Control of the Two-Electron Exchange Interaction in a Nanowire Double Quantum Dot

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The two-electron exchange coupling in a nanowire double quantum dot (DQD) is shown to possess Moriya’s anisotropic superexchange interaction under the influence of both the Rashba and Dresselhaus spin-orbit couplings (SOCs) and a Zeeman field. We reveal the controllability of the anisotropic exchange interaction via tuning the SOC and the direction of the external magnetic field. The exchange interaction can be transformed into an isotropic Heisenberg interaction, but the uniform magnetic field becomes an effective inhomogeneous field whose measurable inhomogeneity reflects the SOC strength. Moreover, the presence of the effective inhomogeneous field gives rise to an energy-level anticrossing in the low-energy spectrum of the DQD. By fitting the analytical expression for the energy gap to the experimental spectroscopic detections [S. Nadj-Perge et al, Phys. Rev. Lett. 108, 166801 (2012)], we obtain the complete features of the SOC in an InSb nanowire DQD.

Introduction.—Achieving an effective manipulation of the electron spins is of essential importance in the spin-based quantum information processing (see, e.g., [1, 2]). It has been shown that the double quantum dot (DQD) is experimentally convenient for implementing logical gate operations [3–6]. In this case, the two-spin manipulation can be based on the exchange interaction in a DQD [7, 8]. Generally, the intrinsic exchange interaction in a system results in a specific alignment of the spins. For example, the ferromagnetic exchange interaction leads to spin polarization [9], and the Dzyaloshinskii-Moriya (DM) exchange interaction induces the spin texture [10–12], which may give rise to skyrmion excitations in magnetic crystals [13, 14]. Therefore, it is of great importance to realize the tunability of the exchange interaction between electrons.

Owing to the spin-orbit coupling (SOC), the spin degree of freedom is correlated with the orbital degree of freedom for electrons [15–20]. In the absence of the SOC, the combined effects of the Coulomb interaction and the Pauli exclusion principle in the DQD give rise to the isotropic Heisenberg exchange interaction between electrons [7, 8]. The presence of the SOC in a semiconductor nanostructures mediates an anisotropic exchange interaction between electrons [21–24]. However, the anisotropic exchange interaction can be mapped via an unitary transformation onto an isotropic Heisenberg interaction in the absence of an external magnetic field [21, 25–28]. Thus, the SOC seems only to have trivial influences on the exchange interaction. However, as shown here, this is not the case when an external magnetic field is present.

In the recent decade, the quasi-one-dimensional nanostructure with SOC has aroused much attention. Specifically, it can implement fast spin manipulations via an electric field [29–32]. Also, it can act as an effective spin splitter between two spin reservoirs [33, 34] and offer a possible platform for searching the Majorana fermions in the superconductor-semiconductor hybrid systems [35–38]. In this Letter, we investigate the two-electron exchange interaction in a symmetric nanowire DQD in the presence of a strong SOC and an external Zeeman field. In the strong intradot Coulomb repulsion regime [39], the effective Hamiltonian describing the two electrons consists of a Zeeman term and a Moriya’s anisotropic superexchange interaction Hamiltonian [25]. This anisotropic exchange interaction depends on the SOC strength in the material and can be manipulated by regulating the direction of the external magnetic field. Furthermore, we show that when the anisotropic exchange interaction is transformed to an isotropic Heisenberg interaction, the uniform magnetic field becomes an effective inhomogeneous field, with the inhomogeneity depending on the SOC strength.

Under the effects of the SOC, there is an energy-level anticrossing, corresponding to the singlet-triplet splitting, in the low-energy part of the two-electron spectrum of the DQD [40–42], which is induced by the inhomogeneity of an effective magnetic field in a symmetric nanowire DQD. More interestingly, based on the effective magnetic field we obtain an analytical expression for the singlet-triplet splitting. By fitting the analytical formula to the experimental curve in Ref. 42, we extract the strength and direction of the SOC in an InSb nanowire DQD. The consistency between our theoretical results and the experimental analyses verifies our theory. Moreover, our new results reveal that the spectroscopy measurements in the presence of an external Zeeman field can identify separately the Rashba and Dresselhaus parts of the SOC. For the existing experiments, the latter is very small for symmetry reasons. However, one can use other crystals, with other symmetry directions, and then both terms may appear [43, 44]. In Ref. [44], the SOC was probed using a different measurement method (i.e., via measuring the spin-flipped tunneling) and the DQD was not in the strong Coulomb blockade limit. Also, as shown in Ref. [45], universal quantum logic gates can be implemented by tuning the anisotropic exchange coupling. Thus, the controllability of the anisotropic exchange interaction which we find is expected to have possible applications in quantum computing.
The effective Hamiltonian of the nanowire DQD.—As shown in Fig. 1(a), we consider a semiconductor nanowire DQD with a strong SOC. For simplicity, the two QDs defined by the local gate electrodes are identical. The electron occupancy of each QD can be adjusted by changing the voltages on the electrodes [46, 47]. Let the x-axis be the direction along the nanowire. The axial confinement of the DQD can then be modeled as a double-well potential, $V(x) = V_0[(x/d)^2 - 1]^2$, with $2d$ being the interdot distance [see Fig. 1(b)].

In the presence of an external magnetic field applied in the $x$–$y$ plane, $\mathbf{B} = B(\cos \varphi, \sin \varphi, 0) \equiv \hat{\mathbf{n}}$, the Hamiltonian of an electron confined in the DQD reads [48, 49]

$$H_0(x) = \frac{\hbar^2}{2m_e} + V(x) + \alpha_R \sigma_z p + \alpha_D \sigma_y p + \frac{g \mu_B B}{2} \sigma_y,$$  
(1)

where $m_e$ is the effective electron mass, $p = -i \hbar \partial / \partial x$, $\alpha_R$ is the Rashba (Dresselhaus) SOC strength, $g$ is the effective Landé factor, $\mu_B$ is the Bohr magneton, and $\sigma^z \equiv \hat{\sigma} \cdot \hat{\mathbf{n}}$, with the Pauli matrices $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Conveniently, by defining a new Pauli matrix $\sigma^y \equiv \hat{\sigma} \cdot \hat{\mathbf{a}}$, the SOI vector is $\hat{\mathbf{a}} = (\cos \theta, \sin \theta, 0)$ with the angle $\theta = \arccot(\alpha_D / \alpha_R)$, the SOC terms can be rewritten in a compact form, i.e.,

$$\alpha_R \sigma_z p + \alpha_D \sigma_y p + \alpha_D \sigma_y \sigma_z p = \alpha \sigma_y p,$$

where $\alpha = \sqrt{\alpha_D^2 + \alpha_R^2}$.

Usually, the electronic eigenstates of a single QD in the coexistence of the Zeeman and SOC terms are analytically obtained by perturbative approaches [17, 18]. In the context of strong SOC, it is optimal to perform an exact analysis of the SOC terms and treat the Zeeman term as a perturbation as long as the Zeeman splitting is much smaller than the orbital splitting, i.e., $g \mu_B B \ll \hbar \omega$, where $\omega = \sqrt{8V_0 / (d^2 m_e)}$. Meanwhile, in the case of small Zeeman splitting, only the lowest Zeeman sublevels in each dot are kept to facilitate the study of the low-energy dynamics of the electron, i.e., the Hund-Mulliken approximation. Let $|\Phi^+_j\rangle$ and $|\Phi^-_j\rangle$ ($j = 1, 2$) denote the two lowest Zeeman sublevels of each QD. In general, the localized eigenstates of the different dots are not orthogonal due to the nonzero overlaps among them. Nevertheless, based on these four localized eigenstates, orthonormal basis states $|\Phi^\ast_{jk}\rangle$ ($j = 1, 2$) can be constructed via the Schmidt orthogonalization [50].

