Ge concentration in wiggly well [70–72], or a single Ge “spike” in the quantum well [73].

Here, we theoretically demonstrate that we can simultaneously circumvent both problems: micromagnets and valley degeneracy, by utilizing vertical double quantum dots (DQDs) [74] in a Si_{0.7}Ge_{0.3}/Si/Si_{1-x}Ge_x/Si/Si_{0.7}Ge_{0.3} double quantum well structure hosting a single electron spin. First, using effective mass theory, we show that the vertical confinement, consisting of the two narrow Si wells separated by a thin Si_{1-x}Ge_x layer, produces a large valley splitting. Realistic device simulation reveals that the DQD system showcases the tunability of the electron g through the top (plunger) gate: $g = 2 \pm \mathcal{O}(10^{-2})$. In the presence of an ac electric field, the device-dependent SOI can enable fast electric dipole spin resonance (EDSR) with a Rabi frequency of $\sim 20 \text{ MHz}$, without any micromagnet. For electron spin resonance (ESR) with an ac magnetic field, the g -tensor tunability provides a powerful electrical control knob, as it allows for shifting the resonance frequency without changing the microwave field itself. Finally, we consider spin shuttling in vertical and horizontal

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DQDs and show that both can generate ultrafast single-qubit rotations in subnanoseconds, owing to the angular difference in the principal axes of g tensors. While vertical DQDs have been experimentally realized for holes in Ge/SiGe double quantum wells [75,76], we are not aware of analogous structures for electrons proposed here.

II. DQD HAMILTONIAN AND DEVICE MODEL

A single electron spin in the Si/Si_{1-x}Ge_x/Si DQD in a heterostructure grown in [001] can be described by a spin-valley Hamiltonian given in the basis $\{|+z, \uparrow\rangle, |+z, \downarrow\rangle, |-z, \uparrow\rangle, |-z, \downarrow\rangle\}$ [77]. Its matrix representation is thus written in the form $\sigma_i \otimes \tau_j$, where σ_i and τ_j ($i, j = \{0, x, y, z\}$) denote the Pauli matrices in the spin and valley energy subspaces, respectively,

$$H_{\text{tot}}^{4 \times 4} = H_{\text{EFA}} + H_{\sigma\tau} + eF_z z \mathbb{I}_{4 \times 4} + \frac{\mu_B}{2} \sigma \cdot \mathbf{g} \cdot \mathbf{B} \mathbb{I}_{2 \times 2}. \quad (1)$$

The first term in Eq. (1) denotes the effective mass Hamiltonian describing the electron dispersion in the $\pm z$ valleys of the lowest conduction band of silicon,

$$H_{\text{EFA}} = \left[\frac{\hbar^2}{2} \left(\frac{(k_z + eA_z(x, y)/\hbar)^2}{m_l} + \frac{k_x^2 + k_y^2}{m_t} \right) + V(\mathbf{r}) + \Xi_u \varepsilon_{zz} \right] \mathbb{I}_{4 \times 4} - 2\Xi'_u \varepsilon_{xy} \mathbb{I}_{2 \times 2} \tau_z. \quad (2)$$

Here, $m_l = 0.916 \times 9.11 \times 10^{-31}$ kg and $m_t = 0.191 \times 9.11 \times 10^{-31}$ kg denote the effective longitudinal and transverse masses of the z valleys. Note that the shear strain ε_{xy} induces a valley splitting term τ_z between the $+z$ and $-z$ valleys. For in-plane magnetic field operation, the vector potential is given by $A_z(x, y) = B_x y - B_y x$. The confinement potential is given by $V(\mathbf{r}) = V(x, y) + V_{\text{DW}}(z)$, where $V(x, y)$ is modeled as 2D parabolic potential in x - y directions, with characteristic lengths $L_x = L_y = L_{ip}$. The z -double-well potential $V_{\text{DW}}(z)$ is modeled as a numerical function of the single Si z -well width L , the Si_{1-x}Ge_x barrier width a , and the barrier height V_b (see Appendix). The modeled z double well and DQD with relevant parameters are shown in Fig. 2(a). The second term in Eq. (1) describes the spin-valley interaction:

$$H_{\sigma\tau} = (V(\mathbf{r})e^{-2ik_0 z} \mathbb{I}_{2 \times 2} + 2\beta_0(k_+ \sigma_+ + k_- \sigma_-) \times e^{2i(2\pi/a_{\text{Si}} - k_0)z}) \tau_- + \text{H.c.}, \quad (3)$$

where $\beta_0 = 8.2$ meV is the Dresselhaus SOI coefficient, calculated using many-body tight binding formalism [77,78]. The third term in Eq. (1) denotes the plunger gate potential, and the fourth term is the Zeeman splitting of the electron spin due to an external magnetic field $\mathbf{B}$. Here, $\mathbf{g}$ denotes the g tensor. The eigenstates of the DQD spin qubit are given by $|\Psi_i\rangle = \sum_{lmnpq} c_i \phi_l(x) \phi_m(y) \phi_n(z) |\sigma_p\rangle \otimes |\tau_q\rangle$. The z -basis states $\phi_n(z)$ are the solutions to the one-dimensional (1D) Schrödinger equation $[\hbar^2 k_z^2 / (2m_l) + V_{\text{DW}}(z)] \phi_n(z) = e_n \phi_n(z)$ (see Appendix B). Similarly, the x - y -basis states are given by harmonic oscillator states $\phi_l(x) \phi_m(y)$. Choosing the basis sizes of $l \in \{1, 2, 3, 4\}$, $m \in \{1, 2, 3, 4\}$, and $n \in \{1, 2, 3, 4, 5, 6, 7, 8\}$, the total Hamiltonian $H_{\text{tot}} |\Psi_i\rangle = E_i |\Psi_i\rangle$ of dimensions 512×512 can be diagonalized to evaluate the DQD qubit energy levels E_i and the corresponding eigenfunction $|\Psi_i\rangle$. We denote the ground and first excited states as $|\Psi_0\rangle$

