

Two-qubit gate with macroscopic singlet-triplet qubits in synthetic spin-one chains in InAsP quantum dot nanowires

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We present a theory of a two-qubit gate with macroscopic singlet-triplet (ST) qubits in synthetic spin-one chains in InAsP quantum dot nanowires. The macroscopic topologically protected singlet-triplet qubits are built with two spin-half Haldane quasiparticles. The Haldane quasiparticles are hosted by a synthetic spin-one chain realized in chains of InAsP quantum dots embedded in an InP nanowire, with four electrons each. The quantum dot nanowire is described by a Hubbard-Kanamori (HK) Hamiltonian derived from an interacting atomistic model. Using exact diagonalization and matrix product states tools, we demonstrate that the low-energy behavior of the HK Hamiltonian is effectively captured by an antiferromagnetic spin-one chain Hamiltonian. Next, we consider two macroscopic qubits and present a method for creating a tunable coupling between the two macroscopic qubits by inserting an intermediate control dot between the two chains. Finally, we propose and demonstrate two approaches for generating highly accurate two-ST qubit gates: (1) by controlling the length of each qubit and (2) by employing different background magnetic fields for the two qubits.

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I. INTRODUCTION

There is currently interest in developing robust qubits with long coherence times for quantum information processing on various platforms. Examples of platforms include superconducting qubits based on macroscopic quantum states [1–4], trapped ions [5–7], quantum photonics [8–11], and semiconductor spin qubits [12–23]. The semiconductor spin qubits approach is particularly attractive for its promise of seamless integration with electronic devices. An important objective of any design is to achieve robustness against quantum noise. To that end, some strategies include realizing topologically protected qubits [24,25], using well-isolated qubits [19,26], and encoding the qubit in composite structures [14,20,27–32]. A notable example of the latter is a qubit encoded in the singlet and triplet states of two electron spins in two gated lateral quantum dots [14,20,23,33], a design that is protected against collective dephasing [34,35]. Another related approach is to encode the qubit in two complex states of a spin cluster, thereby reducing the chance of a bit-flip error [31,32].

Following these ideas, it was proposed to encode the qubit in the low-energy macroscopic quantum states of a synthetic antiferromagnetic spin-one chain [30,36–42]. The low-energy spectrum of an antiferromagnetic spin-one chain consists of a singlet and a triplet separated by a gap from the rest of the spectrum [43], an example of a topological phase of matter [44]. The topologically protected low-energy spectrum can be understood in terms of two spin-half Haldane quasiparticles localized at the two ends of the chain. An array of InAs quantum dots in an InP nanowire with four electrons each was proposed to realize such a chain [30,36–39,41,45,46], with the two spin-half quasiparticles resulting in a singlet-triplet Haldane (STH) qubit. Such a STH qubit

combines the advantages of simple singlet-triplet qubits composed of two electrons in two dots and qubits encoded in clusters of spins (cluster qubits). Importantly, being encoded in topological macroscopic quantum states, unlike the cluster qubit proposal, the gap separating the qubit space from the rest of the spectrum does not go to zero as the system size increases. Instead, it approaches the Haldane gap in the thermodynamic limit, eliminating some of the size trade-offs present in the cluster qubit proposal.

Previously, we have demonstrated how to realize the Haldane qubit in different physical systems [30,36–39,41]. In this work, we demonstrate how to couple two STH qubits and generate two-qubit gates, opening the path toward universal quantum computation with STH qubits. To study various microscopic and effective spin Hamiltonians constructed throughout the paper, we used the exact diagonalization (ED) and matrix product states (MPS) tools [47,48] whenever the Hilbert space size was beyond the scope of ED.

The paper is organized as follows. We start in Sec. II with a description of a single STH qubit realized in a chain of InAs quantum dots in an InP nanowire, for which we construct a Hubbard-Kanamori Hamiltonian and an effective spin-one Hamiltonian. In this section, we also briefly discuss how to generate single-qubit gates using STH qubits. In Sec. III, we construct a microscopic model for on-demand coupling of two STH qubits by an intermediate gated control quantum dot. Here, we demonstrate that two coupled STH qubits, each made of two spin-half Haldane quasiparticles, behave akin to two electronic ST qubits. Then, in Sec. IV, we discuss how to generate two-qubit gates using our proposed coupling scheme. Finally, in Sec. V, we summarize the results of our work and discuss future directions.

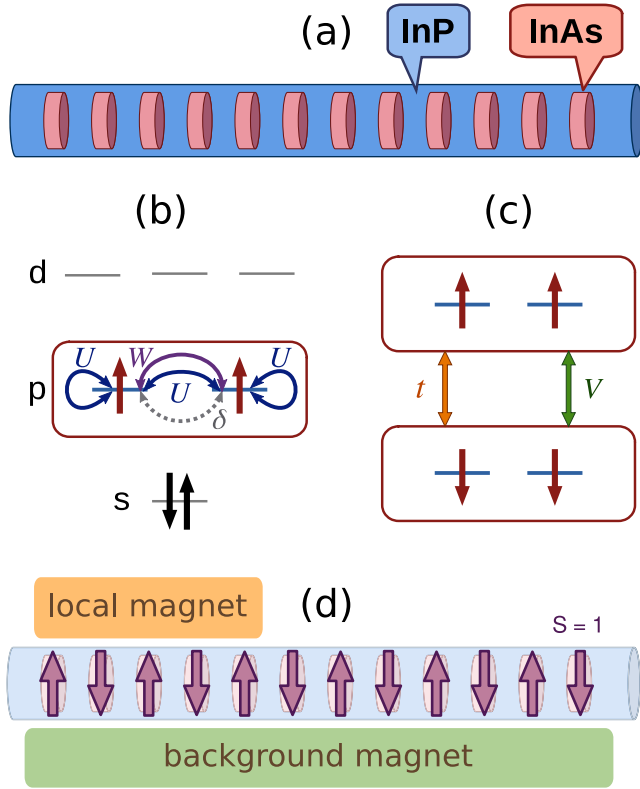


FIG. 1. (a) Schematic of a synthetic spin-one chain as an array of InAs quantum dots in an InP nanowire. (b) The conduction band levels of each dot occupied by four electrons. Our model focuses on the two electrons within the half-filled p shell, as described by Eq. (1). (c) Schematic illustration of the p shells of two adjacent dots as described by Eq. (2). (d) In the low-energy limit, the system behaves like an antiferromagnetic chain of spin-ones, which can be utilized as a macroscopic singlet-triplet qubit. The background magnetic field moves undesired triplets with $S^z = \pm 1$ away from the $S^z = 0$ computational basis, and the controllable local magnet is used to generate single-qubit gates.

II. SINGLET-TRIPLET QUBIT IN SYNTHETIC SPIN-ONE CHAIN

Let us start by describing the synthesis of an effective spin-one chain in an InAsP quantum dot nanowire system. We consider an InP nanowire hosting a sequence of InAsP quantum dots. Experimental fabrication of such quantum dot nanowires has been successfully demonstrated, with theoretical investigations extending to atomic-scale details [39,40]. Figure 1(a) shows a schematic view of such a quantum dot nanowire.

A. Microscopic model of synthetic spin-one chain

The atomistic microscopic model of a InAsP quantum dot has already been developed [39]. Despite hexagonal cross section and disorder due to the low concentration of phosphorus atoms, the electronic states are grouped into shells similar to shells of a two-dimensional (2D) harmonic oscillator. In Fig. 1(b), the conduction band shells of a dot are schematically depicted. As the illustration shows, we populate each dot with

four electrons, where two occupy the s shell and the subsequent two occupy the p shell. We focus on these half-filled p -shell orbitals, which we call $p_{\pm}$, to construct a microscopic electronic Hamiltonian for the dot. As we proceed to consider two such quantum dot nanowires, we designate the Hamiltonian describing dot i in nanowire A as $H_{A,i}$, given by

$$H_{A,i} = U \left[(n_{A,i,+} - 1)(n_{A,i,-} - 1) + \sum_{\alpha=\pm} n_{A,i,\alpha,\uparrow} n_{A,i,\alpha,\downarrow} \right] - 2W \left(\mathbf{s}_{A,i,+} \cdot \mathbf{s}_{A,i,-} + \frac{1}{4} n_{A,i,+} n_{A,i,-} \right) + \frac{\delta}{2} \sum_{\sigma} c_{A,i,+, \sigma}^{\dagger} c_{A,i,-, \sigma} + c_{A,i,-, \sigma}^{\dagger} c_{A,i,+, \sigma}, \quad (1)$$