Expanding the electron field operator in terms of the orthonormal basis states, $\Psi_e(x) = \sum_{j=1,2,n=\pm} g_j \beta_{jr} |\Phi_{jr}\rangle$, we can write the second-quantization form of the Hamiltonian $H_0(x)$ in Eq. (1) as $H_0 = \int dx \Psi_e^\ast(x) H_0(x) \Psi_e(x) = \sum_{j=1,2} \sum_{\sigma} \epsilon_{jr} \beta_{jr} \beta_{jr}^\ast + \sum_{\sigma} \beta_{jr}^\ast \beta_{jr} + \sum_{j=1,2} \sum_{\sigma} \epsilon_{j\sigma} \beta_{jr} \beta_{jr}^\ast + \sum_{\sigma} (2 \beta_{jr} \beta_{jr}^\ast + \epsilon_{j\sigma})$, where $\epsilon^\ast$ (the electron creation (annihilation) operator), $\epsilon_{jr}$ represents the single-electron energy in each QD, where $\beta_{jr}^\ast$ and $\beta_{jr}$ represent, respectively, the spin-conserved and spin-flipped tunnelings between the two QDs [see (50) for their explicit expressions].

When there are two electrons confined in the nanowire DQD, the second-quantization Hamiltonian describing the Coulomb interaction between the electrons is $H_c = \frac{1}{2} \int dx dx' \Psi_e^\ast(x) \Psi_e^\ast(x') \Psi_e(x') \Psi_e(x)$, where $e$ represents the charge of an electron, and $x$ ($x'$) denotes the coordinates of the two electrons along the nanowire axis. Keeping only the leading Coulomb-interaction terms, the Hamiltonian $H_K$ is reduced to $H_K = \frac{U}{2} \sum_{j=1,2} \sum_{\sigma\sigma'} n_{jr} n_{jr}^\ast + \frac{U'}{2} \sum_{j=1,2} \sum_{\sigma} n_{jr} n_{jr}^\ast$, where $n_{jr} = \beta_{jr}^\ast \beta_{jr}$ is the particle number operator, and $U$ ($U'$) denotes the intradot (interdot) Coulomb repulsion. The total Hamiltonian of the system is $H = H_0 + H_c$.

Here we focus on the strong intradot Coulomb repulsion regime, i.e., $U - U' \gg |t_{\sigma\sigma'}|, |t_{\sigma\sigma'}^\ast|$, which means that each QD can only be occupied by one electron. The effective Hamiltonian describing the two electrons can be simplified to [50]

$$H_{\text{eff}} = \Delta_\ast (S_{\pi}^+ + S_{\pi}^-) + J S_1 \cdot S_2 + \vec{D} \cdot \vec{S}_1 \times \vec{S}_2 + \vec{S}_1 \cdot \vec{I} \cdot \vec{S}_2,$$  
(2)

where $S_{\pi j} = \pm (1/2) \sum_{\sigma=\pm} \beta_{jr}^\ast \sigma_{jr} \sigma_{jr}^\ast$, $j = 1, 2$, are the pseudo-spin operators defined by the orthonormal basis, and $\Delta_\ast = g \mu_B Bf$ is the SOC-modified Zeeman splitting [18], with $f = \sqrt{\cos^2(\varphi - \theta) + e^{-2b^2/\sigma^2} \sin^2(\varphi - \theta)}$, $b = \hbar / (m_0 \omega)$ being the “Bohr” radius of the QDs, and $x_{\sigma0} = h / (m_0 \omega)$ the spin-orbit length. The SOC-dependent exchange coupling strengths in Eq. (2) are

$$J = J_0 \cos^2 (2d/x_{\sigma0}), \quad \vec{D} = J_0 \sin (4d/x_{\sigma0}) \vec{v}, \quad \vec{I} = J_0 \sin^2 (2d/x_{\sigma0}) (2\vec{v} \cdot \vec{v} - 1),$$

with the bare exchange coupling strength $J_0 = 4|t_{\pi\pi}^0|^2 / (U - U')$ and the unit vector defined as

$$\vec{v} = \mathbf{e}_z \cos \gamma - \mathbf{e}_x \sin \gamma,$$

where $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ represent the unit vectors in the three-dimensional space of pseudo-spins and $\gamma$ is given by

$$\gamma = \arccos [\cos(\varphi - \theta)/f].$$

(5)
Interestingly, the two-electron exchange interaction in Eq. (2) is shown to possess Moriya’s anisotropic superexchange interaction [25, 26]. Also, it should be noted that the specific form of the confinement potential between the two QDs does not alter the exchange-interaction structure in Eq. (2), but it affects the magnitude of $J_0$. In practice, for a realistic nanowire DQD, the value of $J_0$ can be detected experimentally (see below).

The role of the Zeeman term.—In the absence of the external magnetic field, the Hamiltonian describing an electron in the DQD reads $H'_0(x) = p^2/(2m_e) + V(x) + \alpha_e\sigma^y p + \alpha_{DQ} p^4$. This Hamiltonian possesses time-reversal-symmetry, i.e., $(i\sigma^y K)H'_0(i\sigma^y K)^{-1} = H'_0$, where $K$ is a complex conjugate operator, so there are degenerate states in this case (Kramers pairs). As in the above case of nonzero magnetic field, we can also obtain the effective Hamiltonian of the two electrons in the DQD. However, because of the Kramers degeneracy in the present case, the direction of the anisotropic exchange interaction is not determined, and can be chosen arbitrarily. Here we assume that the DM vector $\vec{v}$ takes the same form as Eq. (4) to facilitate the study, and the effective Hamiltonian of the two electrons is $H'_e = J_0\vec{S}_1 \cdot \vec{S}_2 + D \cdot \vec{S}_1 \times \vec{S}_2 + \sqrt{i} \vec{T} \cdot \vec{S}_2$, with the parameters given in Eq. (3).

Via a unitary transformation, the above anisotropic exchange Hamiltonian $H'_e$ can be mapped onto an isotropic Heisenberg Hamiltonian [21, 25]. $H'_e = J_0\vec{S}_1 \cdot \vec{S}_2$, where the spin operators $\vec{S}_1$ and $\vec{S}_2$ are obtained by rotating $\vec{S}_1$ and $\vec{S}_2$ around the DM vector $\vec{v}$ with angles $-\theta$ and $\theta$, respectively,

$$\begin{align*}
\vec{S}_1 &= \exp(i\theta \hat{\sigma}) \vec{S}_1 \exp(-i\theta \hat{\sigma}), \\
\vec{S}_2 &= \exp(-i\theta \hat{\sigma}) \vec{S}_2 \exp(i\theta \hat{\sigma}),
\end{align*}$$

(6)

where $\theta = 2d/x_{ao}$ and $\hat{\sigma} = (1/2)\hat{\sigma}_z$.

