Qubits Based on Hole Quantum Dots in Strained Ge

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We argue, supported by ab initio calculations, that holes in a Si$_x$Ge$_{1-x}$/Ge/ Si$_x$Ge$_{1-x}$ quantum well possess highly desirable properties as qubits, including a large (>100 meV) intrinsic splitting between the light and heavy hole bands, a very light (∼0.05 $m_0$) effective mass parallel to the Ge well interfaces (potentially leading to high mobilities and tunnel rates, as well as relaxed fabrication demands regarding dot size), and a high natural abundance of nuclear spin-0 isotopes. Compared to electrons in quantum dots, such hole qubits benefit from larger size, and do not suffer from the presence of nearby quantum levels (e.g., valley states) that can compete with electron spins as qubits. The strong spin-orbit coupling in Ge quantum wells may be harnessed to implement electric-dipole spin resonance, leading to gating times of several nanoseconds for single-qubit rotations. The microscopic mechanism of such spin-orbit coupling is discussed, stressing the relevance of coupling terms stemming from the underlying cubic crystal field.

INTRODUCTION

Electron spins in semiconductor quantum dots are promising qubit candidates for scalable quantum computing because of their small size, fast and flexible electrical controls, and fabrication methods that leverage technological advances in the semiconductor industry.1 Recent attention has focused on conduction band electrons in group-IV elements, especially silicon, due to the predominance of naturally abundant, spin-0 nuclear isotopes, yielding spin qubits that have very quiet magnetic environments and, therefore, slow decoherence. Silicon is also protected by intrinsically weak spin-orbit coupling (SOC), which suppresses a potential decoherence channel.2 On the other hand, fast gating through electric-dipole spin resonance (EDSR) requires a sizeable SOC.3 There are also potential disadvantages for electrons in silicon, such as the valley degeneracy of the conduction band, which can interfere with spin control.4 In principle, sharp or specially engineered barriers at the quantum well interface can enhance the valley splitting to mitigate this problem,5 however valley splitting can also be suppressed by unavoidable atomic-scale disorder.6 Hence, there are compelling reasons to consider other group-IV systems, with larger SOC and no valley degeneracy.

Germanium is a natural choice for replacing Si to form qubits,7,8 due to its compatibility with existing growth and fabrication technologies. When sandwiched between strain-relaxed, Ge-rich SiGe alloys, Ge forms a type-I quantum well that can trap either electrons or holes.9 Here, we focus on holes, due to their favorable properties for quantum computing,10,11 several of which already arise in bulk Ge. For example, since the top of the valence band occurs at the Γ point, atomic-scale disorder (e.g., at the quantum-well interface) does not cause interference effects of the type observed between conduction band valleys in Si.12 Moreover, the hole states are formed from p-type atomic orbitals, for which the wavefunction nodes occur at the nuclear sites, suppressing contact hyperfine interactions for the occasional non-zero nuclear spins.13,14 Certain desirable properties are not readily available to holes in bulk Ge, however. For example, cubic symmetry renders the top of the valence band four-fold degenerate, in contrast to conventional paradigms for quantum computing based on two-level systems. Quantum confinement partially solves this problem since the valence bands have different effective masses, with the ground state forming in the two-fold degenerate heavy-hole band. On the other hand, a heavy mass can be unfavorable for confining and manipulating holes, since it implies smaller dots that require greater lithographic precision during fabrication. Heavier masses also tend to suppress tunneling rates and mobilities in a 2D hole gas.15

Here, we present band structure calculations showing that such challenges for Ge hole-spin qubits can be overcome in a compressively strained quantum well. The tetragonal distortion causes a sudden change in the valence band dispersion and a large intrinsic splitting of the degenerate hole bands. The top hole band is of particular interest since its dispersion becomes highly anisotropic, with a larger effective mass along the strain axis, and a very small mass parallel to the quantum well interface, as consistent with recent experiments.17,19 The former is advantageous because the quantum-well confinement further increases the level splitting between the subbands, while the latter enhances the tunneling rates and the mobility. Indeed, 2D Ge hole gases can have mobilities >10⁶ cm²/Vs17, comparable to electrons in GaAs, with the additional benefit of much smaller nuclear spin densities. Such high-quality materials have now been achieved by several groups20 and have recently been fabricated into quantum dots.21,22 Building upon our band struc-
structure calculations, we then explain how to perform EDSR manipulations of the hole spin state— a task that is not trivial since the linear Rashba spin-orbit effect is insufficient to couple qubits with angular momentum differing by more than one quantum and the inversion symmetry of bulk germanium largely suppresses the Dresselhaus effect.