where U denotes the Hubbard repulsion on each orbital, which has the same value as the direct Coulomb interaction between electrons on the two orbitals [39], W is the Coulomb exchange interaction between the electrons on two orbitals, and δ represents the splitting between the two orbitals induced by disorder and deviation from cylindrical symmetry. Notice that there is no spin-orbit term involved, as it is negligible from microscopic calculations [39]. All these terms are graphically depicted in Fig. 1(b). Note that there is no on-site energy for the orbitals, indicating that the energy is measured from the $p_{\pm}$ levels. In writing Eq. (1), we use $n_{A,i,\alpha,\sigma} = c_{A,i,\alpha,\sigma}^{\dagger} c_{A,i,\alpha,\sigma}$ and $n_{A,i,\alpha} = n_{A,i,\alpha,\uparrow} + n_{A,i,\alpha,\downarrow}$, where $c_{A,i,\alpha,\sigma}$ denotes the annihilation operator of spin σ for orbital α at site i of the nanowire A . The spin operators are defined as $s_{A,i,\alpha}^{+} = c_{A,i,\alpha,\uparrow}^{\dagger} c_{A,i,\alpha,\downarrow}$, $s_{A,i,\alpha}^{-} = c_{A,i,\alpha,\downarrow}^{\dagger} c_{A,i,\alpha,\uparrow}$, and $s_{A,i,\alpha}^z = \frac{1}{2}(n_{A,i,\alpha,\uparrow} - n_{A,i,\alpha,\downarrow})$, which then are used to build $\mathbf{s}_{A,i,+} \cdot \mathbf{s}_{A,i,-} = s_{A,i,+}^z s_{A,i,-}^z + \frac{1}{2}(s_{A,i,+}^{+} s_{A,i,-}^{-} + s_{A,i,-}^{+} s_{A,i,+}^{-})$. The Hubbard repulsion U prevents double occupation of the orbitals, while the exchange W aligns the spin of the two electrons on a p shell. Thus, unless the disorder δ is very large, the ground state of an isolated dot is a triplet. Consequently, in the low-energy limit, each dot can be effectively deemed as a spin-one object.

Next, we turn to the Hamiltonian describing the coupling between the p shells of two adjacent dots in the nanowire A ,

$$H_{A,i,i+1} = t \sum_{\alpha,\sigma} (c_{A,i,\alpha,\sigma}^{\dagger} c_{A,i+1,\alpha,\sigma} + \text{H.c.}) + V(n_{A,i} - 2)(n_{A,i+1} - 2), \quad (2)$$

where t is the hopping energy between the same orbitals and the same spins on neighboring dots, and V is direct interdot Coulomb energy. Here we neglect the possible hopping between different orbitals and different spins, due to the symmetry of the wire, and the negligible spin-orbit interaction. We only keep direct Coulomb matrix elements as the other allowed Coulomb matrix elements are negligibly small [39]. In writing Eq. (2), we also used the compact notation $n_{A,i} = n_{A,i,+} + n_{A,i,-}$. These terms are graphically shown between the two dots in Fig. 1(c).

Now, in the spirit of the Hubbard model, one would anticipate that the interdot hopping combined with intradot repulsion results in an effective antiferromagnetic coupling between the dots. In fact, second-order perturbation theory shows that for weak interdot coupling, the low-energy

TABLE I. Parameters of the Hubbard-Kanamori (HK) Hamiltonian in Eq. (1) and Eq. (2), based on a previous atomistic study [39].

	Parameters	Values (meV)
In	U	16
each	W	2.5
dot	δ	0.85
Between	t	0.75
dots	V	7.7

behavior of two dots is the same as two spin-one objects, coupled antiferromagnetically by an exchange matrix element given by $J_{\text{eff}} = 2t^2/(U + W - V)$ [49].

Combining the intradot given by Eq. (1) and the interdot Hamiltonians given by Eq. (2), for a chain, we obtain a Hubbard-Kanamori (HK) electronic Hamiltonian that describes a quantum dot nanowire of length N as

$$H_A = \sum_{i=1}^N H_{A,i} + \sum_{i=1}^{N-1} H_{A,i,i+1}. \quad (3)$$

Following the above discussion and results of exact diagonalization of a two quantum dot system with $N = 8$ electrons, we find that in the limit of small interdot coupling, the HK Hamiltonian behaves like an antiferromagnetic spin-one chain [41].

B. Spin-one chain: A topological singlet-triplet qubit

Now, we proceed to quantitatively confirm that in the limit of weak interdot coupling, the HK Hamiltonian behaves like an antiferromagnetic spin-one chain described by a Heisenberg Hamiltonian,

$$\tilde{H}_A = J_{\text{eff}} \sum_{i=1}^{N-1} \mathbf{S}_{A,i} \cdot \mathbf{S}_{A,i+1}. \quad (4)$$

For this demonstration, we employ the HK parameters listed in Table I, derived from an atomistic study [39]. To compare the low-energy spectra of the HK and Heisenberg Hamiltonians, we pick chains of even length whose ground state is always a singlet. In Fig. 2, we present the results of our density matrix renormalization group (DMRG) computation. Figure 2(a) presents the low-energy spectra of the HK and Heisenberg Hamiltonians, measured from the ground state, for increasing chain length N . As anticipated for an antiferromagnetic spin-one chain, the low-energy spectrum includes a singlet, a triplet, and a quintuplet. Haldane showed [43] that this system possesses a topological gap. In particular, in the thermodynamic limit, the spin-one antiferromagnetic chain features a fourfold degenerate ground state comprising a singlet and three triplets, separated by a topological gap from the rest of the spectrum. Figure 2(a) shows the exponential drop of the singlet-triplet gap Δ with chain length, while the topological Haldane gap Γ converges to a constant value. The spectrum of the HK closely mirrors that of the Heisenberg Hamiltonian, providing quantitative evidence that there exists a set of parameters for which the HK Hamiltonian behaves akin to a chain of spin-ones coupled by

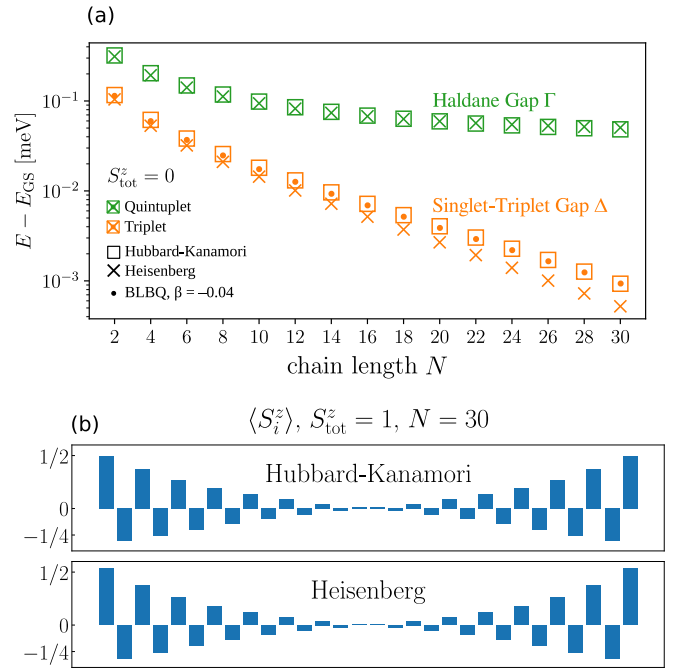


FIG. 2. (a) The low-energy spectra of HK Hamiltonian of Eq. (3) with the parameters of Table I, and an effective spin-one Heisenberg Hamiltonian with $J_{\text{eff}} = 2t^2/(U + W - V) \approx 0.1$ meV. (b) The expectation value of S_i^z operator at each site i , over the lowest triplet state $|T_+\rangle$ with $S_{\text{tot}}^z = 1$, showing the spin-half Haldane quasiparticles, both for HK and Heisenberg chains of length $N = 30$.

an effective antiferromagnetic exchange J_{eff} . In Appendix A, we demonstrate that these features are also robust against spatial fluctuations.