When an external Zeeman field is applied, time-reversal symmetry is broken and the two-electron Hamiltonian takes the form of Eq. (2). If we still perform the rotation for Eq. (2) as done above, the rotated Hamiltonian becomes $H_{eff} = \tilde{H}_0 + \Delta \tilde{H}$, with

$$\begin{align*}
\tilde{H}_0 &= J_0\vec{S}_1 \cdot \vec{S}_2 + \Delta \frac{B_1 + B_2}{2B} \cdot (\vec{S}_1 + \vec{S}_2), \\
\Delta \tilde{H} &= \Delta_{\gamma} \frac{B_1 - B_2}{2B} \cdot (\vec{S}_1 - \vec{S}_2).
\end{align*}$$

(7)

The uniform external magnetic field now becomes an effective \textit{inhomogeneous} magnetic field, with the local effective magnetic fields in the two QDs given by $B_1 = B(\beta_<, \beta_>, \beta_z)$ and $B_2 = B(\beta_-, \beta_-, \beta_z)$, where $\beta_\pm = (\cos \theta - 1) \sin \gamma \cos \gamma$, $\beta_\gamma = \sin \theta \sin \gamma$, and $\beta_z = \cos^2 \gamma + \sin^2 \gamma \cos \theta$. It is easy to find that the eigenstates of $\tilde{H}_0$ are the singlet and triplet states $|S_0\rangle = (1/\sqrt{2})(|\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle)$, $|T_0\rangle = (1/\sqrt{2})(|\uparrow \uparrow\rangle + |\downarrow \downarrow\rangle)$, $|T_-\rangle = |\downarrow \downarrow\rangle$, and $|T_+\rangle = |\uparrow \uparrow\rangle$, with the spin direction determined by the effective field direction $\vec{w} = (B_1 + B_2)/(2B)$: $\vec{w} \cdot \hat{\sigma}_z |T_\pm\rangle = \pm(\Delta_{\gamma} + \Delta_{\gamma}^*) |T_\pm\rangle$, with $\Delta_{\gamma} = \sqrt{1 - \beta_\gamma^2} \Delta_z$. However, $\Delta \tilde{H}$ can lead to the mixing of the triplet and singlet states.

Expanding the Hamiltonian $\tilde{H}_{eff}$ in the subspace spanned by $|T_+\rangle$, $|T_0\rangle$, $|T_-\rangle$ and $|S_0\rangle$, we obtain

$$\tilde{H}_{eff} = \begin{pmatrix}
\frac{\beta_z}{4} + \Delta_z & 0 & 0 & -i \frac{\gamma}{4} \beta_\gamma \Delta_z \\
0 & \frac{\beta_z}{4} & 0 & 0 \\
0 & 0 & \frac{\beta_z}{4} - \Delta_z & -i \frac{\gamma}{4} \beta_\gamma \Delta_z \\
i \frac{\gamma}{4} \beta_\gamma \Delta_z & 0 & i \frac{\gamma}{4} \beta_\gamma \Delta_z & -\frac{3\gamma}{4} \beta_\gamma \Delta_z
\end{pmatrix}. \tag{8}
$$

Below we show that the effect of the SOC can be reflected by the inhomogeneity of the effective magnetic field,

$$\Delta \tilde{B} \equiv \left| \frac{B_1 - B_2}{2B} \right| = |\beta_\gamma|. \tag{9}$$

When there is no difference between the two local effective fields, i.e., $\Delta \tilde{B} = 0$, obviously the eigenstates of the Hamiltonian $\tilde{H}_{eff}$ are the singlet and triplet states $|\Phi_1\rangle = |T_+\rangle$, $|\Phi_2\rangle = |T_0\rangle$, $|\Phi_3\rangle = |T_-\rangle$, and $|\Phi_4\rangle = |S_0\rangle$. Note, though, that there is an energy-level crossing between the singlet and triplet states, i.e., $|\Phi_3\rangle$ and $|\Phi_4\rangle$, at a critical magnetic field $B_0$, where the Zeeman splitting is $\Delta_z = J_0$ (see Fig. 2). However, in the case of two different local effective fields, i.e., $\Delta \tilde{B} \neq 0$, the energy-level crossing is avoided around the critical magnetic field and there is an anticrossing between these two levels (see Fig. 2). For a nanowire DQD with the spin-orbit length $x_{ao} \gg d$, the singlet-triplet splitting at the anticrossing point can be analytically written as $2\Delta_{SO}^{DD} = \sqrt{2} J_0 \Delta \tilde{B}$.

To fit the model with the real system, the parameters of the nanowire DQD used in the following calculations are taken from Ref. 42, with $2d = 50$ nm, $x_{ao} \approx 30$ nm, and $g \approx 32$. Experimentally, it was found that $B_0 = 13.3$ mT for the InSb nanowire DQD [42]. With the values of both $B_0$ and the detected $g$-factor, based on $\Delta_z = J_0$, we can obtain the bare exchange coupling strength $J_0 \approx 24.6$ $\mu$eV. The specific value of the energy splitting $\Delta_{SO}^{DD}$ depends on the magnetic-field direction and the SOC in the nanowire, as explained below.

![Energy spectrum of the nanowire DQD versus the Zeeman-field splitting $\Delta_z$ for different values of the inhomogeneity $\Delta \tilde{B}$.](image-url)
**Dependence on the magnetic-field direction.**—It is known that the magnetic-field direction plays an important role in observing the SOC effects in QDs \([44, 51–54]\). Below we study the influence of the magnetic-field direction on the two-electron exchange interaction in the nanowire DQD.

From the analytical expressions for the DM vector \(\hat{v}\) in Eq. (4) and the angle \(\gamma\) in Eq. (5), it is easy to find that the exchange anisotropy direction in the DQD can be manipulated by regulating the direction of the magnetic field. In Fig. 3(a), the components of the DM vector \(\hat{v}\) versus the angle \(\varphi - \theta\) are shown. For example, when the magnetic-field direction is perpendicular to the SOC direction, i.e., \(\varphi - \theta = \pi/2\) or \(3\pi/2\), the DM interaction points along the \(-e_x\), or \(e_x\), direction. If the two directions are parallel, i.e., \(\varphi - \theta = 0\) or \(\pi\), the DM interaction is along the \(e_z\) or \(-e_z\) direction. However, in this case, the SOC seems to have a trivial contribution to the anisotropic exchange interaction because the effective magnetic field is homogeneous (\(AB = 0\)). In short, we can continuously rotate the DM vector in the \(e_x - e_z\) plane by just varying the magnetic-field direction, as shown in Fig. 3(b).

Furthermore, based on the rotated \(\vec{H}_{\text{eff}}\) and for the SOC-dependent factor \(f \approx 1\), we obtain a specific relationship between \(\Delta^{\text{DD}}_{\text{SO}}\) and \(\varphi\) at the anticrossing point,

\[
\Delta^{\text{DD}}_{\text{SO}} = \frac{\sqrt{5}}{2} J_0 \sin(2d/x_{\text{so}}) \sin(\varphi - \theta). \tag{10}
\]

Interestingly, the cosine dependence of the energy gap \(\Delta^{\text{DD}}_{\text{SO}}\) on the magnetic-field direction angle \(\varphi\) has indeed been detected experimentally, cf. Fig. 4(i) in Ref. [42], i.e., \(\Delta^{\text{DD}}_{\text{SO}} = \Delta_{\text{SO}}(\cos(\varphi - \varphi_0))\), with the fitting parameters \(\Delta_{\text{SO}} \approx 5.2\ \text{meV}\) and \(\varphi_0 \approx 0.02\). By comparing the experimental fitting function with the analytical expression of \(\Delta^{\text{DD}}_{\text{SO}}\) in Eq. (10), we can obtain the formulae for the spin-orbit length \(x_{\text{so}}\) and the spin-orbit angle \(\theta\),

\[
x_{\text{so}} = \frac{2d}{\arcsin(\sqrt{2}\Delta_{\text{SO}}/J_0)}, \quad \theta = \frac{\pi}{2} + \varphi_0. \tag{11}
\]

Using the specific values of the fitting parameters and the bare exchange coupling strength, we find the magnitudes of the spin-orbit parameters, \(x_{\text{so}} = 165\ \text{nm}\), and \(\theta_{\text{ex}} = 0.506\pi\).