RESULTS

An electrically gated double-dot device is sketched in Fig. 1a. The essential components include a SiGe/Ge/SiGe heterostructure, an optional capping layer, and a set of patterned, nanometer-scale metal gates that are isolated from the heterostructure by oxide layers. For simplicity, we consider an accumulation-mode gating scheme (i.e., without dopants) and note that the details of the gate and oxide layers are unimportant for the discussion below. The typical arrangement for trapping holes is to sandwich compressively strained Ge between strain-relaxed SiGe, with barriers that are high enough to form a quantum well. For example, a strain-relaxed Si$_{0.25}$Ge$_{0.75}$ barrier yields a valence-band offset of $\sim 170$ meV [22] which is ample for trapping holes. Heterostructure growth typically begins on a Si wafer. [Here, we assume a Si (001) substrate.] Due to lattice mismatch, the growth of SiGe alloy on Si introduces dislocations, which may be harmful for device operation. Such effects can be mitigated by increasing the Ge content gradually, over several μm, until the desired alloy is achieved; under ideal conditions, the resulting SiGe growth surface will be strain-relaxed and dislocation-free [23]. Alternative approaches, such as reverse grading, have also been employed [24]. A pure Ge quantum well is then grown on the SiGe virtual substrate. The width of the well should be less than the critical thickness for forming additional dislocations; however, this should not be a problem for Ge grown on Ge-rich alloy. For example, the critical Ge thickness for a Si$_{0.25}$Ge$_{0.75}$ barrier is $\sim 30$ nm [23]. Finally, since Ge forms unstable oxides [22] (and similar problems arise for SiGe [25]), it may be desirable to include a capping layer, with a carefully chosen thickness. High-quality dopant-free Ge quantum wells with [13] and without [21] capping layers have already been achieved, with higher mobilities ($>0.5\times 10^{6}$ cm$^2$/V s) obtained in the first case.

A realistic, quantitative prediction for the band structure of strained Ge is key for assessing the viability of hole-spin qubits. Here, we compute the band structure using self-consistent, ab initio density functional theory (DFT), including spin-orbit interactions, following the technical approach described in Methods. For our primitive Bravais lattice we adopt a body-centered tetragonal lattice with a two-atom basis consistent with the diamond structure. For unstrained Ge, the tetragonal lattice parameters are given by $a=b=4.0008$ Å in the plane of the quantum well, and $c=\sqrt{2}a=5.6580$ Å in the growth direction. (See Fig. 1b.) Si$_x$Ge$_{1-x}$ alloy with concentration $x$ has a modified lattice constant, $a(x)$; if the quantum well is grown pseudomorphically, the alloy lattice constant is

FIG. 1. Heterostructure description and band structure. (a) A representative heterostructure for hole-spin qubits, with a 20 nm strained-Ge quantum well epitaxially grown on strain-relaxed Si$_{0.25}$Ge$_{0.75}$ alloy. For this structure, the strain in the Ge layer is $\varepsilon = -1\%$, as defined in the main text. In addition to metal depletion gates (blue) and interspersed oxide layers (yellow), we assume an upper top gate (transparent gray) that can accumulate a 2D hole gas in the quantum well without extrinsic doping. Here, $z$ is defined as the growth direction. (b,c) Computed electronic band structures for relaxed and uniaxially-strained Ge. To the left of each plot we show the corresponding real and reciprocal space crystal structures (lower and upper diagrams, respectively), with lattice constants ($a$ and $c$) and symmetry points (Γ, X, Z, and L), as indicated. (Note that the tetragonal deformation is exaggerated in (c), for clarity.) (d,e) Blown-up band structures corresponding to (b) and (c). Here, we focus on the [100] (X) and [001] (Z) axes because of their relevance for quantum dot formation, and note that [100] and [010] are equivalent. In (b) and (d), cubic symmetry also makes the X and Z points equivalent, and induces a degeneracy between the heavy (higher) and light (lower) hole bands at the Γ point. Except for this one point, the hole bands are all doubly-degenerate.
imposed on the strained Ge. We define the resulting compressive strain as \( \varepsilon(x) = (a(x) - a(0))/a(0) \). For a SiGe alloy, Vegard’s law gives \( \varepsilon(x) = -0.04x \), while Poisson’s ratio gives \( \nu = 0.31 = -[c(x) - c(0)]/[a(x) - a(0)] \), allowing \( c(x) \) to be determined. (See Fig. 1c.) In our simulations, we consider a range of compressive strains.