A bilinear biquadratic (BLBQ) spin Hamiltonian that includes a biquadratic correction $\beta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ —the next term in perturbation theory that conserves total spin—allows us to fit the HK Hamiltonian spectrum even better. In Fig. 2(a), we show that a BLBQ Hamiltonian with a very small $\beta = -0.04$ almost perfectly fits the low-energy spectrum of the HK Hamiltonian. Another possibility to improve the fit is to include spin-exchange interaction with the next-nearest neighbor [50]. Since the needed correction is very small ($|\beta| \ll 1$), we proceed with the Heisenberg model of the HK Hamiltonian for the rest of the paper. The gapped spectrum suggests that one can utilize the isolated singlet and triplet states of a Haldane chain to construct a robust macroscopic singlet-triplet qubit [36]. We refer to such a qubit as a singlet-triplet Haldane (STH) qubit. Similar to a regular ST qubit [20], one can envision an STH qubit as comprising two spin-half quasiparticles. The two spin-half quasiparticles are the emerging fractional particles of the Haldane phase on the two ends of the chain, where the topological phase has an interface with the trivial phase outside the chain [51]. As a way of visualizing these spin-half quasiparticles for a chain of length $N = 30$, in Fig. 2(b) we show the expectation value of S_i^z , i.e., the z component of the spin operator on site i , over the state $|T_+\rangle$, which is the lowest-energy state with $S_{\text{tot}}^z = 1$. The spin-half objects are evident at the two ends of the chain for both the HK and Heisenberg Hamiltonian cases. The nearly identical behavior of $\langle S_i^z \rangle$ in both cases provides further evidence of how closely

the HK Hamiltonian mimics a spin-one Heisenberg chain in the low-energy regime.

C. Generating single-qubit gates

Before moving on to discuss how we couple two STH qubits to generate two-qubit gates, let us briefly describe how one can generate single-qubit gates. Previously, it was shown that single-qubit operations on a STH qubit can be achieved by applying a local magnetic field on the first site of the chain [36]. Here, we demonstrate that any field that does not cover the entire chain is suitable for performing single-qubit operations, thereby relaxing the need for a spatially highly resolved and controllable magnetic field, which is also the main advantage of the cluster qubit proposal [31,32].

Consider the Heisenberg model of the qubit A, now with two sets of magnetic fields as depicted in Fig. 1(d),

$$\tilde{H}_A = J_{\text{eff}} \sum_{i=1}^{N-1} \mathbf{S}_{A,i} \cdot \mathbf{S}_{A,i+1} + b_A \sum_{i=1}^{N_b} S_{A,i}^z + B_A S_{A,\text{tot}}^z, \quad (5)$$

where b_A is a dynamic local magnetic field covering the first N_b sites, and B_A is a uniform background magnetic field covering the entire chain. The computational basis of the STH qubit, much like regular ST qubits, consists of the singlet state $|S\rangle$, which we take to be $|0\rangle$, and the triplet state $|T_0\rangle$ with $S_{\text{tot}}^z = 0$, taken to be $|1\rangle$. These states are separated from the rest of the spectrum by the Haldane gap Γ , which is of the order of $0.4J_{\text{eff}}$. Meanwhile, the gap between them, Δ , diminishes exponentially with the chain length [see Fig. 2(a)]. Turning on the local magnetic field b_A breaks the conservation of total spin S_{tot}^z , causing a mixing between $|S\rangle$ and $|T_0\rangle$, allowing for the generation of single-qubit gates. As in two-electron ST qubits, the uniform background magnetic field B_A serves to push the other two low-energy triplet states $|T_{\pm}\rangle$ away from the computational basis [20], thereby reducing the errors stemming from spin-flipping noises. As we discuss below, the background magnetic field plays a more substantial role in implementing two-qubit operations. Note that since the local field operation still conserves S_{tot}^z , it does not cause leakage to $|T_{\pm}\rangle$ even in the absence of the uniform background magnetic field.

Since the local field breaks S_{tot}^z conservation, it also mixes the computational basis with every other state in the $S_{\text{tot}}^z = 0$ subspace. But as long as $b_A \ll \Gamma$, such leakages remain negligible, as all other states are separated from the computational basis by Γ .

In Fig. 3, we demonstrate the generation of a HADAMARD gate using a STH qubit of length $N = 10$, where the local field is applied to the first $N_b = 5$ sites. For $N = 10$, the singlet-triplet (ST) gap is $\Delta \approx 0.14J_{\text{eff}}$, the Haldane gap is $\Gamma \approx 0.76J_{\text{eff}}$, and the matrix element of the local magnetic field between the singlet and the triplet is $M_b \approx 0.67b_A$. Choosing b_A such that $M_b = \Delta/2$, one can generate a HADAMARD gate by applying the local field for $t_H = \pi/\sqrt{2}\Delta$ duration [52]. To generate Fig. 3, we keep the first 100 states of $\tilde{H}_A$ ($b_A = 0$) to form a new basis for a reduced Hilbert space. Subsequently, we construct the Hamiltonian including the local field. The time evolution is then computed using $e^{-i\tilde{H}_A}$ in the reduced Hilbert space. In the top panel of Fig. 3, solid (dashed) curves

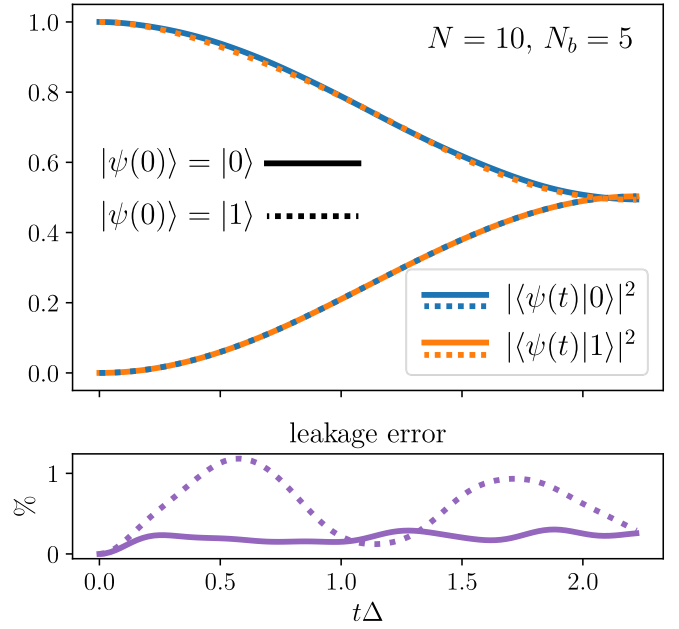


FIG. 3. Implementation of the HADAMARD gate using an STH qubit with a length of $N = 10$, where the local magnetic field b_A is applied to the first $N_b = 5$ sites. The magnetic field is selected such that $M_b = \Delta/2$, where $M_b \approx 0.67b_A$ is the matrix element of the local field between the singlet and the triplet. The solid (dashed) curves illustrate the qubit's evolution when initialized in state $|0\rangle$ ($|1\rangle$). For each scenario, the time evolution of the square of the projections of the chain's state onto the computational basis $|\langle\psi(t)|i = 0, 1\rangle|^2$ is plotted, along with (bottom) the leakage out of the computational basis, as indicated by Eq. (6). The time on the x axis is in units of $1/\Delta$.

show the evolution of the qubit initialized in the $|0\rangle$ ($|1\rangle$) state. It is visible that in both cases, at the end of the operation, the system is in a nearly equal superposition of the $|0\rangle$ and $|1\rangle$ states, as expected for a HADAMARD gate. Note that when the qubit is initialized in $|1\rangle$, there exists a π phase difference between the two projections of $|\psi(t)\rangle$, which is not visible in the plot, as we plot the square of the projections for visual clarity.

As mentioned, there is a small probability of the system leaking out of the computational basis. The leakage is quantified by the projection of the chain's state $|\psi(t)\rangle$ on states outside the computational basis,

$$\epsilon_1 = 1 - \sum_{i=0,1} |\langle\psi(t)|i\rangle|^2. \quad (6)$$

As the bottom panel of Fig. 3 shows, the leakage is well below 1% when the qubit is initialized in the state $|0\rangle$, and it reaches a maximum of approximately 1% when initialized in the state $|1\rangle$. This can be attributed to the smaller separation of the triplet state ($|1\rangle$) from the rest of the spectrum above the Haldane gap.

Notice that to implement the HADAMARD gate, we only needed to control the local magnetic field. Furthermore, with a fixed Δ , we can also generate any phase gate by setting $b_A = 0$. This implies that we can generate all the single-qubit gates by solely controlling the local magnetic field [52].