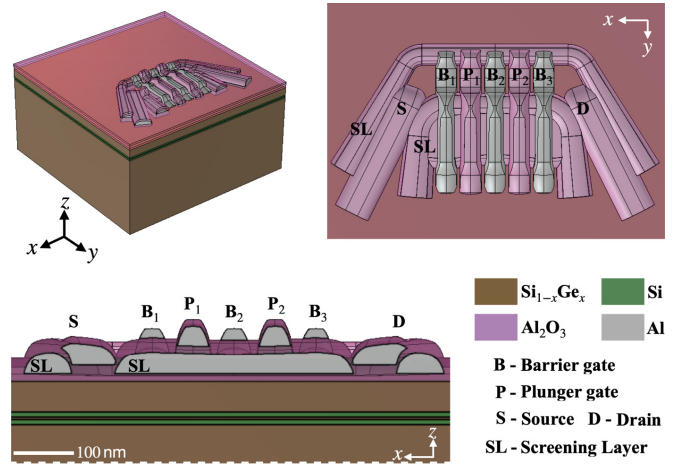


FIG. 1. Realistic device simulation outline. Geometry of the simulated heterostructure with 300 nm regrowth Si_{0.7}Ge_{0.3} layer, followed by the Si/Si_{1-x}Ge_x/Si double-well structure, and then 30 nm Si_{0.7}Ge_{0.3} buffer layer. The trilayer Al gates (from bottom: layer 1 $\rightarrow$ initial SL = screening layer, layer 2 $\rightarrow$ P = plunger, S = source, D = drain gates, and layer 3 $\rightarrow$ B = barrier gates) are 40 nm thick, while the Al₂O₃ oxide layers are 7 nm thick.

and $|\Psi_1\rangle$, respectively. The contraction of the metal gatestack at cryogenic temperatures results in additional shear strain in the DQD, which modifies the SOI and enhances the valley splitting. To this end, we simulate the thermal contraction of a planar DQD device of Si/Si_{1-x}Ge_x heterostructure with a trilayer metallic gate stack on top (Fig. 1). We employ the

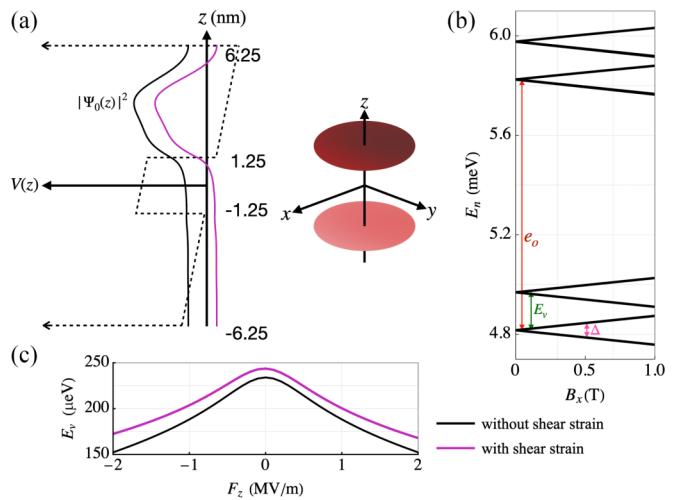


FIG. 2. The vertical DQD schematic. (a) Sketch of the vertical Si/Si_{1-x}Ge_x/Si DQD. The ground-state z -wave-function probability density $|\Psi_0(z)|^2$ at plunger field $F_z = -2$ MV/m, which resides mostly in the top Si well, with finite extent into the bottom well. Here, $L = 5$ nm, $a = 2.5$ nm, and $V_b = 15$ meV ($x = 0.033$). The tunnel coupling in the z double well is $t_c = 1$ meV. The in-plane confinement frequency is $\omega_{ip} = \hbar / (m_l L_{ip}^2)$, where $L_{ip} = 20$ nm. (b) The lowest spin, valley, and orbital states of the DQD without shear strain. Here, $\Delta = 12 \mu\text{eV}$, $E_v = 250 \mu\text{eV}$, and $e_0 = 1$ meV denote the Zeeman, valley, and orbital energy splittings, respectively. (c) Valley splitting E_v as a function of F_z with (purple line) and without (black line) shear strain.

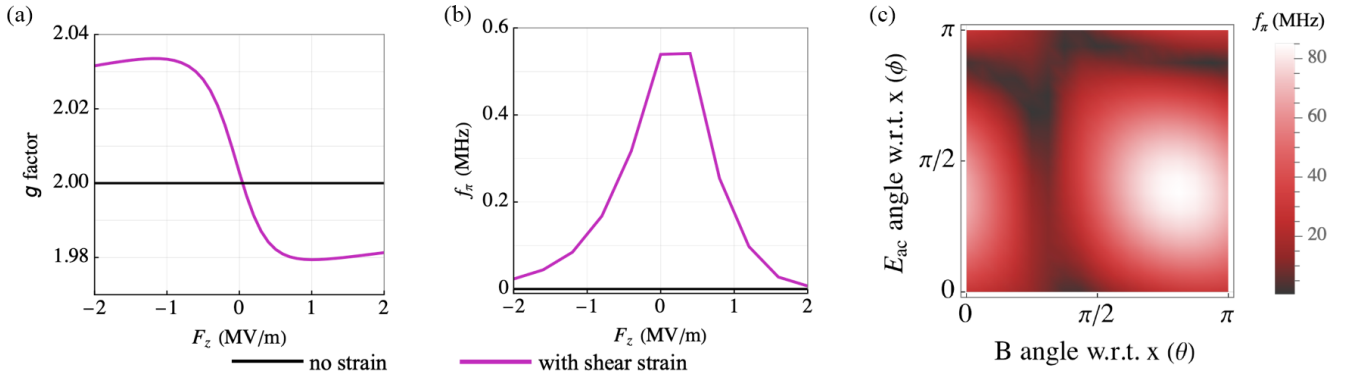


FIG. 3. Electrical control of Si/Si_{0.967}Ge_{0.033}/Si QD spin qubit. (a) The qubit g factor as a function of the P_1 plunger field F_z . The variation around $g_0 = 2$ is a result of strong SOI in the presence of the strain inhomogeneity. (b) EDSR Rabi frequency f_π vs F_z in the presence of an ac electric field along $\hat{z}$. In panels (a) and (b), specific scenarios without the shear strain (black solid line) and with shear strain (purple line) are shown. The magnetic field is $\mathbf{B} = (100, 0, 0)$ mT. (c) 2D map of f_π with the ac electric field in the x - y plane and $F_z = -1$ MV/m. Here, f_π is plotted as a function of the in-plane magnetic field angle θ ($\mathbf{B} = 100(\cos \theta, \sin \theta, 0)$ mT) and in-plane ac electric field angle ϕ ($\mathbf{E}_{ac} = E_{ac}^0 \cos(\omega t)(\cos \phi, \sin \phi, 0)$ with $E_{ac}^0 = 10^4$ V/m).