The band structures of unstrained and strained Ge are compared in Fig. 1b, c. In the unstrained case, the cubic symmetry ensures that the energy dispersion is identical for wavevectors in the plane of the quantum well \((k_x, k_y)\) and the growth direction \((k_z)\). (Here \( x \) refers to the \([100]\) axis, not the alloy composition.) In strained Ge, the \( X \) and \( Z \) points are inequivalent; both are shown in the figure. The most important band-structure properties for quantum dots can be read off at the energy band edges. Focusing on holes, we show blown-up views of the top of the valence band in Fig. 1d, e. Since the quantum dot wave functions are constructed mainly from Bloch states at the very top of the band, the essential physics is captured in the curvature of the band at the \( \Gamma \) point (proportional to the inverse effective mass), and the energy splitting that lifts the light and heavy-hole degeneracy.

We first consider the anisotropy of the effective mass, as induced by strain. Figure 2 shows our results for the in-plane \((m^x_z)\) and out-of-plane \((m^z_z)\) masses. The corresponding strain is also shown on the top axis. We find that the in-plane mass of the top two bands changes abruptly near \( x=0 \), corresponding to pure Ge. Remarkably, the top band now has the lightest mass over the experimental regime of interest. We therefore refrain from referring to heavy or light holes, adopting instead the terminology “first” (or “top”), and “second” bands. For \( m^x_z \), the top band retains the heaviest mass for all \( x \) considered here, and is a smooth function of the strain. Our results are in reasonable agreement with recent experiments that obtain a range of values, \( m^x_z/m_0 = 0.065 - 0.17 \). For the strain levels shown here, \( m^x_z \) appears to change abruptly, although smooth behavior is recovered for blown-up results in the range \( x=0 - 0.01 \).

Next, we consider energy splittings of the valence band at the \( \Gamma \) point. Additional \( k \cdot p \) calculations, described in Methods, provide insights into the DFT results for the valence band-edge splittings. This allows us to decouple SOC and strain effects, as shown in Fig. 3 where we separately sweep \( \varepsilon \) and the strain (represented by the split-off energy difference \( \Delta \) of bulk Ge) from zero to values consistent with \( x=0.25 \). By following the progression from a single sixfold-degenerate band (center panel) to three twofold-degenerate bands (outer panels), we see that SOC and strain effects are both needed to split the top bands. We note that the hybridization of the top bands occurs indirectly via strain-induced coupling to the split-off band. Since this mixing is weak, the predominant components of the total angular momentum in the top band, which defines the qubit, remains \( j=3/2 \) and \( m_j=\pm 3/2 \), as indicated in the figure. Therefore, flipping the qubit requires a total momentum change of \( 3\hbar \), which cannot be achieved via single-photon processes. This does not preclude using EDSR to implement gate operations however, as we discuss below.

For the \( k \cdot p \) calculations reported in Fig. 3, strain is introduced perturbatively, yielding results that are quantitatively inaccurate for high strain levels. In Fig. 4, we report more extensive results from self-consistent DFT calculations that do not suffer from this problem. For example, the energy difference between the top and split-off bands at \( x=0 \) is found to be \( \Delta=0.29 \text{ eV} \), which is quite close to the experimental value of 0.296 eV. (The latter was simply inserted as an input parameter into the \( k \cdot p \) theory.) For \( x=0.25 \), the DFT and \( k \cdot p \) methods differ somewhat, yielding a DFT result of \( \Delta=0.53 \text{ eV} \) (nearly 50% larger than the \( k \cdot p \) prediction).