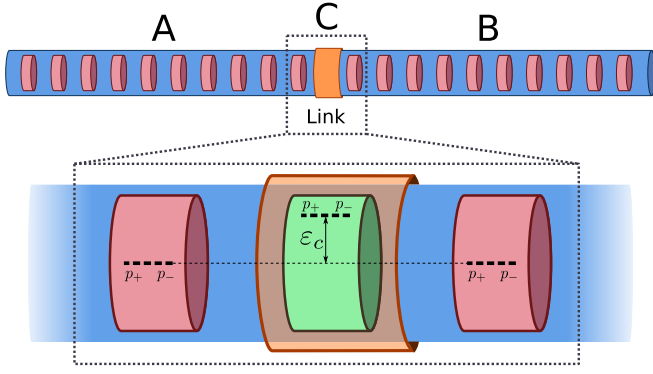


FIG. 4. Schematic illustrating two STH qubits coupled via a link consisting of a gated control dot. The gate voltage ε_c shifts the p shells of the control dot relative to its neighbors.

Note that since the energies of the two computational states are separated by Δ , the initialization of this qubit is relatively simple, through the system relaxing to the state $|0\rangle$, while keeping the background magnetic field off. The readout process, however, poses a more significant challenge. The original approach for two-dot ST qubits is not practical for these large macroscopic STH qubits, as it relies on charge transfer [20]. Instead, optical approaches, such as those proposed in Refs. [53] and [54], should be the suitable readout mechanisms in this case.

III. COUPLING TWO SINGLET-TRIPLET HALDANE QUBITS

In this section, we first describe how to make a tunable coupling between two STH qubits, A and B, each realized in a quantum dot nanowire. Then, using the effective spin Hamiltonian of the two coupled STH qubits, we compare their coupling with that of two coupled simple electron-based ST qubits, each consisting of two spin-half electrons.

A. Microscopic model of the inter-chain coupling

Consider two STH qubits, A and B, coupled by a tunable link, as depicted in Fig. 4. The tunable link is made of another quantum dot, labeled C and referred to as the “control dot,” which is gated by a gate tunable with applied voltage ε_c . As shown in Fig. 4, adjusting the gate voltage shifts the states of the control dot relative to its neighbors. When the p shell of the control dot is out of resonance with their neighbors, the two ends of qubits A and B are effectively decoupled. Lowering ε_c , an effective coupling between the two ends of A and B develops, which, as we demonstrate, acts as a tunable effective antiferromagnetic spin coupling between the two ends of the two STH qubits.

The Hamiltonian describing the two coupled STH qubits is given by

$$H = \varepsilon_c n_C + H_C + H_{AC} + H_{BC} + H_A + H_B, \quad (7)$$

where n_C is the electron number operator at the control dot, H_C describes the control dot without the detuning ε_c as in Eq. (1), H_{AC} and H_{BC} describe the hopping and Coulomb interaction between the last dots of qubits A and B and the control dot

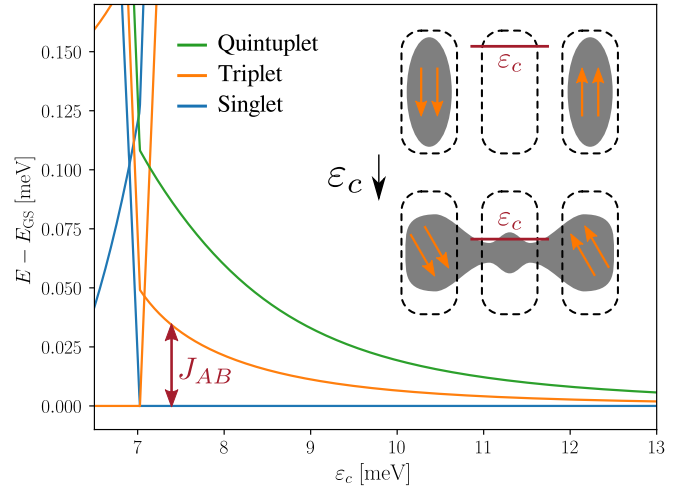


FIG. 5. The low-energy spectrum of three dots, each populated by four electrons, as schematically illustrated in the inset. The gate voltage of the control dot, ε_c , varies along the x axis. At high ε_c , the p shells of the control dot are empty and the two side dots are effectively decoupled. Decreasing ε_c forms a bridge between the two side dots, antiferromagnetically coupling the two effective spin-ones on the side dots. The singlet-triplet gap gives the value of the effective coupling J_{AB} . Going below a critical value of ε_c , a phase transition occurs and the system can no longer be viewed as two antiferromagnetically coupled spin-ones.

as in Eq. (2), and H_A and H_B are the HK Hamiltonians as in Eq. (3), describing each qubit in isolation.

To demonstrate that the link, realized by the gated control dot, functions as an effective tunable spin coupling between the two ends of the two STH qubits, let us focus on the link and consider three dots populated by four electrons. Two electrons belong to qubit A and two electrons belong to a dot of qubit B. Using the HK parameters listed in Table I, Fig. 5 shows the low-energy spectrum of the three-dot system as a function of ε_c . Recalling that two antiferromagnetically coupled spin-ones form a singlet, a triplet, and a quintuplet, one can observe that once ε_c exceeds a critical value, the spectrum of the three-dot system resembles that of two antiferromagnetically coupled spin-ones. In this regime, the changing singlet-triplet gap gives the value of the tunable effective spin coupling J_{AB} . It is evident how this coupling quickly diminishes as ε_c increases, allowing the two ends of qubits A and B to be perceived as two decoupled spin-one objects for large enough ε_c . Therefore, by adjusting ε_c , we can control J_{AB} and effectively switch it on and off.

B. Spin model of two coupled STH qubits

Let us now consider the effective spin Hamiltonian of two coupled STH qubits, A and B, given by

$$\tilde{H} = \tilde{H}_A + \tilde{H}_B + J_{AB} \mathbf{S}_{A,N} \cdot \mathbf{S}_{B,N}, \quad (8)$$

where $\tilde{H}_A$ and $\tilde{H}_B$ are Heisenberg Hamiltonians, as described in Eq. (4), representing qubits A and B in isolation. The last term describes how the last dots of qubits A and B are coupled by the tunable coupling J_{AB} .

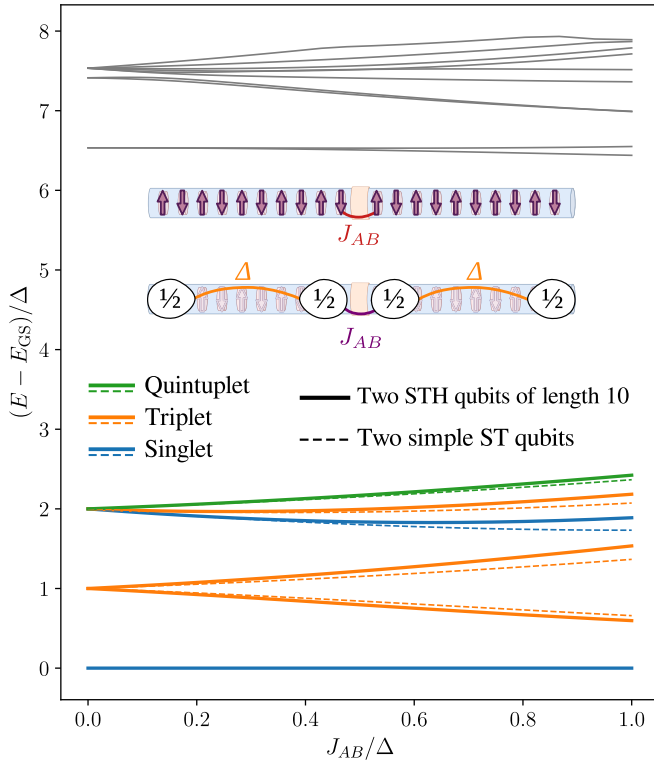


FIG. 6. The spectrum of two coupled STH qubits (solid curves) of length $N = 10$, described by $\tilde{H}$ in Eq. (8), plotted against J_{AB}/Δ , where $\Delta \approx 0.14J_{\text{eff}}$ is the singlet-triplet gap of a single chain. Energies are measured from the ground state and are normalized to Δ . The inset illustrates how STH qubits can be modeled as antiferromagnetic spin-one chains, with the low-energy spectrum of each spin-one chain viewed as two spin-half quasiparticles coupled by an exchange equal to Δ . For comparison, the spectrum of two coupled simple ST qubits (dashed curves), described by Eq. (9), is also presented. The color of each curve indicates the total spin of the corresponding state. $\tilde{H}$ exhibits higher-energy states beyond the six lowest-energy states, separated from the low-energy manifold by a Haldane gap. The first few of these higher-energy states are shown as gray curves.