For the spin-orbit length in an InSb nanowire DQD, the discrepancy between the theoretical result \(x_{\text{so}} = 165\ \text{nm}\) and the experimental estimate in Ref. [42], \(l_{\text{so}} = 230\ \text{nm}\), mainly originates from the different quantitative methods. In the experiments, the spin-orbit length was quantified using an approximation method \([55]\), \((2d/l_{\text{so}}) = (\Delta_{\text{SO}}/J_0)\), and then from Eq. (11) the ratio of \(l_{\text{so}}\) to \(x_{\text{so}}\) can be identified as \(l_{\text{so}}/x_{\text{so}} \approx \sqrt{2}\).

Using the definition of the spin-orbit angle \(\theta \equiv \arccot(\alpha_{\text{ex}}/\alpha_{\text{ex}}\text{eff})\), in the absence of the Dresselhaus SOC, i.e., \(\theta = \pi/2\) or \(3\pi/2\), it follows from Eq. (10) that the magnitude of \(\Delta^{\text{DD}}_{\text{SO}}\) reaches its maximal (minimal) value when the magnetic field is parallel (perpendicular) to the nanowire axis. Obviously, it is the presence of a small Dresselhaus SOC that gives rise to \(\theta_{\text{ex}} = 0.506\pi\). The absolutely dominant role of the Rashba SOC, which would imply \(\theta_{\text{ex}} = 0.5\pi\), was predicted by the symmetry analysis of the nanowire DQD in Ref. [42]. Our fit, which does give a small Dresselhaus contribution, must result from deviations of the finite sample from the ideal crystal \([56]\). On the other hand, the consistency between our theoretical results (Fig. 4) and the experimental detections \([42]\) validates the controllability of the exchange interaction in the nanowire DQD by varying the direction of the external magnetic field.

**Conclusions.**—We have studied the two-electron anisotropic exchange interaction in a nanowire DQD under the influence of a strong SOC and a Zeeman field. As in the case of zero magnetic field, the exchange interaction can be mapped onto an isotropic Heisenberg interaction, but the uniform external magnetic field becomes then an effective inhomogeneous field and the inhomogeneity of this effective magnetic field reflects the SOC strength. Also, we reveal the controllability of the anisotropic exchange interaction by tuning the direction of the external magnetic field and obtain an analytical expression for the dependence of the singlet-triplet splitting on the magnetic-field direction, as detected in an InSb nanowire DQD \([42]\). Our theory provides a tool to explore the novel properties of the exchange interaction in a nanowire DQD under the strong SOC and also offers a complete method to detect the separate Rashba and Dresselhaus SOCs in the nanowire experimentally.
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[1] R. Hanson and D. D. Awschalom, Coherent manipulation of single spins in semiconductors, Nature (London) 453, 1043 (2008).
[2] R. Hanson, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, Spins in few-electron quantum dots, Rev. Mod. Phys. 79, 1217 (2007).
[3] J. R. Petta, A. C. Johnson, J. M. Taylor, E. A. Laird, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Coherent Manipulation of Coupled Electron Spins in Semiconductor Quantum Dots, Science 309, 2180 (2005).
[4] Z. Shi, C. B. Simmons, J. R. Prance, J. K. Gamble, T. S. Koh, Y.-P. Shim, X. Hu, D. E. Savage, M. G. Lagally, M. A. Eriksson, M. Friesen, and S. N. Coppersmith, Fast Hybrid Silicon Double-Quantum-Dot Qubit, Phys. Rev. Lett. 108, 140503 (2012).
[5] T. S. Koh, J. K. Gamble, M. Friesen, M. A. Eriksson, and S. N. Coppersmith, Pulse-Gated Quantum-Dot Double-Hybrid Qubit, Phys. Rev. Lett. 109, 250503 (2012).
[6] B. Bertrand, H. Flentje, S. Takada, M. Yamamoto, S. Tarucha, A. Ludwig, A. D. Wieck, C. Bäuerle, and T. Meunier, Quantum Manipulation of Two-Electron Spin States in Isolated Double Quantum Dots, Phys. Rev. Lett. 115, 096801 (2015).
[7] G. Burkard, D. Loss, and D. P. DiVincenzo, Coupled quantum dots as quantum gates, Phys. Rev. B 59, 2070 (1999).
[8] J. M. Taylor, J. R. Petta, A. C. Johnson, A. Yacoby, C. M. Marcus, and M. D. Lukin, Relaxation, dephasing, and quantum control of electron spins in double quantum dots, Phys. Rev. B 76, 035315 (2007).
[9] N. Atodiresei, J. Brede, P. Lazić, V. Caciuc, G. Hoffmann, R. Wiesendanger, and S. Blügel, Design of the Local Spin Polarization at the Organic-Ferromagnetic Interface, Phys. Rev. Lett. 105, 066601 (2010).
[10] P. Kim and J. H. Han, Orbital Dzyaloshinskii-Moriya exchange interaction, Phys. Rev. B 87, 205119 (2013).
[11] F. Freimuth, R. Bamler, Y. Mokrousov, and A. Rosch, Phase-space Berry phases in chiral magnets: Dzyaloshinskii-Moriya interaction and the charge of skyrmions, Phys. Rev. B 88, 214409 (2013).
[12] I. Dzyaloshinskii, A thermodynamic theory of “weak” ferromagnetism of antiferromagnetics, Phys. Chem. Solids 4, 241 (1958); T. Moriya, Anisotropic Superexchange Interaction and Weak Ferromagnetism, Phys. Rev. 120, 91 (1960).
[13] S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, and P. Böni, Skyrmion Lattice in a Chiral Magnet, Science 323, 915 (2009).
[14] X. Z. Yu, Y. Onose, N. Kanazawa, J. H. Park, J. H. Han, Y. Matsui, N. Nagaosa, and Y. Tokura, Real-space observation of a two-dimensional skyrmion crystal, Nature (London) 465, 901 (2010).
[15] Yu. A. Bychkov, and E. I. Rashba, Oscillatory effects and the magnetic susceptibility of carriers in inversion layers, J. Phys. C. 17, 6039 (1984); G. Dresselhaus, Spin-Orbit Coupling Effects in Zinc Blende Structures, Phys. Rev. 100, 580 (1955).
[16] S. Nadj-Perge, S. M. Frolov, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Spin-Orbit qubit in a semiconductor nanowire, Nature (London) 468, 1084 (2010).
[17] M. Trif, V. N. Golovach, and D. Loss, Spin dynamics in InAs nanowire quantum dots coupled to a transmission line, Phys. Rev. B 77, 045434 (2008).
[18] R. Li, J. Q. You, C. P. Sun, and F. Nori, Controlling a Nanowire Spin-Orbit Qubit via Electric-Dipole Spin Resonance, Phys. Rev. Lett. 111, 086805 (2013).
[19] Y. Ban, X. Chen, E. Ya Sherman, and J. G. Muga, Fast and Robust Spin Manipulation in a Quantum Dot by Electric Fields, Phys. Rev. Lett. 109, 206602 (2012).
[20] L. S. Levitov and E. I. Rashba, Dynamical spin-electric coupling in a quantum dot, Phys. Rev. B 67, 115324 (2003).
[21] T. A. Kaplan, Single-band Hubbard model with spin-orbit coupling, Z. Phys. B: Condensed Matter 49, 313 (1983).
[22] S. Gangadharaiah, J. Sun, and O. A. Starykh, Spin-Orbit-Mediated Anisotropic Spin Interaction in Interacting Electron Systems, Phys. Rev. Lett. 100, 156402 (2008).
[23] R. Li and J. Q. You, Anisotropic exchange coupling in a nanowire double quantum dot with strong spin-orbit coupling, Phys. Rev. B 90, 035303 (2014).
[24] F. Baruffa, P. Stano, and J. Fabian, Theory of Anisotropic Exchange in Laterally Coupled Quantum Dots, Phys. Rev. Lett. 104, 126401 (2010).
[25] L. Shekhtman, O. Entin-Wohlman, and A. Aharony, Moriya’s anisotropic superexchange interaction, frustration, and Dzyaloshinskys weak ferromagnetism, Phys. Rev. Lett. 69, 836 (1992).
[26] L. Shekhtman, A. Aharony, and O. Entin-Wohlman, Bond-dependent symmetric and antisymmetric superexchange interactions in La$_3$CuO$_4$, Phys. Rev. B 47, 174 (1993).
[27] K. V. Kavokin, Anisotropic exchange interaction of localized conduction-band electrons in semiconductors, Phys. Rev. B 64, 075305 (2001).
[28] H. Imamura, P. Bruno, and Y. Utsumi, Twisted exchange interaction between localized spins embedded in a one- or two-dimensional electron gas with Rashba spin-orbit coupling, Phys. Rev. B 69, 121303(R) (2004).
[29] J. W. G. van den Berg, S. Nadj-Perge, V. S. Priabiag, S. R. Plissard, E. P. A. M. Bakkers, S. M. Frolov, and L. P. Kouwenhoven, Fast Spin-Orbit Qubit in an Indium Antimonide Nanowire, Phys. Rev. Lett. 110, 066806 (2013).
[30] K. D. Petersson, L. W. McFaul, M. D. Schroer, M. Jung, J. M. Taylor, A. A. Houck, and J. R. Petta, Circuit quantum electrodynamics with a spin qubit, Nature (London) 490, 380 (2012).
[31] A. F. Sadreev and E. Ya. Sherman, Effect of gate-driven spin resonance on the conductance through a one-dimensional quantum wire, Phys. Rev. B 88, 115302 (2013).
[32] J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Gate Control of Spin-Orbit Interaction in an Inverted In$_{5/3}$Ga$_{47}$As/In$_{52.5}$Al$_{47.5}$As Heterostructure, Phys. Rev. Lett. 78, 1335 (1997).
[33] R. I. Shekhter, O. Entin-Wohlman, and A. Aharony, Suspended Nanowires as Mechanically Controlled Rashba Spin Splitters, Phys. Rev. Lett. 111, 176602 (2013); Mechanically controlled spin-selective transport, Phys. Rev. B 90, 045401 (2014).
[34] R. I. Shekhter, O. Entin-Wohlman, M. Jonson, and A. Aharony,
Rashba Splitting of Cooper Pairs, Phys. Rev. Lett 116, 217001 (2016).