The energies reported in Figs. 3 and 4 were obtained without including the quantum well confinement energies. This confinement energy is different for the top and second bands, due to differences in effective masses. We can estimate the latter corrections for a triangular potential well by assuming a uniform vertical electric field when \( z < 0 \), and an infinite barrier when \( z > 0 \). Here, we estimate the electric field as \( F_z \approx e\rho/\epsilon \) (the field required to accumulate a density of \( \rho = 4 \times 10^{11} \text{ cm}^{-2} \) in the 2D hole gas), and we linearly interpolate the dielectric constant in the SiGe \( x=\) barrier layer: \( \epsilon(x)=(16.2 - 4.5x)\epsilon_0 \). The corresponding potential energy is given by \( eF_z z \). For a quantum well of width 20 nm, the vertical extent of the wavefunction is less than the well width, allowing us to ignore the bottom edge of the well. We assume this to be true for all the relevant excited subbands as well. The triangular potential has known solutions giving a confinement energy of 2.34 \( E_0 \) for the first subband and 4.09 \( E_0 \) for the second subband, where \( E_0 = (\hbar^2 e^4 p^2)/(2m^x_z \epsilon^2) \) is
FIG. 3. Energy levels calculated at the Γ point, using the $k \cdot p$ method with no magnetic field, allowing us to artificially decouple the effects of SOC (represented by the split-off band gap $\Delta$ of bulk Ge) and strain ($\varepsilon$). The five panels show results when these two parameters are independently varied between zero and their final values, which correspond to a strained quantum well with $x=0.25$. Level degeneracies are indicated by color: black for six-fold, blue for four-fold, and red for two-fold. The point symmetry groups and corresponding irreducible representations for hole states are indicated in each case. The central panel represents the case with no SOC and no strain, in which the $p_x$, $p_y$, and $p_z$ orbitals and both spin states are degenerate. Moving to the right, the strain is increased without including SOC, yielding a four-fold degenerate band spanned by $p_x$ and $p_y$, and a two-fold degenerate $p_z$ band. Including SOC, the $p$ orbitals hybridize, creating states with different combinations of orbitals (represented now as tori) and spins, resulting in three doublets. Moving from the central panel to the left, including SOC but no strain yields a split-off, doubly-degenerate $j=1/2$ band and a four-fold degenerate $j=3/2$ band, as consistent with bulk, relaxed Ge at the Γ point. We represent these states in a classical picture as having orbital angular momenta and spins either parallel (upper quadruplet) or anti-parallel (lower doublet). The different values of orbital angular momenta are represented by the colors of the orbital (darker tones for lower $m_j$) and by the inclination of the green vectors with relation to the vertical direction. Including strain, the bands hybridize such that $j$ is no longer a good quantum number. Of course, the fully strained spectrum is the same as on the far right-hand side of the figure.

FIG. 4. Energy differences between the hole bands at the Γ point, computed using DFT, as a function of the Si concentration in the substrate, $x$. Upward blue triangle symbols refer to the splitting between the top of the valence band and the split-off band, while downward green triangles show the difference between the top band and the second highest band.

dot tunnel couplings (0-200 $\mu$eV), and exchange interactions (0-200 $\mu$eV), suggesting that confinement will not affect the energy ordering of the hole bands, nor compromise the energy separation of the top band. Vertical confinement does cause additional band mixing, underscoring the fact that $j$ and $m_j$ are not good quantum numbers and that the qubit is a hybrid of different total angular momenta. Lateral confinement, on the other hand, will lead to vanishingly small band mixing in the highly strained case.

Since the valence band has a large SOC, it is natural to explore single-qubit gate operations based on EDSR, similar to what was proposed for heavy holes in III-V semiconductors with Dresselhaus interactions. While bulk Dresselhaus terms are absent in group-IV materials, we argue here that in Ge, Rashba spin-orbit interaction terms stemming from the lack of spherical symmetry of the valence band can be used to achieve fast EDSR. The effective Hamiltonian for holes in the top band is $H_0 + H_{SO}$, where $H_0 = \hbar^2 (k_x^2 + k_y^2)/2m^*_v$ is a simplified model of the in-plane kinetic energy, and the Rashba spin-orbit Hamiltonian is the sum of two terms:

$$H_{SO} = i\alpha_{R2} (k_+^3 \sigma_- - k_-^3 \sigma_+) + i\alpha_{R3} (k_+ k_- \sigma_+ - k_- k_+ \sigma_-),$$