heat transfer module in COMSOL MULTIPHYSICS with relevant material parameters [79,80] to generate maps of the inhomogeneous shear strain across the device (see Appendix A).

III. ELECTRICAL TUNABILITY OF THE ELECTRON SPIN QUBIT

With full knowledge of the energy spectrum of a single electron spin in the vertical DQD (under P_1) with $L_{ip} = 20$ nm, $L = 5$ nm, $a = 2.5$ nm, and $V_b = 15$ meV ($x = 0.033$), we now examine the spin qubit properties and their electrical tunability. The dependence of the lowest spin, valley, and orbital energy levels on an external magnetic field $\mathbf{B} \parallel \hat{x}$ [Fig. 2(b)] reveals a valley splitting of $E_v \simeq 250 \mu\text{eV}$ and a Zeeman splitting of $\Delta = E_2 - E_1 = g\mu_B B \simeq 10 \mu\text{eV}$ (2.42 GHz) for $|\mathbf{B}| = 100$ mT. The large valley splitting originates from the vertical double-well geometry, which enhances coherent coupling between the $+z$ and $-z$ valleys through interface-induced Fourier components of the confinement potential near $2k_0$ [81–83]. Random alloy disorder is not included in the effective mass approximation employed here, which captures the average band-edge physics of the Si/Si_{1-x}Ge_x heterostructure. Atomistic studies have shown that alloy disorder can induce intervalley scattering and sample-dependent valley splittings [84,85]. Nevertheless, in the vertical DQD, the valley splitting is primarily geometry controlled rather than disorder dominated. In fact, it can be shown that with realistic gate-induced strain in the vertical DQD, the valley splitting at finite plunger gate field is consistently large, exceeding $150 \mu\text{eV}$ across the relevant operating regime (see Appendix A). Therefore, we expect alloy disorder to introduce device-to-device variability without qualitatively altering either the large valley splitting or the micromagnet-free electrical control mechanisms demonstrated in the proposed vertical DQD architecture.

As mentioned before, the lack of intrinsic SOI in Si implies that electrical manipulation of electron spin requires a nearby micromagnet; however, their large footprint and limited local tunability hinder the scalability of planar spin qubit devices. In the DQD device, strong SOI originates from (1) the atomistic

Dresselhaus-type spin-valley interaction, as given by the second term in Eq. (3); (2) the spatially varying gate-induced strain, which effectively produces an inhomogeneous electric field that the dot wave function experiences when shaken; and (3) the structural inversion asymmetry (SIA) introduced by the plunger gate field F_z . We demonstrate that the SOI in the vertical DQD opens up multiple micromagnet-free approaches to electrical spin manipulation. First, the presence of shear strain changes the g factor by $\delta g \approx 1\%$ when the field of the top/plunger gate is varied from negative to positive, essentially pushing the qubit wave function into the bottom or the top Si well [Fig. 3(a)]. Although small, this g -factor tunability via the plunger gate allows one to turn the spin rotations on and off electrostatically. The $\delta g \approx 1\%$ change corresponds to the 10 MHz shift in qubit Larmor frequency, which can help avoid frequency-dependent impedance mismatches and standing-wave resonances in the microwave transmission line, often separated by ≈ 10 MHz. Additionally, this tunability implies that local control in quantum dot arrays would be possible exclusively via the plunger gates. Moreover, for $\mathbf{B} = B_x \hat{x}$, an out-of-plane ac electric field $\mathbf{E}_{ac} = E_{ac}^0 \cos(\omega t) \hat{z}$ supplied through the plunger gate can induce a transverse magnetic field $\propto B_x \frac{\partial g_{xy}}{\partial F_z} E_{ac}^0 \cos(\omega t) \hat{z} \sigma_y$. This leads to g -tensor modulation resonance (g -TMR), a particular mechanism of EDSR where the spin exhibits Rabi oscillations when driven in a changing g tensor. We evaluate $f_\pi = 550$ kHz for $\mathbf{E}_{ac} \parallel \hat{z}$ [Fig. 3(b)], where the EDSR Rabi frequency f_π in the presence of an ac electric field $\mathbf{E}_{ac} = E_{ac}^0 \cos(\omega t) \hat{n}$ is calculated as follows:

$$\hbar f_\pi = e E_{ac}^0 |\langle \Psi_0 | \hat{n} \cdot \mathbf{r} | \Psi_1 \rangle|, \quad (4)$$

where E_{ac}^0 is the amplitude and $\hat{n}$ is the direction of the ac drive. Note that f_π for $\mathbf{E}_{ac} \parallel \hat{z}$ can be enhanced by improving the g -factor gradient through geometric means, up to a few MHz (see Appendix A). The amplitude is assumed to be $E_{ac}^0 = 10^4$ V/m [28,86].