[35] M. T. Deng, S. Vaitiekenas, E. B. Hansen, J. Danon, M. Leijinse, K. Flensberg, J. Nygård, P. Krostrup, and C. M. Marcus, Majorana bound states in a coupled quantum-dot hybrid-nanowire system, Science 354, 1557 (2016).

[36] S. Li, N. Kang, P. Caroff, and H. Q. Xu, 0-π phase transition in hybrid superconductor-InSb nanowire quantum dot devices, Phys. Rev. B 95, 014515 (2017).

[37] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Majorana Fermions and a Topological Phase Transition in Semiconductor-Superconductor Heterostructures, Phys. Rev. Lett. 105, 077001 (2010).

[38] J. D. Sau and S. Das Sarma, Realizing a robust practical Majorana chain in a quantum-dot-superconductor linear array, Nature Commun. 3, 964 (2012).

[39] W. G. van der Wiel, S. De Franceschi, J. M. Elzerman, T. Fujisawa, S. Tarucha, and L. P. Kouwenhoven, Electron transport through double quantum dots, Rev. Mod. Phys. 75, 1 (2002).

[40] A. Pfund, I. Shorubalko, K. Ensslin, and R. Leturcq, Spin-state mixing in InAs double quantum dots, Phys. Rev. B 76, 161308(R) (2007).

[41] C. Fasth, A. Fuhrer, M. T. Björk, and L. Samuelson, Tunable double quantum dots in InAs nanowires defined by local gate electrodes, Nano Lett. 5(7), 1487 (2005).

[42] J.-Y. Wang, S. Huang, Z. Lei, D. Pan, J. Zhao, and H. Q. Xu, Measurements of the spin-orbit interaction and Landé g factor in a pure-phase InAs nanowire double quantum dot in the Pauli spin-blockade regime, Appl. Phys. Lett. 109(5), 120 (2016).

[43] Z.-H. Liu, R. Li, X. Hu, and J. Q. You, Spin-orbit coupling and electric-dipole spin resonance in a nanowire double quantum dot, Sci. Rep. 8, 2302 (2018).

[44] C. Fasth, A. Fuhrer, L. Samuelson, V. N. Golovach, and D. Loss, Direct Measurement of the Spin-Orbit Interaction in a Two-Electron InAs Nanowire Quantum Dot, Phys. Rev. Lett. 98, 266801 (2007).

[45] S. Nadj-Perge, V. S. Pribyag, J. W. G. Berg, K. Zuo, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Spectroscopy of Spin-Orbit Quantum Bits in Indium Antimonide Nanowires, Phys. Rev. Lett. 108, 166801 (2012).

[46] J.-Y. Wang, G.-Y. Huang, S. Huang, J. Xue, D. Pan, J. Zhao, J. Zhao, and H. Q. Xu, Anisotropic Pauli spin-blockade effect and spin-orbit interaction field in an InAs nanowire double quantum dot, arXiv: 1803.07277.

[47] A. Hofmann, V. F. Maisi, T. Krähenmann, C. Reichl, W. Wegscheider, K. Ensslin, and T. Ihn, Anisotropy and Suppression of Spin-Orbit Interaction in a GaAs Double Quantum Dot, Phys. Rev. Lett. 119, 176807(2017).

[48] L.-A. Wu and D. A. Lidar, Universal quantum logic from Zee-
I. DERIVATION OF THE ORTHONORMAL BASIS STATES

First, we calculate the localized eigenstates that construct the orthonormal basis states. Near the minima of the axial confinement potential $V(x) = V_0[(x/d)^2 - 1]^2$, the confining potential can be expanded harmonically as $V_{1/2}(x) = (m_e\omega^2/2)(x \pm d)^2$, where $\omega = \sqrt{8V_0/(d^2m_e)}$. Then, the Hamiltonian in Eq. (1) of the main text becomes

$$H_{1/2}(x) = \frac{p^2}{2m_e} + \frac{m_e\omega^2}{2}(x \pm d)^2 + \alpha_R \sigma^y p + \alpha_D \sigma^x p + \frac{g\mu_B B}{2}\sigma^n. \quad \text{(S1)}$$

Based on the local harmonic potential, in the absence of the external magnetic field, the localized electron wavefunctions in a single nanowire dot can be solved analytically. In this case, the ground states of the electron confined in the left and right dots are degenerate:

$$|\Phi^{1/2}_1\rangle = \frac{1}{\sqrt{\pi x_0/2 m_e}} e^{-i(x \pm d)/x_0} e^{-(x \pm d)^2/(2x_0^2)} |\uparrow\rangle,$$

$$|\Phi^{1/2}_1\rangle = \frac{1}{\sqrt{\pi x_0/2 m_e}} e^{i(x \pm d)/x_0} e^{-(x \pm d)^2/(2x_0^2)} |\downarrow\rangle, \quad \text{(S2)}$$

where $x_0 = \hbar/(m_e \omega)$ is the spin-orbit length, $x_0 = \sqrt{8V_0/(d^2m_e)}$ is the characteristic length, while $|\uparrow\rangle$ and $|\downarrow\rangle$ are the two eigenstates of $\sigma^z$: $\sigma^z |\uparrow\rangle = |\uparrow\rangle$ and $\sigma^z |\downarrow\rangle = -|\downarrow\rangle$.