(1)

where $k_\pm = k_x \pm ik_y$, and $\sigma_\pm = \sigma_x \pm i\sigma_y$ are Pauli spin matrices. Here, the $\alpha_{R2}$ term stems from the spherically symmetric part of the Luttinger-Kohn Hamiltonian, while the $\alpha_{R3}$ term arises from its cubic-symmetric components. It is important to note that only the latter

the characteristic energy and $m^*_v$ depends on both $x$ and the band index, as per Fig. 2. For example when $x=0.25$, we obtain an effective energy separation of 140 meV between the lowest confined quantum well states at the top band and the second band. On the other hand, the energy difference between the lowest and first excited bound states in the quantum well, within the top band, is 27.7 meV, which therefore corresponds to the lowest leakage state for the qubit. Hence, we conclude that band and subband excitations of the qubit level are much larger than other relevant energy scales, including the temperature of the hole reservoirs (5-15 $\mu$eV), inter-
changes the photon number by ±1; therefore, this is the term we focus on for EDSR.

EDSR qubit gate operations can be implemented in a quantum dot by applying a microwave signal to one of the nearby top gates, yielding an ac electric field parallel to the quantum well, $E_{ac}$. In the presence of a perpendicular magnetic field $B_z$, the EDSR Hamiltonian for the qubit is given by

$$H_{EDSR} = \frac{g}{2} \mu_B B_z \sigma_z + e E_{ac} x \cos(\omega t) \sigma_x,$$  \hspace{1cm} (2)

where $x$ is the lateral position operator for the hole, and $\omega$ is the driving frequency. Denoting the orbital energy splitting as $\hbar \omega_0$, we derive in Supplementary Section 4 an expression for the EDSR Rabi frequency, $f_R \propto E_{ac} \alpha R_3$, under resonant driving conditions ($\hbar \omega = g \mu_B B_z$).

In Fig. 5, we evaluate $f_R$ as a function of the dot radius $a_0$ and the vertical electric field, $F_z$. In particular, for a typical field of 4.8 MV/m and dot radii in the range 30-60 nm, we obtain Rabi frequencies of order 0.1 GHz, corresponding to a 5 ns gate time for an $X_\pi$ gate.

**DISCUSSION**

In Table I we summarize the main results of this work for hole spins in Ge/SiGe quantum wells and compare them to other important candidates for quantum dot spin qubits including electrons in Si/SiGe quantum wells, holes in Ge/Si core shell nanowires, and electrons in GaAs/AlGaAs quantum wells. For Ge/SiGe, we assume alloy barriers with a Si concentration of $x=0.25$. While all four of these systems have favorable properties for qubits, the Ge/SiGe system appears especially well suited due to its full gamut: high mobility, well separated energy levels, all-electrical control for EDSR, low effective mass, and weak hyperfine interactions.

To conclude, we comment on the expected decoherence mechanisms affecting Ge hole spins. As mentioned above, hyperfine interactions are suppressed for hole spins due to the $p$-orbital character of the valence band and the low natural abundance (<8%) of Ge isotopes with nonzero nuclear spin, which can be further reduced by isotopic purification. On the other hand, charge noise is ubiquitous in semiconductor devices, particularly in their gate oxides. Although the poor quality of Ge oxides could exacerbate this problem, the simple inclusion of a Si capping layer would bring Ge/SiGe on par with other Si-based qubits. Similarly, phonon noise should be similar in Ge and Si-based devices; in both cases, phonon effects are much weaker than in GaAs charged spin qubits, due to the absence of piezoelectric phonons.

We therefore conclude that hole spins in Ge quantum wells should be relatively well protected from their environment, making them particularly strong candidates for quantum dot qubits.

**METHODS**

**Density Functional Theory**

Calculations were performed using the FP-LAPW method embodied in the WIEN2k code. In the WIEN2k implementation of the APW+lo method, the wavefunctions are expanded in spherical harmonics inside non-overlapping atomic spheres, with “muffin-tin” radii $R_{MT}$, and in-plane waves in the remaining space of the unit cell (the interstitial region). In the present calculations we assume $R_{MT}=0.95$ Å for Ge, and use 405 $k$-points in the irreducible wedge of the Brillouin zone. The maximum orbital angular momentum for the expansion of the wavefunctions in spherical harmonics inside the spheres is $l_{max}=10$. The plane wave expansion of the wavefunctions in the interstitial region extends to $K_{max}=9.0/R_{MT}=9.47$ Å$^{-1}$, and the charge density is Fourier expanded up to $G_{max}=12$ Ry. All these values were checked and found to yield numerical convergence. We use DFT to describe electron-electron interactions within the modified Becke-Johnson exchange potential.
LDA correlations, which gives accurate calculations of band gaps in semiconductors.