As mentioned, the low-energy behavior of a single chain can be interpreted as two emerging spin-half quasiparticles coupled by an exchange coupling equal to the singlet-triplet gap, Δ . In this picture, which is schematically illustrated in Fig. 6, we anticipate that coupling qubits A and B by $\mathbf{S}_{A,N} \cdot \mathbf{S}_{B,N}$ will be analogous to coupling one spin-half quasiparticle of qubit A to one spin-half quasiparticle from qubit B.

On the other hand, two simple ST qubits A and B, each composed of two spin-halves, coupled in the same fashion, can be described by

$$\hat{H} = \Delta(\mathbf{s}_{A,1} \cdot \mathbf{s}_{A,2} + \mathbf{s}_{B,1} \cdot \mathbf{s}_{B,2}) + J_{AB}\mathbf{s}_{A,2} \cdot \mathbf{s}_{B,2}, \quad (9)$$

where $\mathbf{s}_{X,i}$ denotes the spin-half number i of qubit X , Δ is the coupling in each ST qubit, and J_{AB} couples the two ends of qubit A and B. Since $\hat{H}$ conserves the total spin, the computational basis of the two simple ST qubits evolves in the subspace $S_{\text{tot}}^z = 0$, which is a six-dimensional space spanned by $\{|SS\rangle, |ST_0\rangle, |T_0S\rangle, |T_0T_0\rangle, |T_+T_-\rangle, |T_-T_+\rangle\}$, where each component represents the tensor product of a state from qubit A and a state from qubit B. Notice how the two

components $|T_{\pm}T_{\mp}\rangle$ do not belong to the computational basis. In this basis and with this ordering, $\hat{H}$ has the following structure:

$$\hat{H} = \begin{bmatrix} H_{QQ} & H_{Q\bar{Q}} \\ H_{\bar{Q}Q} & H_{\bar{Q}\bar{Q}} \end{bmatrix}, \quad (10)$$

with

$$H_{QQ} = \begin{bmatrix} -\Delta & 0 & 0 & \chi J_{AB} \\ 0 & 0 & \chi J_{AB} & 0 \\ 0 & \chi J_{AB} & 0 & 0 \\ \chi J_{AB} & 0 & 0 & \Delta \end{bmatrix}, \quad (11a)$$

$$H_{\bar{Q}\bar{Q}} = \begin{bmatrix} -\chi J_{AB} & \chi' J_{AB} & -\chi' J_{AB} & \chi'' J_{AB} \\ -\chi J_{AB} & -\chi' J_{AB} & \chi' J_{AB} & \chi'' J_{AB} \end{bmatrix}, \quad (11b)$$

$$H_{Q\bar{Q}} = \begin{bmatrix} \Delta - \chi'' J_{AB} & 0 \\ 0 & \Delta - \chi'' J_{AB} \end{bmatrix}, \quad (11c)$$

where the energy is measured from the $|ST_0\rangle$ state, and for $\hat{H}$ in Eq. (9), we have $\chi = \chi' = \chi'' = 1/4$. In Appendix B, we show how to analytically determine the spectrum of $\tilde{H}$ comprising two singlets, three triplets, and one quintuplet. This spectrum is plotted in Fig. 6 by dashed lines as a function of J_{AB}/Δ .

Now, considering that the low-energy spectrum of $\tilde{H}$ in Eq. (8) primarily consists of the low-energy singlets and triplets of the STH qubits A and B, and given that $\tilde{H}$ also conserves total spin, its low-energy spectrum should be well approximated in a similar six-dimensional basis, comprising the computational basis along with the two additional states $|T_{\pm}T_{\mp}\rangle$. In Appendix C, we provide a rigorous proof of why the projection of $\tilde{H}$ onto this basis follows the structure shown in Eq. (11). But for STH qubits, unlike the simple ST qubits, χ , χ' , and χ'' are not identical and they generally vary depending on the size of the chain. For two STH qubits of length $N = 10$, they are approximately given by $\chi \approx 0.34$, $\chi' \approx 0.30$, and $\chi'' \approx 0.26$.

In Fig. 6, we present the low-energy spectrum of two coupled STH qubits with a length of $N = 10$, described by $\tilde{H}$ in Eq. (8), computed using exact diagonalization. The solid curves represent the energy levels of $\tilde{H}$ measured from the ground state as a function of J_{AB}/Δ , where Δ is the singlet-triplet gap of a single chain, approximately given by $0.14J_{\text{eff}}$. It is evident that the spectrum, normalized to Δ , closely follows the spectrum of two simple ST electron-spin-based qubits described by Eq. (9). The color of the curves corresponds to the total spin of the respective state, which is consistent for the lowest six states in both systems. The $S_{\text{tot}}^z = 0$ subspace of two coupled simple ST qubits is, of course, six dimensional, but for two coupled STH qubits described by $\tilde{H}$, the $S_{\text{tot}}^z = 0$ subspace is much larger and contains many higher-energy states. However, these states are all separated from the six-dimensional low-energy spectrum by a Haldane gap. We display the first few of these higher-energy states as gray curves in Fig. 6.

IV. GENERATING TWO-QUBIT GATES

Now that we have established how to couple two STH qubits, we proceed to demonstrate how to generate two-qubit

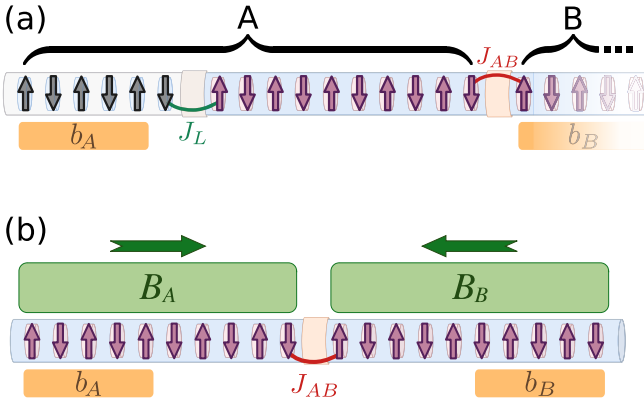


FIG. 7. (a) Two STH qubits A and B, with variable lengths coupled by J_{AB} . The local magnetic fields b_A and b_B are applied at different ends of each qubit, following Levy's prescription [55]. By toggling J_L on and off, we control the length of each STH qubit, effectively switching off and on Δ , the singlet-triplet gap of each qubit. (b) Two coupled STH qubits with fixed lengths, and hence fixed Δ . The local fields required for generating single-qubit gates are applied at the same ends. By applying two different background magnetic fields B_A and B_B behind qubits A and B, the undesired states $|T_{\pm}T_{\pm}\rangle$ are pushed away from the computational basis, thereby reducing the leakage error.

gates using this coupling. It is well known that for a quantum computer to be universal, it is sufficient to be able to generate all single-qubit gates, along with any two-qubit gate that is “locally equivalent” to the CNOT gate [52]. In Appendix D, we describe the concept of locally equivalent two-qubit gates and demonstrate how one can generate a gate locally equivalent to CNOT using a Hamiltonian with the structure of H_{QQ} in Eq. (11a).

The primary challenge in generating two-qubit gates from ST qubits is apparent from the previous section, where we presented the spectrum of two coupled qubits. This challenge arises from the two undesired states $|T_{\pm}T_{\pm}\rangle$, which couple to the computational basis. For conventional ST qubits, Levy addressed this challenge by devising a unique sequence to produce the CONTROLLED-Z (CZ) gate [55], which is locally equivalent to the CNOT gate. In Levy's sequence, the undesired states fully decouple from the computational basis at the end of the sequence. Crucial to this sequence is (a) the application of one of the local magnetic fields on the coupled ends of the qubits and the other on the noncoupled one, and (b) the ability to decouple the spin-halves comprising each ST qubit, that is, to be able to set $\Delta = 0$ in our language. The first requirement can be fulfilled for STH qubits as well, as illustrated in Fig. 7(a). However, the second requirement presents a serious challenge, as Δ remains fixed for a given chain length in STH qubits.

To address this challenge, we can leverage the fact that the singlet-triplet gap Δ in Haldane chains decreases exponentially with the chain length. Therefore, by connecting and disconnecting a few more dots at the end of each STH qubit, we can effectively switch Δ on and off. This may be achievable by incorporating an additional controllable link within each STH qubit, labeled J_L in Fig. 7(a). When J_L is activated, the chain becomes longer, turning Δ off, and when it is

deactivated, Δ is turned on. It is important to carefully design the internal link of each qubit so that when J_L is activated, it accurately replicates the J_{eff} coupling between other dots of the chain, ensuring a properly uniform Haldane chain of increased length.