The degeneracy of the localized states is lifted in the presence of the external magnetic field. The Zeeman term can be treated as a perturbation in the calculations as long as $g\mu_B B \ll \hbar \omega$ [1, 2]. Thus, up to the lowest order, the localized wavefunctions can be calculated as

$$|\Phi^{1/2}_1\rangle = \cos(\gamma/2) |\Phi^{1/2}_1\rangle - i \sin(\gamma/2) |\Phi^{1/2}_1\rangle,$$

$$|\Phi^{-1/2}_1\rangle = -\sin(\gamma/2) |\Phi^{1/2}_1\rangle - i \cos(\gamma/2) |\Phi^{1/2}_1\rangle, \quad \text{(S3)}$$

where the angle $\gamma$ is given in Eq. (5) of the main text. The energy difference between the quasi-spin states $|\Phi^\uparrow_1\rangle$ and $|\Phi^\downarrow_1\rangle$ is modified by the spin-orbit coupling (SOC) effect,

$$\Delta_x = g\mu_B B f, \quad \text{(S4)}$$

with $f = \sqrt{\cos^2(\varphi - \theta) + e^{-2\xi_0^2/x_0^2} \sin^2(\varphi - \theta)}$ being a SOC-dependent factor [2]. Therefore, we have obtained four localized wavefunctions (two for the left dot and two for the right dot). These four localized states $|\Phi^\uparrow_1\rangle$ and $|\Phi^\downarrow_1\rangle$ are not orthogonal to each other, because

$$s_d = \langle \Phi^\uparrow_1 | \Phi^\downarrow_1 \rangle = \langle \Phi^\uparrow_1 | \Phi^\downarrow_1 \rangle^*$$

$$= e^{-d^2/x_0^2} \left[ \cos(2d/x_0) - i \sin(2d/x_0) \cos \gamma \right],$$

$$s_x = \langle \Phi^\uparrow_1 | \Phi^\downarrow_1 \rangle = \langle \Phi^\uparrow_1 | \Phi^\downarrow_1 \rangle^*$$

$$= -ie^{-d^2/x_0^2} \sin(2d/x_0) \sin \gamma, \quad \text{(S5)}$$

which are usually not identical to zero.

According to the Schmidt diagonalization, we define two orthonormal basis states

$$|\Phi_1\rangle = \frac{1}{\sqrt{\tau_1}} \left( |\Phi^\uparrow_1\rangle - \varsigma |\Phi^\downarrow_1\rangle \right),$$

$$|\Phi_2\rangle = \frac{1}{\sqrt{\tau_1}} \left( |\Phi^\uparrow_1\rangle - \varsigma^* |\Phi^\downarrow_1\rangle \right), \quad \text{(S6)}$$

where

$$\varsigma = \frac{1}{s_d} \left( 1 - \sqrt{1 - |s_d|^2} \right),$$

$$\tau_1 = 1 + |\varsigma|^2 - 2\text{Re}\{\varsigma s_d\}, \quad \text{(S7)}$$

with the explicit expressions of $s_d$ and $s_x$ given in Eq. (S5). In addition, we introduce two auxiliary states which are orthogonal to $|\Phi_1\rangle$ and $|\Phi_2\rangle$,

$$|\Phi_1^\uparrow\rangle = \frac{1}{\sqrt{\tau_2}} \left( |\Phi^\uparrow_1\rangle - \xi^* |\Phi^\downarrow_1\rangle - \xi_2 |\Phi^\downarrow_2\rangle \right),$$

$$|\Phi_2^\uparrow\rangle = \frac{1}{\sqrt{\tau_2}} \left( |\Phi^\uparrow_2\rangle - \xi^*_2 |\Phi^\downarrow_1\rangle - \xi^*_1 |\Phi^\downarrow_2\rangle \right), \quad \text{(S8)}$$

with $\xi^*_1 = -s_d^* \varsigma^*/\sqrt{\tau_1}$, $\xi^*_2 = s_d^* / \sqrt{\tau_1}$, and $\tau_2 = 1 - |\xi^*_1|^2 - |\xi^*_2|^2$. Note that there exists an overlap between $|\Phi_1\rangle$ and $|\Phi_2^\uparrow\rangle$. Nevertheless, we can derive the other two orthonormal basis states using these auxiliary states, just in the same way as for $|\Phi_1\rangle$ and $|\Phi_2\rangle$. In terms of the localized states, the other two orthonormal basis states can be written as

$$|\Phi_1\rangle = \frac{1}{\sqrt{\tau_2}} \left( |\Phi^\uparrow_1\rangle - \xi_1 |\Phi^\downarrow_1\rangle + \xi_2 |\Phi^\downarrow_2\rangle - \xi_3 |\Phi^\downarrow_3\rangle \right),$$
\[ |\Phi_{2\uparrow}\rangle = \frac{1}{\sqrt{\tau_2}} \left( |\Phi_{+}\rangle - \xi^*_{2} |\Phi_{-}\rangle \right), \quad (S9) \]

where

\[ \xi_1 = \frac{1}{\rho} \left( 1 - \sqrt{1 - |\rho|^2} \right), \]
\[ \xi_2 = \frac{1}{\tau_1} \left( -2\xi^* s_x + \xi_1 s_x (1 + |\xi|^2) \right), \]
\[ \xi_3 = \frac{1}{\tau_1} \left( 2\xi_1 s_x - s_x (1 + |\xi|^2) \right), \quad (S10) \]
\[ \tau_2 = \frac{\tau_1}{\tau_1 - s_y^2 (|\xi|^2 + 1)} \left( 1 + \xi_1^2 - 2\text{Re}[\xi_1 \rho] \right), \]

with \( \rho = (s_y^2 \tau_1 + 2s_y^2 s_x^2) / (\tau_1 - s_y^2 (|\xi|^2 + 1)) \).

II. THE SECOND-QUANTIZATION FORM OF THE SINGLE-ELECTRON HAMILTONIAN

Based on the orthonormal basis states, we can obtain the expansion of the electron field operator \( \Psi(x) = \sum_{j=1,2} c_j^\dagger \Phi_j \) and derive the second-quantization form of the single-electron Hamiltonian \( H_0(x) \) in Eq. (1) of the main text,

\[ H_0 = \int dx \Psi^\dagger(x) H_0(x) \Psi(x) = H_e + H_t, \quad (S11) \]

with

\[ H_e = \sum_{j=1,2} \sum_{\sigma} \varepsilon_{j\sigma} c_j^{\dagger} c_j, \]
\[ H_t = \sum_{\sigma} \left( t_{\sigma} c_1^{\dagger} c_{2\sigma} + t'_{\sigma} c_1^{\dagger} c_{2\sigma} + \text{h.c.} \right), \quad (S12) \]

where the parameters of the Hamiltonian can be calculated by using the orthonormal basis states,

\[ \varepsilon_{j\sigma} = \langle \Phi_{j\sigma} | H_0(x) | \Phi_{2\sigma} \rangle, \]
\[ t_{\sigma} = \langle \Phi_{1\sigma} | \Delta V_2(x) | \Phi_{2\sigma} \rangle, \]
\[ t'_{\sigma} = \langle \Phi_{1\sigma} | \Delta V_2(x) | \Phi_{2\sigma} \rangle. \quad (S13) \]