**k·p Theory**

The k·p calculations summarized in Fig. 3 were performed using a 6×6 Hamiltonian, which accounts for strain through the Bir-Pikus model. The deformation potentials used are obtained within a linear approximation for the dependence of the energy bands on strain. To determine the EDSR Rabi frequency, we adopt the reduced 4×4 Hamiltonian, describing just the top two valence bands, as detailed in Supplementary Section 1. For the quantum well confinement, we assume a circular parabolic potential, as described in Supplementary Section 3. The form and magnitude of the Rashba spin-orbit interaction is determined using the method described in ref.\(^1\) We take into account the Zeeman-split ground and first orbital excited states, which are coupled by the spin-orbit interaction, and eliminate the excited states via a Schrieffer-Wolff transformation.

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**SUPPLEMENTAL MATERIAL**

In this Supplemental Material we provide details of the theoretical treatment of electric dipole spin resonance (EDSR) in Ge quantum dots, as reported in the main text. The main parts of the derivations are only sketched here, since details of the spin-orbit calculations are given in ref.\(^1\) In Section S1, we describe the Hamiltonian of the top two valence bands. The vertical and lateral confinement of holes in quantum dots is described in Sections S2 and S3, respectively. The EDSR physics, including the Rabi frequency, is described in Section S4. Physically relevant limits on dot size and magnetic field are discussed briefly in Section S5.

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**S1. LUTTINGER-KOHN-PIKUS-BIR HAMILTONIAN**

The starting point for our EDSR calculation is the 4×4 Luttinger-Kohn-Pikus-Bir Hamiltonian \( H_{LKPB} \), which, in the basis of \( J_z \) eigenstates \( \{|\frac{1}{2}, \frac{1}{2}\}, |\frac{1}{2}, -\frac{1}{2}\}, |\frac{1}{2}, \frac{1}{2}\}, |\frac{1}{2}, -\frac{1}{2}\}\) is given by

\[
H_{LKPB}(k^2, k_z) = \begin{pmatrix}
P + Q & 0 & L & M \\
0 & P + Q & M^* & -L^* \\
L^* & M & P - Q & 0 \\
M^* & -L & 0 & P - Q
\end{pmatrix},
\]

(S1)

where

\[
P = P_k + P_z, \quad Q = Q_k + Q_z, \\
L = L_k + L_z, \quad M = M_k + M_z.
\]

(S2)

Here, the \( k \) subscripts denote the Luttinger-Kohn Hamiltonian matrix elements given by\(^5\)

\[
P_k = \frac{\mu}{2} \gamma_1 (k^2 + k_z^2), \quad Q_k = -\frac{\mu}{2} \gamma_2 (2k_x^2 - k_z^2),
\]

\[
L_k = -\sqrt{3} \mu \gamma_3 k_x k_z, \quad M_k = -\frac{\sqrt{3} \mu}{2} (\gamma k_x^2 + \delta k_z^2),
\]

(S3)

while the \( \varepsilon \) subscripts denote the Pikus-Bir strain matrix elements given by\(^5\)

\[
P_\varepsilon = -a_\varepsilon (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}), \\
Q_\varepsilon = -\frac{b_\varepsilon}{\sqrt{3}^2} (\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{xy}), \\
L_\varepsilon = \frac{\sqrt{3}^2}{2} b_\varepsilon (\varepsilon_{xx} - \varepsilon_{yy} - i\varepsilon_{xy}), \quad M_\varepsilon = d(\varepsilon_{xx} - i\varepsilon_{xy}).
\]