Demonstrating a Levy sequence on two STH qubits with variable lengths, sufficiently long to effectively turn off Δ , poses a significant computational challenge, particularly in tracking the time evolution of a system with a massive Hilbert space. Additionally, designing and fabricating STH qubits with variable lengths could present its own set of challenges. Therefore, we propose a simpler scheme where Δ remains constant in each STH qubit. As we discuss below, this is achieved by introducing different background magnetic fields for the two coupled qubits.

Using different background magnetic fields

Introducing two different background magnetic fields for the two STH qubits modifies the spin Hamiltonian describing the coupled qubits to

$$\tilde{H}_{AB} = \tilde{H} + B_A S_{A,\text{tot}}^z + B_B S_{B,\text{tot}}^z, \quad (12)$$

where $\tilde{H}$, as given in Eq. (8), describes the coupled qubits without background magnetic fields. The addition of the background magnetic fields further modifies the structure of H_{QQ} as

$$H_{QQ} = \begin{bmatrix} \Delta - \chi'' J_{AB} + B_{AB} & 0 \\ 0 & \Delta - \chi'' J_{AB} - B_{AB} \end{bmatrix}, \quad (13)$$

with $B_{AB} = B_A - B_B$. This implies that when the two background magnetic fields are different and $B_{AB} \neq 0$, the two undesired states $|T_{\pm}T_{\pm}\rangle$ are displaced from the $|T_0T_0\rangle$ component of the computational basis by B_{AB} . The greater the B_{AB} , the lower the leakage of the computational basis into $|T_{\pm}T_{\pm}\rangle$. However, it is important to be cautious about the higher-energy states, as they can come down due to the nonzero B_{AB} and potentially interfere with the computational basis, resulting in leakage. The first of such states is $|Q_-T_+\rangle$, comprising the quintuplet in the $S_{A,\text{tot}}^z = -1$ subspace and $|T_+\rangle$ of qubit B. In the absence of coupling, $|Q_-T_+\rangle$ is positioned $\Gamma - B_{AB}$ above $|T_0T_0\rangle$, where Γ is the Haldane gap, while $|T_+T_-\rangle$ is B_{AB} above $|T_0T_0\rangle$, and $|T_-T_+\rangle$ is $B_{AB} - 2\Delta$ below $|SS\rangle$. Therefore, minimal interference from the outside of the computational basis can be achieved around the point where $\Gamma - B_{AB} = B_{AB} - 2\Delta \rightarrow B_{AB} = \Delta + \frac{\Gamma}{2}$. Assuming the fields have the same magnitude, $|B_A| = |B_B| = \frac{\Delta}{2} + \frac{\Gamma}{4}$, this choice guarantees that the higher-energy polarized states in each qubit, such as $|Q_{2\pm}\rangle$, are also kept away from the computational basis.

In Fig. 8, the solid curves show the evolution of two STH qubits, each with a length of $N = 10$, coupled by $J_{AB} = \Delta/2$, and subjected to $B_{AB} = \Delta + \frac{\Gamma}{2}$. To generate this plot, we use the low-energy product states as the basis of the reduced Hilbert space, formed by the products of states from $S_{A,\text{tot}}^z = m$ and $S_{B,\text{tot}}^z = -m$. We progressively incorporate higher-energy states until the convergence of leakage, quantified by

$$\epsilon_2 = 1 - \sum_{i,j=0,1} |(\psi(t)|ij)|^2, \quad (14)$$

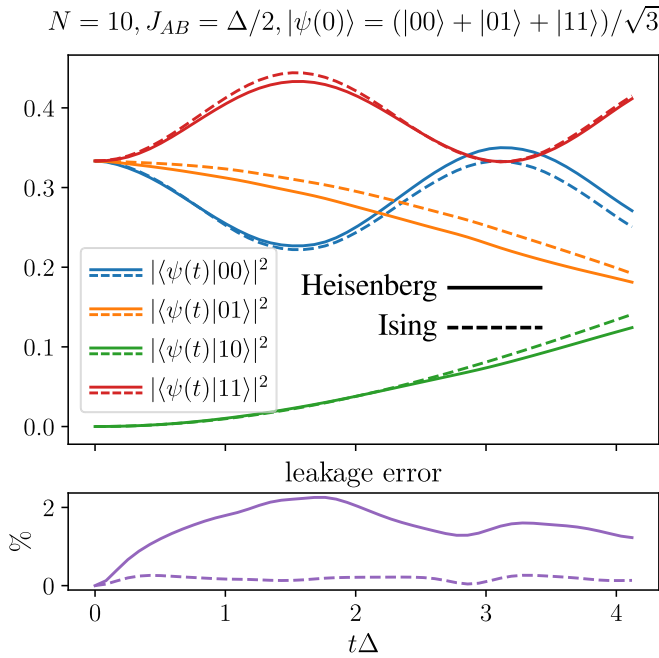


FIG. 8. Time evolution of two coupled STH qubits each with a length of $N = 10$, as governed by $\tilde{H}_{AB}$ in Eq. (12) (solid curves), with a coupling energy of $J_{AB} = \Delta/2$, half of the singlet-triplet gap of each qubit. Here, $B_{AB} = \Delta + \frac{\Gamma}{2}$, where Γ is the Haldane gap of each qubit, selected to minimize the leakage error depicted in the lower panel, calculated using Eq. (14). The two-qubit system was initialized in the state $|\psi(0)\rangle = (|00\rangle + |01\rangle + |11\rangle)/\sqrt{3}$, and as $|\psi(t)\rangle$ evolves, the squares of its projections onto the four components of the computational basis are plotted in different colors. The duration of the evolution was chosen to be t_c , the time needed for a coupling pulse in the process of generating a gate locally equivalent to CNOT. This value was determined using the procedure outlined in Appendix D 1. Time on the x axis is measured in units of $1/\Delta$. The dashed curves show the evolution and leakage of the same two qubits coupled by an Ising interaction.

where $|\psi(t)\rangle$ is the state of the coupled system at time t , and i and j go over the computational basis. In this case, we included 338 product states in the basis.

As the leakage panel of Fig. 8 shows, the maximum leakage is about 2%. But note that one can always reduce the leakage by choosing smaller J_{AB} . In Appendix D 1, we demonstrate that for any given J_{AB} , it is possible to create a gate locally equivalent to CNOT by applying the coupling J_{AB} twice, with a local transformation in between. We also show how to find the duration of the coupling pulses, denoted as t_c , for any J_{AB} . In Fig. 8, we use the t_c value obtained for $J_{AB} = \Delta/2$ as the duration of the time evolution.

To produce the time evolution depicted in Fig. 8, we initialize the two-qubit system in the state $|\psi(0)\rangle = (|00\rangle + |01\rangle + |11\rangle)/\sqrt{3}$. We choose this initial state to ensure that the two-qubit system evolves through all four components of the computational basis. We can see that being initialized in $|\psi(0)\rangle$ and with the small leakage, the two-qubit system primarily evolves within the computational basis. The evolution appears to comprise two nearly independent rotations, one involving the components $|00\rangle$ and $|11\rangle$, and the other involving $|01\rangle$ and $|10\rangle$. This behavior arises from the structure of H_{QQ}

in Eq. (11a), which couples $|01\rangle$ and $|10\rangle$ with $\omega_1 = \chi J_{AB}$, and $|00\rangle$ and $|11\rangle$ with $\omega_2 = \sqrt{\omega_1^2 + \Delta^2}$, thus resulting in a faster evolution of the two-qubit system among the latter components. If we choose two very large background magnetic fields for the two qubits in opposite directions, we can effectively push away all the spin-polarized states of the system from the computational basis. In this limit, the coupling effectively becomes an Ising coupling. Therefore, the only product states that can interfere with the computational basis are the pairs made of non-spin-polarized states, where each state belongs to the $S_{\text{tot}}^z = 0$ subspace of its own chain. Among these states, the closest to the computational basis are $|SQ_0\rangle$ and $|Q_0S\rangle$, consisting of the nonmagnetic first quintuplet of one chain and the ground-state singlet of the other chain. When the two chains are not coupled, these states are separated from the computational basis by $\Gamma - \Delta$.