Notably, ESR due to a fixed frequency ac magnetic field $\mathbf{B}_{ac} = B_{ac}^0 \cos(\omega_{ESR} t)$ applied perpendicular to $\mathbf{B}$ can be electrically controlled via local gates by exploiting the g -factor variation in the vertical DQD. Indeed, by shifting the

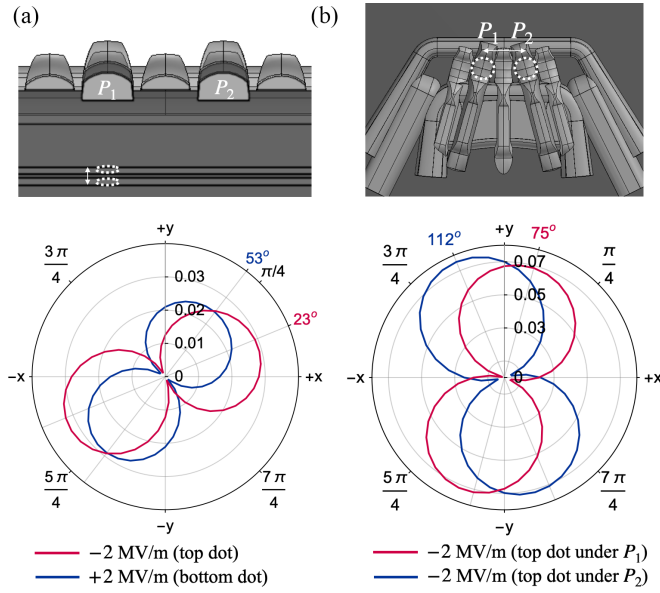


FIG. 4. g -factor anisotropy in DQDs in the presence of gate-induced strain. The quantity plotted is $|g(\theta) - 2|$, where $g(\theta) = \frac{\Delta(\theta)}{\mu_B B}$, and the Zeeman splitting Δ varies with the magnetic field angle, $\mathbf{B} = B(\cos \theta, \sin \theta, 0)$. (a) The polar plot of $|g(\theta) - 2|$ for a vertical DQD under plunger gate P_1 with $F_z = 2$ MV/m and $F_z = -2$ MV/m. (b) Polar plot of $|g(\theta) - 2|$ for left (under P_1) and right (under P_2) dots with rotated plunger gates at $F_z = -2$ MV/m. The plunger gates P_1 and P_2 are rotated by 30° with respect to each other.

electron wave function, the Zeeman splitting Δ of its spin can be tuned to resonance so that $\Delta = \hbar\omega_{\text{ESR}}$. Typical ESR powers of 5 dBm in experiments yield an ac magnetic field amplitude of 0.1 mT after device dissipation, leading to $f_\pi = 2.8$ MHz [87]. Achieving resonance control requires tuning Δ beyond the ESR linewidth (~ 100 kHz [88]), which is satisfied for $\delta g \sim 0.01$ and typical $\omega_{\text{ESR}} \sim 5$ GHz. An in-plane ac electric field $\mathbf{E}_{\text{ac}} = E_{\text{ac}}^0 \cos(\omega t)(\cos \phi \hat{x} + \sin \phi \hat{y})$ could facilitate strong iso-Zeeman EDSR. Here, the qubit is driven at a constant g factor via a transverse magnetic field originating from the net effect of SOI and $\mathbf{E}_{\text{ac}}$. We calculate fast EDSR of up to $f_\pi = 80$ MHz with an in-plane ac electric field [Fig. 3(c)]. While iso-Zeeman EDSR is significantly faster than g -TMR, the latter is more robust against charge noise. This is due to the reliance of iso-Zeeman EDSR on SOI, which exposes the qubit to electric field fluctuations from nearby charge traps. Therefore, g -TMR at higher magnetic fields could potentially lead to full electrical control of the vertical DQD spin qubit using only the plunger gate [89].

Finally, we examine the in-plane g -factor anisotropy, which can facilitate single-qubit rotations via spin hopping [1,45,90,91]. Including gate-induced strain, we present the polar plot of the deviation of the g factor from $g_0 = 2$ for a sweep of $B_x - B_y$, where $|\mathbf{B}| = 100$ mT. The directions of maximum and minimum $|g(\theta) - 2|$ define the principal axes of the in-plane g tensor. A pulse can be engineered to periodically shuttle the qubit between the top and bottom dots with wait times τ_b at the bottom dot and τ_t at the top dot (see Appendix C). We calculate the difference between g -tensor principal axes to be $\sim 30^\circ$ [see Fig. 4(a)], so a $\pi/2$ spin rotation is

achieved after $2(\tau_t + \tau_b)$ sequences consisting of three hoppings, with an S -gate time of $T_g = 0.6$ ns. Shuttling in the x direction, between the top dots under P_1 and P_2 plunger gates, is considered as well. We find that when the plunger gates are tilted by 30° with respect to each other, a 37° difference is produced in the in-plane principal axes of the g tensor [see Fig. 4(b)]. The deviation of the g factor from $g_0 = 2$ is also enhanced. Horizontal DQD shuttling has the advantage of requiring smaller pulse voltages [91]. In contrast, vertical DQD shuttling requires larger pulse amplitudes but offers the benefit of ultrafast qubit manipulation using a single plunger gate.

IV. CONCLUSION

We have shown that vertical DQDs in $\text{Si}/\text{Si}_{1-x}\text{Ge}_x$ heterostructures enable large valley splitting and exhibit micromagnet-free full electrical control of an electron spin qubit. An in-plane ac electric field generates fast EDSR with a gate time of ~ 30 ns. An out-of-plane ac electric field supplied via the top gate also produces 100 kHz Rabi frequency. Combined with the g -factor tunability, this potentially provides a mechanism by which the spin qubit can be entirely controlled via the plunger gate. We also establish that the angular difference in the g -tensor principal axes between vertically and horizontally neighboring quantum dots facilitates spin-hopping-based spin rotation. The path forward is to study the two-spin problem and investigate the feasibility of universal gate operations in this architecture.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [92].

APPENDIX A: GEOMETRY DEPENDENCY: VALLEY SPLITTING, SHEAR STRAIN, AND ELECTRICAL TUNABILITY IN THE VERTICAL DQD

Three-dimensional finite element method simulations of the strain distribution at 0.1 K are performed using the Structural Mechanics module in COMSOL MULTIPHYSICS. The metal gate electrodes are modeled as stress-inducing layers on top of the $\text{Si}/\text{Si}_{1-x}\text{Ge}_x$ heterostructure, and the resulting strain tensor is evaluated throughout the DQD region (Fig. 5). Standard material parameters for Si and $\text{Si}_{1-x}\text{Ge}_x$ from the literature have been used [79,80]. Few of the relevant $\text{Si}_{1-x}\text{Ge}_x$ parameters are listed in Table I.