To facilitate the calculations, we write the Hamiltonian \( H_0(x) \) as \( H_0(x) = H_j(x) + \Delta V_j(x) \), with \( \Delta V_j \equiv V(x) - V_j(x) \) denoting the potential deviation from \( V_j(x) \). Then, based on the orthogonality of \( |\Phi_{j\sigma}\rangle \), the spin-dependent tunnelings can be calculated as

\[ t_{\sigma} = \langle \Phi_{1\sigma} | \Delta V_2(x) | \Phi_{2\sigma} \rangle, \]
\[ t'_{\sigma} = \langle \Phi_{1\sigma} | \Delta V_2(x) | \Phi_{2\sigma} \rangle. \quad (S14) \]

Up to the first order of \( \exp(-d^2/d\Omega^2) \), the spin-conserved and spin-flipped tunnelings can be explicitly written as

\[ t_{\psi} = t'_{\psi} = -3 \left( 1 + \frac{d^2}{d\omega^2} \right) V_0 s_d, \quad (S15) \]

The single-electron energy is given by

\[ \varepsilon_{j\psi} = \frac{3d^2}{4d^2} V_0 + \frac{1}{2} (\hbar \omega - \alpha^2) \pm \frac{1}{2} \gamma \mu_B B f. \quad (S16) \]

III. DERIVATION OF THE ANISOTROPIC EXCHANGE HAMILTONIAN

As given in the main text, when keeping only the leading Coulomb-interaction terms, the second-quantization Hamiltonian describing the Coulomb interaction between two electrons in a nanowire double quantum dot (DQD) reduces to

\[ H_e = \frac{U}{2} \sum_{j=1}^2 \sum_{\sigma} n_{j\sigma} n_{j\sigma}, \]
\[ H_t = U' \sum_{j\neq j'} \sum_{\sigma \sigma'} n_{j\sigma} n_{j'\sigma'}, \quad (S17) \]

where \( n_{j\sigma} = c_{j\sigma}^{\dagger} c_{j\sigma} \) is the particle number operator and \( U \) (\( U' \)) represents the intradot (interdot) Coulomb repulsion. When the single-electron Hamiltonian \( H_0 \) in Eq. (S11) is included, the total Hamiltonian of the two electrons in the nanowire DQD is

\[ H = H_0 + H_c. \quad (S18) \]

In the regime of strong intradot coulomb repulsion, i.e., \( U - U' \gg |t_{\sigma}|, |t'_{\sigma}| \), each QD can only be occupied by one electron, and the Hilbert space we investigate is restricted to the subspace defined by the projection operator

\[ P = \frac{1}{2} \sum_{j \neq j'} \sum_{\sigma \sigma'} n_{j\sigma} n_{j'\sigma'} (1 - n_{j\sigma})(1 - n_{j'\sigma'}). \quad (S19) \]

Then, the effective Hamiltonian reads

\[ H_{\text{eff}} = PHP - PHQ \frac{1}{QHQ - E} QHP, \quad (S20) \]

where the projection operator \( P \) is given in Eq. (S19) and \( Q = 1 - P \), while \( E \) is the ground-state energy of the nanowire DQD. In the strong repulsion regime, \( QHQ - E \) can be approximated as \( U - U' \). Based on the definition of the projection operator, the first term on the right side of Eq. (S20) can be rewritten as

\[ PHP = \left( \varepsilon_{1\uparrow} - \varepsilon_{1\downarrow} \right) S_{1\uparrow}^z + \left( \varepsilon_{2\uparrow} - \varepsilon_{2\downarrow} \right) S_{2\uparrow}^z + \frac{\varepsilon_{1\uparrow} + \varepsilon_{1\downarrow} + \varepsilon_{2\uparrow} + \varepsilon_{2\downarrow}}{2} + 4U', \quad (S21) \]

where \( S_{j\sigma} = (1/2) \sum_{\sigma' = \sigma \pm \hat{\rho}} c_{j\sigma}^{\dagger} \sigma_{\sigma'\sigma} c_{j\sigma'} \) are the pseudo-spin operators, and the explicit forms of \( \varepsilon_{j\sigma} \) \((j = 1, 2; \sigma = \uparrow, \downarrow)\) are given in Eq. (S16).

In a QD, the electron occupancy can only be affected by the tunneling Hamiltonian \( H_t \), so \( PHQ \) can be simplified as \( PH_i Q \). Similarly, we have \( QHP = QH_i P \) and
\( \mathbf{P} \mathbf{H} \mathbf{P} = 0 \). Thus, the second term on the right side of Eq. (S20) can be rewritten as \(-\mathbf{P} \mathbf{H}_t^2 \mathbf{P} / (U - U')\). Taking the explicit form of \( H_t \) into consideration, \( \mathbf{P} \mathbf{H}_t^2 \mathbf{P} \) can be expanded as

\[
\mathbf{P} \mathbf{H}_t^2 \mathbf{P} = \sum_{\sigma, \sigma'} \left[ |t_{\sigma \sigma'}|^2 (\mathbf{P} c_\sigma^\dagger c_{\sigma'} \mathbf{P} \mathbf{c}_{\sigma} \mathbf{c}_{\sigma'}^\dagger + \mathbf{P} c_{\sigma}^\dagger \mathbf{c}_{\sigma'} \mathbf{P} \mathbf{c}_{\sigma} \mathbf{c}_{\sigma'}^\dagger) + |t_{\sigma \sigma'}|^2 (\mathbf{P} c_\sigma^\dagger c_{\sigma'} \mathbf{P} \mathbf{c}_{\sigma} \mathbf{c}_{\sigma'}^\dagger + \mathbf{P} c_{\sigma}^\dagger \mathbf{c}_{\sigma'} \mathbf{P} \mathbf{c}_{\sigma} \mathbf{c}_{\sigma'}^\dagger) \right]
\]

Using the identity relations [3]

\[
c_{\sigma} c_{\sigma'}^\dagger = \frac{1}{2} \delta_{\sigma \sigma'} (n_{\sigma \uparrow} + n_{\sigma \downarrow}) + \mathbf{S}_j \cdot \mathbf{\hat{\sigma}}_{\sigma \sigma'},
\]

with \( \mathbf{\hat{\sigma}} = (\sigma_x, \sigma_y, \sigma_z) \), we can rewrite Eq. (S22) as

\[
\mathbf{P} \mathbf{H}_t^2 \mathbf{P} = 2|t|^2 \left( \frac{1}{2} - 2\mathbf{S}_1 \cdot \mathbf{S}_2 \right) + 2|t|^2 \left( \frac{1}{2} + 2\mathbf{S}_1 \cdot \mathbf{S}_2 - 4\mathbf{S}_1 \cdot \mathbf{S}_2 \right)
\]

\[
+ 4i(t_{\sigma \sigma'} - t_{\sigma' \sigma})(\mathbf{S}_1 \cdot \mathbf{S}_2 - \mathbf{S}_1 \cdot \mathbf{S}_2) + W_1 + W_2 + W_3,
\]

where

\[
W_1 = (t_{\sigma \sigma'} - t_{\sigma' \sigma}) t_{\sigma}^\dagger c_{\sigma} (c_{\sigma}^\dagger c_{\sigma} + c_{\sigma} c_{\sigma}^\dagger),
\]

\[
W_2 = (t_{\sigma \sigma'} - t_{\sigma' \sigma}) t_{\sigma}^\dagger c_{\sigma} (c_{\sigma}^\dagger c_{\sigma} + c_{\sigma} c_{\sigma}^\dagger),
\]

\[
W_3 = (t_{\sigma \sigma'} - t_{\sigma' \sigma}) t_{\sigma}^\dagger (c_{\sigma}^\dagger c_{\sigma} + c_{\sigma} c_{\sigma}^\dagger).
\]