(S4)

where \( \mu = \hbar^2/m_0 \), \( m_0 \) is the bare electron mass, \( \gamma_1, \gamma_2, \) and \( \gamma_3 \) are the Luttinger parameters, \( \gamma = (\gamma_2 + \gamma_3)/2 \), \( \delta = (\gamma_2 - \gamma_3)/2 \), \( k^2 = k_x^2 + k_y^2 + k_z^2 \), \( k_\pm = k_x \pm ik_y \), and \( \{\varepsilon_{ij}\} \) are the strain tensor components, with \( \varepsilon_{xx} = \varepsilon_{yy} \) corresponding to \( \varepsilon (x) \) in the main text. In this work we consider cases where \( \varepsilon_{xx} \neq \varepsilon_{yy} \neq \varepsilon_{zz} \), \( \varepsilon_{xx} = -2(C_{12}/C_{11}) \varepsilon_{xy} \) and \( \varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0 \), so that \( L_\varepsilon = 0 \) and \( M_\varepsilon = 0 \). The resulting spin splits the fourfold-degenerate valence band into two twofold-degenerate bands. For a Si\(_{1-x}\)Ge\(_x\) quantum well with \( x = 0.25 \), we have \( \varepsilon_{xx} = \varepsilon_{yy} = -0.010 \), \( \varepsilon_{zz} = 0.009 \), yielding an energy splitting of 0.089 eV between the top two valence bands, which is somewhat smaller than the DFT results reported in Fig. 4 of the main text.
S2. TWO-DIMENSIONAL SUBBANDS

The hole confinement potential plays an important role in the calculation of Rashba spin-orbit coupling. As described in the main text, holes are confined vertically in a SiGe/Ge/SiGe heterostructure. Taking the z-axis as the quantum well growth direction, we model the quantum well confining potential \( V(z) \) as

\[
V(z) = eF_z z,
\]

where \( F_z \) is the average electric field across the quantum well.

We can include subband confinement effects into the hole energy dispersion by diagonalizing the matrix \( \hat{H} \), whose elements are given by

\[
\hat{H} = \langle \nu | H_{\text{LKPB}}(k^2, \hat{z}_z) + V(z) | \nu \rangle,
\]

where \( | \nu \rangle \) denotes the subband wave function in one of the top two valence bands and \( \hat{z}_z = -i \frac{\partial}{\partial z} \). Here, we adopt the modified infinite-square-well wave functions \( \phi_{\nu}(z) \) defined in ref. [56]

\[
\phi_{\nu}(z) = \sin \left( \frac{\pi}{d} \left( z + \frac{d}{2} \right) \right) \exp \left[ -b_{\nu} \left( \frac{z + 1/2}{d} \right) \right],
\]

where \( F_z \) has been subsumed into the variational parameter, \( b_{\nu} \), which is determined by minimizing equation (S6) at \( k=0 \), and \( d \) is the thickness of the quantum well. Throughout this work, we set \( d=20 \text{~nm} \).

Performing a Schrieffer-Wolff transformation on equation (S6) to eliminate the coupling between the top two valence bands, we obtain the effective Hamiltonian for the top band in a Ge heterostructure, \( H_0 + H_{\text{SO}} \), where \( H_0 \) and \( H_{\text{SO}} \) are defined in the main text.

S3. QUANTUM DOT SPECTRUM

We now also include a lateral confinement \( V(x,y) \). In the presence of an out-of-plane magnetic field \( B_z \) and an in-plane ac electric field of amplitude \( E_{\text{ac}} \), the total Hamiltonian for a circular dot is given by

\[
H = H_0 (k \rightarrow -i \nabla - eA/\hbar) + H_{\text{SO}} (k \rightarrow -i \nabla - eA/\hbar) + (g/2) \mu_B B_z \sigma_z + V(x,y) + eE_{\text{ac}} x \cos(\omega t) \sigma_x, \tag{S8}
\]

where \( A = (B_z/2)(-y, x, 0) \),

\[
V(x,y) = \frac{1}{2} m^*_z \omega_0 (x^2 + y^2), \tag{S9}
\]

\( \hbar \omega_0 \equiv \hbar^2/m^*_z a_0^2 \), \( a_0 \) is the quantum dot radius in the absence of a magnetic field, and the other parameters are described in the main text. Note that in the simulations described below and in the main text, we adopt effective mass parameters obtained from our DFT calculations.