The dominant contribution to the large valley splitting originates from coherent interference of intervalley coupling at the two Si/SiGe interfaces defining the vertical double

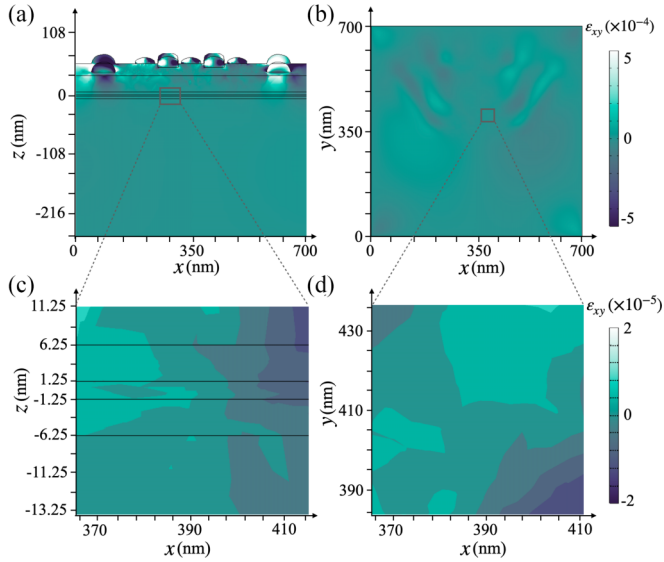


FIG. 5. Simulated shear strain in the DQD due to the metal gate electrodes atop the Si/Si_{1-x}Ge_x heterostructure. (a) The xz map of the $\varepsilon_{xy}(x, y, z)$ shear strain tensor component in the simulated DQD device. (b) Similarly, the xy map of $\varepsilon_{xy}(x, y, z)$. (c), (d) The 2D maps of $\varepsilon_{xy}(x, y, z)$ in the DQD under plunger gate P_1 . The Si/Si_{1-x}Ge_x/Si ($x = 0.033$ here) layers are indicated in panel (c). The DQD centered at point (390, 410, 0) nm spans the following range: $x \in [370, 410]$ nm, $y \in [390, 430]$ nm, $z \in [-6.25, 6.25]$ nm.

well. We first examine the dependence of the valley splitting on the barrier height, set by the Ge concentration x in the Si_{1-x}Ge_x barrier. Varying x from 1.1% to 5.5%, we find that for $V_b = 15$ meV, corresponding to $x = 3.3\%$ (Si_{0.967}Ge_{0.033}), the valley splitting is maximized [Fig. 6(a)]. In the absence of shear strain, varying the barrier width a between 2 and 3 nm yields oscillations in the valley splitting ranging from 260 down to 25 μ eV. When realistic gate-induced shear strain is included, these oscillations are substantially modified, with the valley splitting varying between 275 and 90 μ eV [Fig. 6(b)]. Furthermore, at finite plunger fields $|F_z| > 0$, the oscillations are suppressed and a uniformly large valley splitting of order 150 μ eV emerges [Fig. 6(c)]. This behavior reflects the interference of interface-induced intervalley coupling contributions from the

TABLE I. Si_{1-x}Ge_x parameters as a function of Ge fraction x . For $x = 0$, these parameters correspond to Si. Note that the value of thermal conductivity K has been taken from the plot in Ref. [80] highlighting its nontrivial variation with x .

Parameters	Values
Lattice constant, a_l	$(5.43 + 0.20x + 0.03x^2) \times 10^{-10}$ m
Density, ρ	$(2.3 + 3.5x - 0.5x^2) \times 10^3$ g cm ⁻³
Young's modulus, E	$(130.2 - 28.1x) \times 10^9$ Pa
Thermal expansion coefficient, α	$(2.60 + 2.55x) \times 10^{-6}$ K ⁻¹
Heat capacity, C_p	$\frac{19.6+2.9x}{72.6x+28.1(1-x)} \times 10^3$ J kg ⁻¹ K ⁻¹
Band gap, E_g	$1.12 - 0.41x + 0.008x^2$ eV
Poisson's ratio, ν	$0.278 - 0.005x$
Relative permittivity, ε_r	$11.7 + 4.5x$

two barrier interfaces. Since $2k_0 \approx 9.5$ nm⁻¹, the relative phase of these contributions is sensitive to changes in the barrier width on the scale of a monolayer (~ 0.14 nm). Consistently, we find that the valley splitting exhibits peak-to-peak oscillations when a is varied by approximately 0.16 nm. Gate-induced strain breaks the symmetry between the two interfaces, modifying the relative weighting of their contributions and thereby elevating the minimum valley splitting to 90 μ eV. Importantly, while the valley splitting exhibits oscillations on the monolayer scale at zero plunger field, gate-induced strain in realistic devices and plunger field strongly suppress this sensitivity, yielding a robust lower bound ~ 150 μ eV that is insensitive to atomic-scale variations in barrier thickness. To place in context the various spin manipulation pathways described in the main text, we now discuss in detail the mechanisms enabling different modes of electrical control of the spin qubit. A transverse oscillatory magnetic field $\mathbf{B}_{\text{eff}}(t) \perp \mathbf{B}$ is necessary to be in resonance with the qubit Zeeman splitting to rotate the spin polarization, i.e., to flip the spin. In the presence of SOI, an alternating electric field $\mathbf{E}_{\text{ac}}$ can also produce spin flips. The ac electric field essentially “shakes” the QD wave function back and forth in the direction of the field. This oscillatory dipole mixes the $\Delta n = 1$ orbital levels, conserving the spin polarization. The SOI, on the other hand, can also induce $\Delta n = 1$ orbital mixing; importantly, it connects opposite spin directions. The