In this limit, where the coupling is effectively an Ising coupling, one can imagine that the leakage will be smaller for the same coupling energy J_{AB} . To illustrate this point, we also present, with dashed curves, the time evolution of the same two STH qubits now coupled by an Ising interaction instead of the Heisenberg interaction of Eq. (8). It is evident that with an Ising interaction, the leakage is significantly reduced for the same J_{AB} . However, the problem with choosing two very large magnetic fields in the background of the qubits is that it transforms the computational basis into highly excited states. Therefore, such a scenario may not be stable enough for executing a long sequence of unitary operations. The significantly reduced leakage observed with Ising coupling prompts speculation on effective methods to generate Ising coupling between two quantum dots without relying on strong background magnetic fields. This intriguing question remains open for future investigations.

V. CONCLUSION

Starting from a microscopic model, we investigated the coupling of two singlet-triplet Haldane (STH) qubits realized in a quantum dot nanowire with four electrons in each dot through a gated control dot. By computing the energy spectrum of the fermionic system, we demonstrated that each quantum dot nanowire behaves like a topological Haldane chain with Haldane quasiparticles at both ends. Furthermore, we established the equivalence between controlling the detuning of the control dot and controllable antiferromagnetic coupling between the ends of the two STH qubits. We showed that the low-energy behavior of two coupled STH qubits, effectively made of two spin-half Haldane quasiparticles each, resembles that of two simple ST qubits, each made of two real spin-halves.

Using the spin model, we focused on the issue of decoupling $|T_+T_- \rangle$ states from the computational basis while generating two-qubit gates. We proposed that by using an internal link in each STH qubit, one can vary their length and effectively switch the singlet-triplet gap Δ on and off, thereby enabling the use of Levy sequence for generating two-qubit gates [55].

Furthermore, we demonstrated that resolving the leakage problem without altering the length of the STH qubits is

attainable by employing different background magnetic fields for the two qubits. Additionally, we showed that interchain Ising coupling could substantially decrease leakage, and discussed its potential realization through the use of very large magnetic fields in the background. We anticipate exploring alternative methods for achieving Ising coupling that do not rely on the use of large magnetic fields in the future. Exploring other avenues for coupling these STH qubits, such as photon bus, remains an interesting direction for future research. We hope this work motivates future experimental work on macroscopic quantum states in semiconductor nanostructures.

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APPENDIX A: THE ROBUSTNESS OF THE TOPOLOGICAL STATE AGAINST SPATIAL FLUCTUATIONS

Here, we demonstrate that the topological gap of the simulated Haldane chain in quantum dots is robust against spatial fluctuations in the parameters of the Hamiltonians that describe the chain. Let us describe a chain with spatial fluctuations by the noisy variation of Eq. (3),

$$H_{A,\text{noisy}} = \sum_{i=1}^N \gamma_1(i) H_{A,i} + \sum_{i=1}^{N-1} \gamma_2(i) H_{A,i,i+1}, \quad (\text{A1})$$

where $\gamma_1(i)$ and $\gamma_2(i)$ are drawn from a Gaussian noise distribution centered at 1 with variable variance.

As explained in the main text, with the parameters in Table I, Eq. (3) can be approximated by an effective spin-one Heisenberg Hamiltonian given in Eq. (4). Similarly, the noisy Hamiltonian given in Eq. (A1) can be approximated by a noisy Heisenberg Hamiltonian as

$$\tilde{H}_{A,\text{noisy}} = J_{\text{eff}} \sum_{i=1}^{N-1} \tilde{\gamma}(i) \mathbf{S}_{A,i} \cdot \mathbf{S}_{A,i+1}, \quad (\text{A2})$$

where $\tilde{\gamma}(i)$ is also drawn from a Gaussian noise distribution centered at 1 with variable variance.

To produce Fig. 9, we considered a noisy chain of length $N = 10$ and generated many noisy series for γ_1 , γ_2 , and $\tilde{\gamma}$, each with a random standard deviation drawn from a uniform distribution between 0 and 5%. For each sample, we show the energy of the first three levels in $S_{\text{tot}}^z = 0$ subspace, measured from the ground state and normalized to J_{eff} . The colors represent the total spin of the states: blue for a singlet, orange for triplet, and green for quintuplet. It can be observed that the singlet is always the ground state, followed by a triplet and a quintuplet, with the latter being separated from the first two by a larger Haldane gap. It is also evident that the Haldane

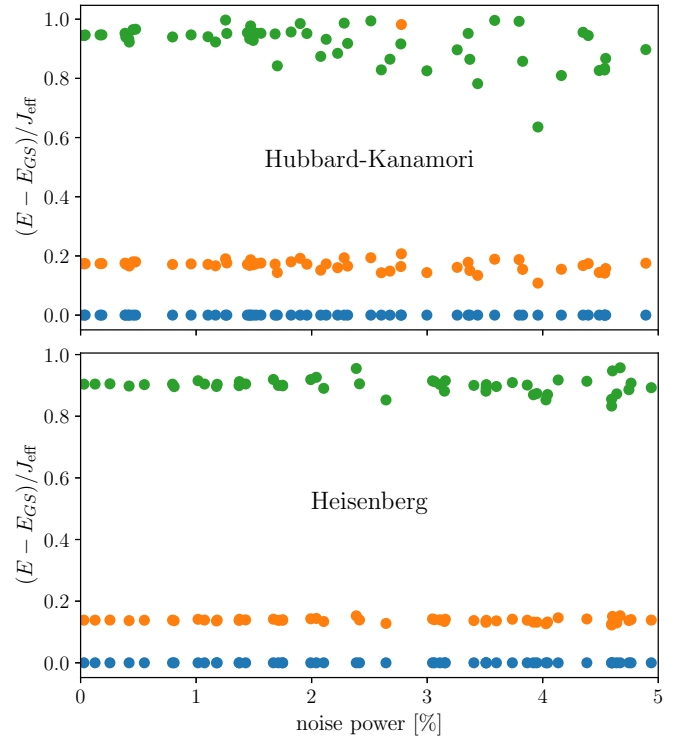


FIG. 9. The first three energy levels in the $S_{\text{tot}}^z = 0$ subspace of the noisy Hamiltonians in Eq. (A1) (upper panel) and Eq. (A2) (lower panel) against the noise power of each sample, given by the standard deviation of the Gaussian distributions from which γ_1 , γ_2 , and $\tilde{\gamma}$ are drawn. For the noisy HK Hamiltonian (upper panel), the values from Table I are used. The colors represent the total angular momentum of each state: blue for a singlet, orange for a triplet, and green for a quintuplet.

gap is less robust against noise in the more realistic case of a noisy HK Hamiltonian (upper panel). Notice the one case where the third state, though still separated by a large gap from the singlet and the first triplet, is another triplet rather than a quintuplet.

APPENDIX B: TWO COUPLED SIMPLE ST QUBITS

Consider $\hat{H}$ in Eq. (9) that describes two coupled simple ST qubits. Since $\hat{H}$ conserves total spin, its spectrum consists of two singlets, three triplets, and one quintuplet. The quintuplet is $|Q_{TT}\rangle \propto 2|T_0T_0\rangle + |T_+T_- \rangle + |T_-T_+ \rangle$ and its energy is given by $E_{Q_{TT}} = \Delta + J_{AB}/4$. Next observe that one of the triplets is $|T_{ST+}\rangle \propto |ST_0\rangle + |T_0S\rangle$ and its energy is given by $E_{T_{ST+}} = J_{AB}/4$. This leaves us with two 2D subspaces, one for the singlets and the other for the remaining two triplets. Finding the eigenstates of 2D Hamiltonians is straightforward. We find that the two remaining triplets are $|T_{ST-}\rangle \propto C_1(|ST_0\rangle - |T_0S\rangle) - J_{AB}(|T_+T_- \rangle - |T_-T_+ \rangle)$ and $|T_{TT}\rangle \propto J_{AB}(|ST_0\rangle - |T_0S\rangle) + C_1(|T_+T_- \rangle - |T_-T_+ \rangle)$, with $C_1 = \Delta + \sqrt{\Delta^2 + J_{AB}^2}$; their energy is given by $E_{T_{ST-}} = -\frac{1}{2}\sqrt{\Delta^2 + J_{AB}^2} + \Delta/2 - J_{AB}/4$ and $E_{T_{TT}} = \frac{1}{2}\sqrt{\Delta^2 + J_{AB}^2} + \Delta/2 - J_{AB}/4$. In the limit of $J_{AB} \ll \Delta$, $|T_{ST-}\rangle$ is primarily made of one singlet and one triplet, while $|T_{TT}\rangle$ is primarily made of two triplets. And, finally, we find that the two singlets

are $|S_{TT}\rangle \propto C_2(|T_+T_- \rangle + |T_-T_+ \rangle - |T_0T_0\rangle) - 3J_{AB}|SS\rangle$ and $|S_{SS}\rangle \propto J_{AB}(|T_+T_- \rangle + |T_-T_+ \rangle - |T_0T_0\rangle) + C_2|SS\rangle$, with $C_2 = 2\sqrt{4\Delta^2 - 2\Delta J_{AB} + J_{AB}^2 + 4\Delta - J_{AB}}$; their energy is given by $E_{S_{TT}} = \frac{1}{2}\sqrt{4\Delta^2 - 2\Delta J_{AB} + J_{AB}^2} - J_{AB}/4$ and $E_{S_{SS}} = -\frac{1}{2}\sqrt{4\Delta^2 - 2\Delta J_{AB} + J_{AB}^2} - J_{AB}/4$. The ground state is $|S_{SS}\rangle$ and, in the limit of $J_{AB} \ll \Delta$, it is primarily made of two singlets, while $|S_{TT}\rangle$ is primarily made of two triplets. This spectrum is shown in Fig. 6 by dashed curves as a function of J_{AB}/Δ .