FIG. S1. Calculated values of (a) the EDSR Rabi frequency \( f_R \) and (b) the EDSR gate time \( \tau_R=1/f_R \) as a function of dot radius \( a_0 \). Simulation parameters are \( B_z=0.06 \text{~T} \), \( E_{\text{ac}}=0.1 \text{~MV/m} \), \( d=20 \text{~nm} \), \( x=0.25 \) (yielding \( \xi_{zz}=\xi_{yy}=-1\% \) and \( \xi_{zz}=0.9\% \)), and \( F_z = 4.5 \text{~MV/m} \).

The eigenstates of \( H_0 \) are the Fock-Darwin states, with the ground state given by \( \phi_0 = 1/\sqrt{\alpha_0} \exp \left[ -(x^2+y^2)/2a_0^2 \right] \), and excited states given by \( \phi_{\pm 1} = \frac{2}{\alpha_0} \exp \left[ (x \pm iy) \right] \exp \left[ -(x^2+y^2)/2a_0^2 \right] \). We note that the \( \alpha_{R2} \) term in \( H_{\text{SO}} \) (see main text) cannot be used for EDSR because it connects \( n=0 \) to \( n=3 \), whereas the \( \alpha_{R3} \) term connects \( n=0 \) to \( n=1 \). Hence, we shall only consider the \( \alpha_{R3} \) term in what follows.

S4. EDSR HAMILTONIAN

We now, finally, evaluate the quantum dot Hamiltonian \( H \) in the 3D Fock-Darwin basis set. Performing a Schrieffer-Wolff transformation to eliminate the coupling to the excited states, we obtain the EDSR Rabi frequency

\[
f_R = \frac{-eE_{\text{ac}} \mu_B B_z}{2a_0^2 \hbar} \left[ \left( \frac{1}{\Delta_1} + \frac{1}{\Delta_2} \right) - \left( \frac{1}{\Delta_3} + \frac{1}{\Delta_4} \right) \right],
\]

where

\[
\begin{align*}
\Delta_1 & \equiv -\hbar \omega - \frac{1}{2} \hbar \omega_c, \\
\Delta_2 & \equiv -\hbar \omega - \frac{1}{2} \hbar \omega_c - g \mu_B B_z, \\
\Delta_3 & \equiv -\hbar \omega + \frac{1}{2} \hbar \omega_c + g \mu_B B_z, \\
\Delta_4 & \equiv -\hbar \omega + \frac{1}{2} \hbar \omega_c,
\end{align*}
\]

and we assume resonant driving with \( \omega = \sqrt{\omega_0^2 + \omega_c^2}/4 \) and \( \omega_c \equiv eB_z/m^*_z \). We note that \( f_R=0 \) when \( B_z=0 \), as readily verified by expanding equation (S10) in terms of \( B_z \). Hence, to leading order, \( f_R \) is linear in \( B_z \).

Figure S1 shows the dependence of the Rabi frequency \( f_R \) and the \( X_{2\pi} \) gate time \( \tau_R=1/f_R \) on the dot radius \( a_0 \). We see that increasing \( a_0 \) results in a shorter \( \tau_R \). However
we note that at sufficiently large $a_0$, our perturbative treatment eventually breaks down.

**S5. WELL DEFINED QUBITS**

Typical qubit readout and initialization involves tunneling between the quantum dot and a nearby hole reservoir. The qubit is well defined if this process is well resolved with respect to thermal broadening of the Fermi level in the reservoir. Since typical electron or hole temperatures are of order 50-100 mK, this corresponds to an energy broadening of $k_B T = 5$-$10 \text{ µeV}$. Characteristic energies in the dot must therefore be somewhat larger than 10 µeV to allow proper qubit operation. In Section S4, we considered large dots that decrease the Rabi frequency. There is clearly a limit to such expansion, as set by the dot energy level spacing $\hbar \omega_0$, yielding a maximum dot radius of $\sim 125$ nm.

By the same argument, the Zeeman energy, which defines the spin qubit, must also satisfy $g \mu_B B \gtrsim k_B T$. The Landé $g$-factor has previously been estimated for bulk Ge using $k \cdot p$ methods similar to our calculation of the spin-orbit coupling, obtaining $g \approx 20$, and the eventual requirement that $B \gtrsim 0.06 \text{ T}$, which is the field value used in our simulations in Fig. S1 and Fig. 5 of the main text.

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