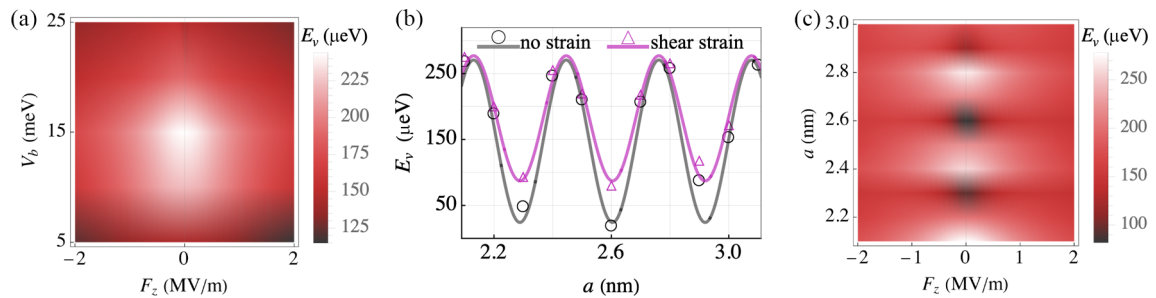


FIG. 6. Valley Splitting dependence on barrier height and width. (a) 2D map of the valley splitting E_v as a function of plunger voltage F_z and Si_{1-x}Ge_x barrier height V_b . $V_b = 15$ ($x = 3.3\%$) exhibits the largest valley splitting. (b) Valley splitting E_v as a function of the barrier width a at $F_z = 0$. The circles and solid fit line in black denote the results without strain, while triangular markers and solid fit line in purple show results with strain. The oscillation in the valley splitting can be fit to a period of 0.31 nm. (c) 2D map of E_v as a function of F_z and barrier width a in the presence of gate-induced shear strain.

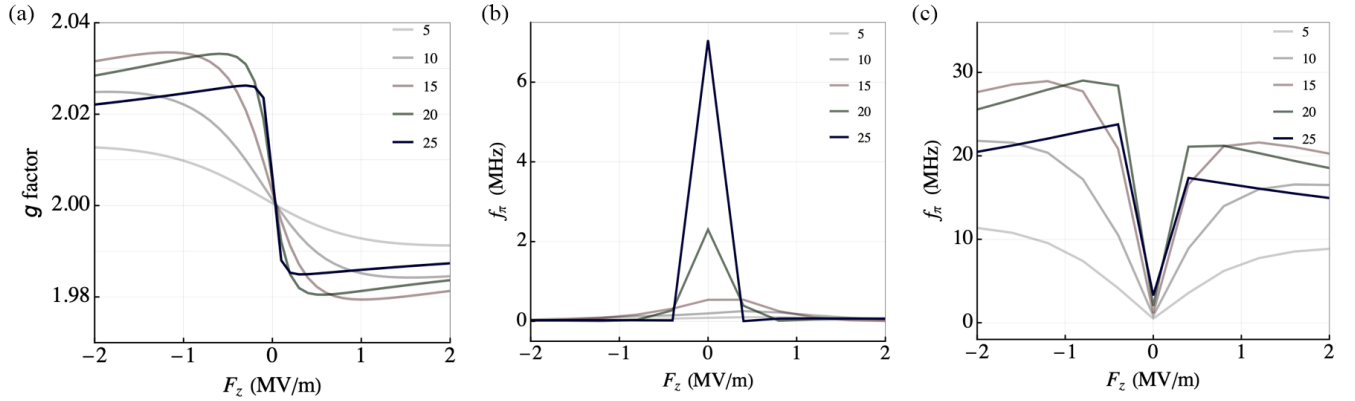


FIG. 7. Electrical tunability with varying barrier height. (a) g factor as a function of plunger voltage F_z for different $\text{Si}_{1-x}\text{Ge}_x$ barrier heights V_b (plot legends given in meV). (b) EDSR Rabi frequency f_π as a function of F_z at different barrier heights V_b ; $\mathbf{B} \parallel \hat{\mathbf{x}}$, $\mathbf{E}_{\text{ac}} \parallel \hat{\mathbf{z}}$. (c) f_π vs F_z at different barrier heights V_b ; $\mathbf{B} \parallel \hat{\mathbf{x}}$, $\mathbf{E}_{\text{ac}} \parallel \hat{\mathbf{x}}$. The barrier width is $a = 2.5$ nm.

net effect of SOI and $\mathbf{E}_{\text{ac}}$ is thus an effective magnetic field, resulting in Rabi oscillation of the spin polarization, given that this effective magnetic field is perpendicular to the externally applied static $\mathbf{B}$. In the DQD device, the SOI originates from (1) the atomistic Dresselhaus-type spin-valley interaction; (2) the spatially varying gate-induced strain, which effectively produces an inhomogeneous electric field that the dot wave function experiences when shaken; and (3) the SIA introduced by the plunger gate field F_z . The iso-Zeeman EDSR gives rise to fast Rabi oscillations with in-plane ac electric field. Additionally, the variation of the g tensor via the plunger gate can result in g -TMR. For $\mathbf{B} = B_x \hat{\mathbf{x}}$, coherent single-qubit rotation with $\mathbf{E}_{\text{ac}} \parallel \hat{\mathbf{z}}$ is possible via driving term $\propto B_x \frac{\partial g_{xy}}{\partial F_z} E_{\text{ac}}^0 \cos(\omega t) \hat{z} \sigma_y$.

We also examine the effect of varying the barrier height on the electrical tunability of the electron spin qubit. With increasing barrier height, the slope of the g factor increases, while $V_b = 15$ meV ($x = 3.3\%$) produces the largest variation [Fig. 7(a)]. As anticipated, the EDSR Rabi frequency for microwave drive via the plunger gate enhances with increasing maximum $\frac{\partial g}{\partial F_z}$ close to $F_z = 0$ [Fig. 7(b)]. EDSR with in-plane

ac electric field ($\mathbf{E}_{\text{ac}} \parallel \hat{\mathbf{x}}$) is the fastest for $V_b = 15$, close to plunger field value where $\frac{\partial g}{\partial F_z} \approx 0$ (Fig. 7).