With Eq. (S23), we have the following relationships:

\[
c_{\sigma \sigma'} c_{\sigma' \sigma} = S_z^\sigma + i S_y^\sigma, \quad c_{\sigma \sigma'} c_{\sigma' \sigma} = S_z^\sigma - i S_y^\sigma,
\]

\[
c_{\sigma \sigma'} c_{\sigma' \sigma} = \frac{1}{2} - S_z^\sigma, \quad c_{\sigma \sigma'} c_{\sigma' \sigma} = \frac{1}{2} + S_z^\sigma,
\]

which can be used to simplify the terms in Eq. (S25). Then, we obtain

\[
W_1 = -2(t_{\sigma \sigma'} - t_{\sigma' \sigma}) t_{\sigma}^\dagger (S_1^\sigma S_2^\sigma + i S_2^\sigma S_1^\sigma) + S_1^\sigma (S_2^\sigma - i S_2^\sigma)),
\]

\[
W_2 = -2(t_{\sigma \sigma'} - t_{\sigma' \sigma}) t_{\sigma}^\dagger (S_1^\sigma S_2^\sigma - i S_2^\sigma S_1^\sigma) + S_2^\sigma (S_1^\sigma + i S_2^\sigma)),
\]

\[
W_3 = -2(S_1 \cdot S_2 - S_1^\sigma S_2^\sigma)(t_{\sigma \sigma'} - t_{\sigma' \sigma}) (t_{\sigma \sigma'} - t_{\sigma' \sigma}^2) + 2i(S_1 \times S_2) \cdot (t_{\sigma \sigma'} - t_{\sigma' \sigma}^2).
\]

Because \( t_{\sigma \sigma'} = t_{\sigma' \sigma}^\dagger \) and \( t_{\sigma \sigma'}^\dagger = t_{\sigma' \sigma} \) [cf. Eq(S15)], \( W_1 + W_2 \) and \( W_3 \) can be finally simplified as

\[
W_1 + W_2 = 4(t_{\sigma \sigma'} - t_{\sigma' \sigma}) t_{\sigma}^\dagger S_1^\sigma S_2^\sigma + S_1^\sigma S_2^\sigma,
\]

\[
W_3 = -2(S_1 \cdot S_2 - S_1^\sigma S_2^\sigma)(t_{\sigma \sigma'} - t_{\sigma' \sigma} - 2|t_{\sigma \sigma'}|^2) + 2i(S_1 \times S_2) \cdot (t_{\sigma \sigma'} - t_{\sigma' \sigma}^2).
\]

By substituting Eqs. (S21), (S24) and (S28) into Eq. (S20), the effective Hamiltonian reads

\[
H_{\text{eff}} = \mathbf{P} \mathbf{H} \mathbf{P} - \mathbf{P} \mathbf{H} (Q \mathbf{H} Q - E)^{-1} \mathbf{Q} \mathbf{H} \mathbf{P}
\]

\[
= \Delta_x (S_1^\sigma + S_2^\sigma) + \frac{2 t_{\sigma \sigma'}^2 + 2 |t_{\sigma \sigma'}|^2}{U - U'} S_1 \cdot S_2 - 4i \frac{(t_{\sigma \sigma'} + t_{\sigma' \sigma}) t_{\sigma}^\dagger S_1 \cdot S_2}{U - U'} + 8 \frac{|t_{\sigma \sigma'}|^2}{U - U'} S_1^\sigma S_2^\sigma.
\]
When the explicit expressions in Eq. (S15) are used, we obtain the simplified form of the effective Hamiltonian

$$H_{\text{eff}} = \Delta_{\text{z}}(S_{1z}^2 + S_{2z}^2) + JS_{1} \cdot S_{2} + \hat{D} \cdot S_{1} \times S_{2} + S_{1} \hat{\Gamma} \cdot S_{2}, \quad (S30)$$

which is Eq. (2) in the main text and the exchange coupling strengths are given by

$$J = J_0 \cos^2 (2d/x_{\text{so}}), \quad \hat{D} = J_0 \sin (4d/x_{\text{so}}) \hat{v}, \quad \hat{\Gamma} = J_0 \sin^2 (2d/x_{\text{so}}) (2\hat{v} \hat{v} - 1), \quad (S31)$$

with the unit vector $\hat{v} = e_z \cos \gamma - e_x \sin \gamma$.

The exchange interaction consists of three parts: the antiferromagnetic $J$ term (i.e., the isotropic Heisenberg interaction), the Dzyaloshinskii-Moriya (DM) interaction ($\hat{D}$ term), and the symmetric tensor $\hat{\Gamma}$ term (a ferromagnetic term). It follows from Eq. (S31) that the strengths of the exchange couplings depend on the relative spin-orbit parameter $2d/x_{\text{so}}$. Due to the short-range character of the exchange interaction, i.e., $J_0 \propto \exp(-d^2/x_0^2)$, we only consider the case of varying the spin-orbit length $x_{\text{so}}$. In Fig. S1, the exchange interaction strengths, $J$, $|\hat{D}|$ and $\|\hat{\Gamma}\|$, as a function of the SOC strength, i.e., $1/x_{\text{so}}$, are shown. Experimentally, the Rashba SOC can be tuned by an external electric field [4, 5]. In the present study, we concentrate on the case of a strong SOC. The two-electron exchange interaction is dominated by the antiferromagnetic interaction in the weak SOC regime, but the DM interaction becomes important in the strong SOC regime. In the ultrastrong SOC regime, the ferromagnetic term becomes important as well. At present, most of the semiconductor nanowire DQDs are in the weak SOC regime, but the SOC in an InSb or InAs nanowire DQD nearly falls in the strong-coupling regime [6–8], which indicates the importance of the anisotropic DM interaction in the spin dynamics.

FIG. S1. (color online) Exchange-coupling strengths $J$, $|\hat{D}|$, and $\|\hat{\Gamma}\|$ (in units of $J_0$) as a function of the SOC strength, i.e., $1/x_{\text{so}}$. The solid (black) and dot-dashed (red) curves represent the variations of $J$ and $|\hat{D}|$, respectively.

[1] M. P. Nowak and B. Szafran, Spin-polarization anisotropy in a narrow spin-orbit-coupled nanowire quantum dot, Phys. Rev. B 87, 205436 (2013).
[2] R. Li, J. Q. You, C. P. Sun, and F. Nori, Controlling a Nanowire Spin-Orbit Qubit via Electric-Dipole Spin Resonance, Phys. Rev. Lett. 111, 086805 (2013).
[3] N. Nagaosa, Quantum Field Theory in Strongly Correlated Electronic Systems (Springer-Verlag, Berlin, 1999).
[4] D. Liang and X. Gao, Strong tuning of Rashba spin-orbit interaction in single InAs nanowires, Nano Lett. 12(6), 3263 (2012).
[5] J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Gate Control of Spin-Orbit Interaction in an InGaAs/InAlAs Heterostructure, Phys. Rev. Lett. 76, 1335 (1997).
[6] S. Nadj-Perge, S. M. Frolov, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Spin-Orbit qubit in a semiconductor nanowire, Nature (London) 468, 1084 (2010).
[7] K. D. Petersson, L. W. McFaul, M. D. Schroer, M. Jung, J. M. Taylor, A. A. Houck, and J. R. Petta, Circuit quantum electrodynamics with a spin qubit, Nature (London) 490, 380 (2012).
[8] S. Nadj-Perge, V. S. Pribiag, J. W. G. Berg, K. Zuo, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Spectroscopy of Spin-Orbit Quantum Bits in Indium Antimonide Nanowires, Phys. Rev. Lett. 108, 166801 (2012).