APPENDIX B: THE z -DOUBLE-WELL POTENTIAL BASIS

The double-well potential is given by

$$V(\mathbf{r}) = V_{\text{DW}}(z) + \frac{m_t}{2} \left(\left[\frac{\hbar}{m_t L_x^2} \right]^2 x^2 + \left[\frac{\hbar}{m_t L_y^2} \right]^2 y^2 \right). \quad (\text{B1})$$

The z -basis states are calculated by solving the following equation: $[-\frac{\hbar^2 \partial^2}{2m_t} + V_{\text{DW}}] \phi_n(z) = e_n \phi_n(z)$. The piecewise function describing the double-well potential is as follows:

$$V_{\text{DW}}(z, a, L, V_b) = \begin{cases} V_0, & L + \frac{a}{2} \leq z < \infty, \\ 0, & \frac{a}{2} < z < L + \frac{a}{2}, \\ V_b, & -\frac{a}{2} \leq z \leq \frac{a}{2}, \\ 0, & -(L + \frac{a}{2}) < z < -\frac{a}{2}, \\ V_0, & -\infty < z \leq -(L + \frac{a}{2}). \end{cases} \quad (\text{B2})$$

Below, we provide the full form of the transcendental equation and basis solutions for even and odd bound ($e_n < V_b$) and unbound ($e_n > V_b$) states. Note that $\gamma = \sqrt{\frac{2mL^2 V_b}{\hbar^2}}$ and $r = \frac{a}{2L}$. For $e_n < V_b$, even:

$$\gamma \pi \sqrt{\frac{e_n}{V_b}} (1+r) = n\pi + \tan^{-1} \left[-F \frac{1 + \frac{e_n}{F\sqrt{V_0^2 - e_n^2}}}{1 - \frac{e_n F}{\sqrt{V_0^2 - e_n^2}}} \right],$$

where $F = \frac{\cos(\gamma \sqrt{\frac{e_n}{V_b}} \pi r) \cosh(\gamma \sqrt{1 - \frac{e_n}{V_b}} \pi r) - \sqrt{\frac{V_b}{e_n} - 1} \sin(\gamma \sqrt{\frac{e_n}{V_b}} \pi r) \sinh(\gamma \sqrt{1 - \frac{e_n}{V_b}} \pi r)}{\sin(\gamma \sqrt{\frac{e_n}{V_b}} \pi r) \cosh(\gamma \sqrt{1 - \frac{e_n}{V_b}} \pi r) + \sqrt{\frac{V_b}{e_n} - 1} \cos(\gamma \sqrt{\frac{e_n}{V_b}} \pi r) \sinh(\gamma \sqrt{1 - \frac{e_n}{V_b}} \pi r)}, \quad (\text{B3})$

$$\phi_n(z) = \mathbf{N} \times \begin{cases} \frac{\text{num}(F) \cos(\gamma \sqrt{\frac{e_n}{V_b}} \pi (1+r)) + \text{den}(F) \sin(\gamma \sqrt{\frac{e_n}{V_b}} \pi (1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi (1+r)}} e^{\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r), \\ \text{num}(F) \cos(-\gamma \sqrt{\frac{e_n}{V_b}} \pi \frac{z}{L}) + \text{den}(F) \sin(-\gamma \sqrt{\frac{e_n}{V_b}} \pi \frac{z}{L}), & -L(1+r) < z < -Lr, \\ \cosh(\gamma \sqrt{1 - \frac{e_n}{V_b}} \pi \frac{z}{L}), & -Lr \leq z \leq Lr, \\ \text{num}(F) \cos(\gamma \sqrt{\frac{e_n}{V_b}} \pi \frac{z}{L}) + \text{den}(F) \sin(\gamma \sqrt{\frac{e_n}{V_b}} \pi \frac{z}{L}), & Lr < z < L(1+r), \\ \frac{\text{num}(F) \cos(\gamma \sqrt{\frac{e_n}{V_b}} \pi (1+r)) + \text{den}(F) \sin(\gamma \sqrt{\frac{e_n}{V_b}} \pi (1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi (1+r)}} e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r). \end{cases} \quad (\text{B4})$$

For $e_n < V_b$, odd:

$$\gamma\pi\sqrt{\frac{e_n}{V_b}}(1+r) = n\pi + \tan^{-1} \left[-F \frac{1 + \frac{e_n}{F\sqrt{V_0^2 - e_n^2}}}{1 - \frac{e_n F}{\sqrt{V_0^2 - e_n^2}}} \right],$$

$$\text{where } F = \frac{\cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \sinh(\gamma\sqrt{1 - \frac{e_n}{V_b}}\pi r) - \sqrt{\frac{V_b}{e_n} - 1} \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \cosh(\gamma\sqrt{1 - \frac{e_n}{V_b}}\pi r)}{\sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \sinh(\gamma\sqrt{1 - \frac{e_n}{V_b}}\pi r) + \sqrt{\frac{V_b}{e_n} - 1} \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \cosh(\gamma\sqrt{1 - \frac{e_n}{V_b}}\pi r)},$$

$$\phi_n(z) = \mathbf{N} \times \begin{cases} -\frac{\text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r)) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi(1+r)}} e^{\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r), \\ -\text{num}(F) \cos(-\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}) - \text{den}(F) \sin(-\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}), & -L(1+r) < z < -Lr, \\ \sinh(\gamma\sqrt{1 - \frac{e_n}{V_b}}\pi \frac{z}{L}), & -Lr \leq z \leq Lr, \\ \text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}), & Lr < z < L(1+r), \\ \frac{\text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r)) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi(1+r)}} e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r). \end{cases} \quad (\text{B5})$$

For $e_n > V_b$, even:

$$\gamma\pi\sqrt{\frac{e_n}{V_b}}(1+r) = n\pi + \tan^{-1} \left[-F \frac{1 + \frac{e_n}{F\sqrt{V_0^2 - e_n^2}}}{1 - \frac{e_n F}{\sqrt{V_0^2 - e_n^2}}} \right],$$

$$\text{where } F = \frac{\cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \cos(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r) + \sqrt{1 - \frac{V_b}{e_n}} \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \sin(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r)}{\sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \cos(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r) - \sqrt{1 - \frac{V_b}{e_n}} \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \sin(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r)}, \quad (\text{B6})$$

$$\phi_n(z) = \mathbf{N} \times \begin{cases} \frac{\text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r)) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi(1+r)}} e^{\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r), \\ \text{num}(F) \cos(-\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}) + \text{den}(F) \sin(-\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}), & -L(1+r) < z < -Lr, \\ \cos(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi \frac{z}{L}), & -Lr \leq z \leq Lr, \\ \text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}), & Lr < z < L(1+r), \\ \frac{\text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r)) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi(1+r)}} e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r). \end{cases} \quad (\text{B7})$$

For $e_n > V_b$, odd:

$$\gamma\pi\sqrt{\frac{e_n}{V_b}}(1+r) = n\pi + \tan^{-1} \left[-F \frac{1 + \frac{e_n}{F\sqrt{V_0^2 - e_n^2}}}{1 - \frac{e_n F}{\sqrt{V_0^2 - e_n^2}}} \right],$$

$$\text{where } F = \frac{\cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \sin(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r) - \sqrt{1 - \frac{V_b}{e_n}} \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \cos(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r)}{\sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \sin(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r) + \sqrt{1 - \frac{V_b}{e_n}} \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi r) \cos(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi r)},$$

$$\phi_n(z) = \mathbf{N} \times \begin{cases} -\frac{\text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r)) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi(1+r)}} e^{\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r), \\ -\text{num}(F) \cos(-\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}) - \text{den}(F) \sin(-\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}), & -L(1+r) < z < -Lr, \\ \sin(\gamma\sqrt{\frac{e_n}{V_b} - 1}\pi \frac{z}{L}), & -Lr \leq z \leq Lr, \\ \text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi \frac{z}{L}), & Lr < z < L(1+r), \\ \frac{\text{num}(F) \cos(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r)) + \text{den}(F) \sin(\gamma\sqrt{\frac{e_n}{V_b}}\pi(1+r))}{e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi(1+r)}} e^{-\gamma V_b^{-1} \sqrt{V_0^2 - e_n^2} \pi z/L}, & -\infty < z \leq -L(1+r). \end{cases} \quad (\text{B8})$$

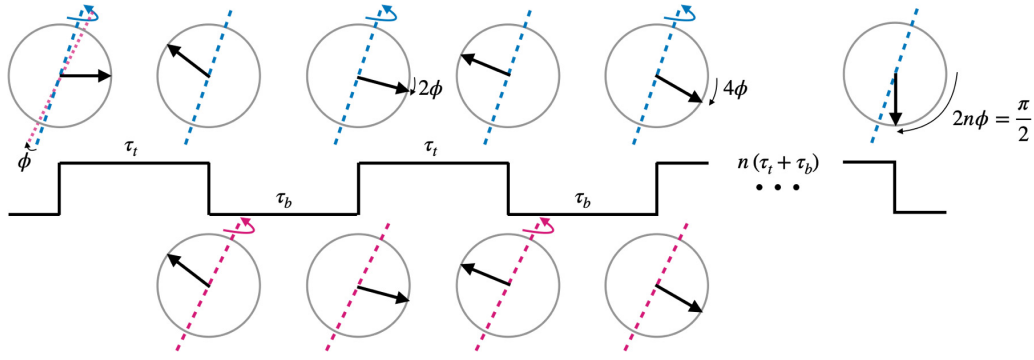


FIG. 8. Schematic of the pulsing sequence of hopping between top and bottom Si dots. The in-plane principal axis of the g tensor is denoted in blue (red) for the top (bottom) QD, with an angular difference ϕ between them. Each $(\tau_t + \tau_b)$ sequence of hopping back and forth generates 2ϕ net rotation of the spin. Hence, after n such sequences, for example, single-qubit S gate ($\pi/2$ rotation) can be achieved if $2n\phi = \pi/2$.

The transcendental equation can be solved on a graph by plotting the left-hand side and right-hand side and identifying the intersecting points to produce e_n solutions for each case. The normalization coefficient N can be obtained by using $\int_{-\infty}^{\infty} |\phi_n(z)|^2 dz = 1$. Also, num() and den() denote the numerator and denominator of the expression in parentheses, respectively. For this work, we approximate $V_0 \gg e_n$ (the infinite outer boundary of the double well), in which case $1 + \frac{F \sqrt{V_0^2 - e_n^2}}{e_n F} \approx 1$.

The x - y basis is described by the following set of equations:

$$\begin{aligned} \phi_l(x) &= \frac{1}{\sqrt{2^l l! L_x \sqrt{\pi}}} e^{-\frac{x^2}{2L_x^2}} H_l(x/L_x), \\ \phi_m(y) &= \frac{1}{\sqrt{2^m m! L_y \sqrt{\pi}}} e^{-\frac{y^2}{2L_y^2}} H_m(y/L_y). \end{aligned} \quad (\text{B9})$$

APPENDIX C: HOPPING-BASED SPIN ROTATION MECHANISM

An anisotropic g tensor can be harnessed to realize single-qubit rotations via a spin hopping (or shuttling) sequence between the top and bottom dots of the DQD structure. As demonstrated in Fig. 8, the spin could be initialized in the top QD in the direction of the applied magnetic field $\mathbf{B} \parallel \mathbf{x}$. The spin is allowed to precess from $-\pi/2$ to $\pi/2$ about the principal g -tensor axis for τ_t time, followed by the spin hopping to the bottom QD. The spin then precesses from $-\pi/2$ to $\pi/2$ about the principal g -tensor axis of the bottom QD for τ_b time. When shuttled back to the top QD, the angular difference ϕ between the two g -tensor axes would produce a 2ϕ rotation of the original spin orientation $\parallel \mathbf{x}$. By repeating this pulsing sequence n times, a $\pi/2$ rotation of the spin about the z axis, for example, can be achieved if $2n\phi = \pi/2$. The gate time for this rotation is estimated as $T_g^{\pi/2} = \frac{n}{f_L}$, where $f_L = \frac{g\mu_B B}{h}$ is the Larmor frequency of the electron spin qubit ($f_L \simeq 2.8$ GHz for the electron spin at $|\mathbf{B}| = 100$ mT).

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