APPENDIX C: THE STRUCTURE OF COUPLING MATRIX $\tilde{H}_{AB}$

Here, we demonstrate that the coupling operator

$$\begin{aligned} \tilde{H}_{AB} &= \mathbf{S}_{A,N} \cdot \mathbf{S}_{B,N} \\ &= S_{A,N}^z S_{B,N}^z + \frac{1}{2}(S_{A,N}^+ S_{B,N}^- + S_{A,N}^- S_{B,N}^+), \end{aligned} \quad (\text{C1})$$

which appears in Eq. (8), has the same structure as described in Eqs. (10) and (11) within the subspace spanned by $\{|SS\rangle, |ST_0\rangle, |T_0S\rangle, |T_0T_0\rangle, |T_+T_- \rangle, |T_-T_+ \rangle\}$.

Before starting the proof, observe that we can write a product state of two chains in terms of their configurations as

$$|ij\rangle = \sum_{p,q} a_{ip} b_{jq} |p; q\rangle, \quad (\text{C2})$$

where we are concerned with $i, j \in \{S, T_0, T_+, T_-\}$, and $p(q)$ are configurations of a single chain of length N like $p = p_1 \cdots p_N$, with $p_k \in \{0, \pm 1\}$. Let us also introduce inverted configuration $\bar{p}$, for which $\bar{p}_k = -p_k$ for all k 's. Then, since the Hamiltonian does not distinguish between $\pm \hat{z}$ directions, for all eigenstates of a single chain in its $S_{\text{tot}}^z = 0$ subspace, we have $|a_{ip}| = |a_{i\bar{p}}|$.

1. The structure of H_{QQ}

For the H_{QQ} block, we need to show that the only nonzero matrix elements are those located on the antidiagonal of H_{QQ} , corresponding to the terms proportional to J_{AB} in Eq. (11a). Notice that in this block, the only relevant terms of $\tilde{H}_{AB}$ are the Ising part $S_{A,N}^z S_{B,N}^z$. Then, using the orthonormality of the configurations, we can write

$$\langle i' j' | S_{A,N}^z S_{B,N}^z | ij \rangle = \sum_{p,q} p_N q_N a_{i'p}^* a_{ip} b_{jq}^* b_{j'q}. \quad (\text{C3})$$

If $i = i'$ or $j = j'$, we have $|a_{ip}|^2$ or $|b_{jq}|^2$ in the summand of Eq. (C3). But since the sum in Eq. (C3) goes over all p 's and q 's, and we have $p_N |a_{ip}|^2 + \bar{p}_N |a_{i\bar{p}}|^2 = q_N |b_{jq}|^2 + \bar{q}_N |b_{j\bar{q}}|^2 = 0$, then $\langle i' j' | S_{A,N}^z S_{B,N}^z | ij \rangle = 0$, unless $i \neq i'$ and $j \neq j'$, which is on the antidiagonal of H_{QQ} . Moreover, since H_{QQ} is Hermitian, to complete the proof, we just need to show $\langle SS | S_{A,N}^z S_{B,N}^z | T_0 T_0 \rangle = \langle ST_0 | S_{A,N}^z S_{B,N}^z | T_0 S \rangle$. To see that, we realize that since the Hamiltonian is real, its eigenvectors are also real, and therefore

$$\begin{aligned} \langle SS | S_{A,N}^z S_{B,N}^z | T_0 T_0 \rangle &= \sum_{p,q} p_N q_N a_{Sp} a_{T_0p} b_{Sq} b_{T_0q} \\ &= \langle ST_0 | S_{A,N}^z S_{B,N}^z | T_0 S \rangle = \chi. \end{aligned} \quad (\text{C4})$$

2. The structure of $H_{\bar{Q}\bar{Q}}$

Here, we derive the structure of the matrix elements of $\tilde{H}_{AB}$ between $|T_+T_- \rangle$ and the computational basis, and the procedure is the same for $|T_-T_+ \rangle$. Notice that $\frac{1}{2}S_{A,N}^- S_{B,N}^+$ is the only term in $\tilde{H}_{AB}$, given in Eq. (C1), that produces a nonzero matrix element between $|T_+T_- \rangle$ and the computational basis.

Let us start by making a few observations. First, observe that we have $S_{\text{tot}}^\pm |T_0\rangle = \sqrt{2}|T_\pm\rangle$ and $S_{\text{tot}}^\pm |S\rangle = S_{\text{tot}}^\pm |T_\pm\rangle = 0$, where $S_{\text{tot}}^\pm = \sum_n S_n^\pm$. Second, observe that using the commutation relation $[S^+, S^-] = 2S^z$ and the first observation, we have $\langle S | S_N^\mp | T_\pm \rangle = \frac{1}{\sqrt{2}} \langle S | S_N^\mp S_{\text{tot}}^\pm | T_0 \rangle = \mp \sqrt{2} \langle S | S_N^z | T_0 \rangle$. Similarly, we also have $\langle T_0 | S_N^\mp | T_\pm \rangle = \frac{1}{\sqrt{2}} \langle T_\pm | S_{\text{tot}}^\pm S_N^\mp | T_\pm \rangle = \pm \sqrt{2} \langle T_\pm | S_N^z | T_\pm \rangle$. Here, we suppressed the chain indices A and B to stay general.

Then, using the second observation, we can write $\langle SS | \tilde{H}_{AB} | T_+T_- \rangle = \frac{1}{2} \langle SS | S_{A,N}^- S_{B,N}^+ | T_+T_- \rangle = -\langle SS | S_{A,N}^z S_{B,N}^z | T_0T_0 \rangle = -\chi$, which gives us the first column of $H_{\bar{Q}\bar{Q}}$, in agreement with the form in Eq. (11).

Next, for the following two columns of $H_{\bar{Q}\bar{Q}}$, it is evident that we should have $|\langle ST_0 | \tilde{H}_{AB} | T_\pm T_\mp \rangle| = |\langle T_0S | \tilde{H}_{AB} | T_\mp T_\pm \rangle|$, as the Hamiltonian does not have a preferred direction, and as it is symmetric with respect to the two chains. To complete the proof, we show that $\langle ST_0 | \tilde{H}_{AB} | T_+T_- \rangle = \langle T_0S | \tilde{H}_{AB} | T_-T_+ \rangle = \chi'$, and the other two matrix elements have the opposite sign. As mentioned, we can write $|T_+T_- \rangle$ as

$$|T_+T_- \rangle = \sum_{p,q} a_p b_q |p; q\rangle \quad (\text{C5a})$$

$$\rightarrow |T_-T_+ \rangle = \sum_{p,q} a_p b_q |q; p\rangle. \quad (\text{C5b})$$

Consequently, we have

$$\frac{1}{2} S_{A,N}^- S_{B,N}^+ |T_+T_- \rangle = \sum_{p,q} a_p b_q |p'; q'\rangle, \quad (\text{C6a})$$

$$\frac{1}{2} S_{A,N}^+ S_{B,N}^- |T_-T_+ \rangle = \sum_{p,q} a_p b_q |q'; p'\rangle, \quad (\text{C6b})$$

where p' and q' are configurations that we obtain by flipping the last spin down and up in each chain, respectively. It is evident that Eq. (C6a) and Eq. (C6b) are the same up to switching between the A and B configurations, which implies that we have $\langle ST_0 | S_{A,N}^- S_{B,N}^+ | T_+T_- \rangle = \langle T_0S | S_{A,N}^+ S_{B,N}^- | T_-T_+ \rangle$, as we claimed.

Finally, for the last elements of $H_{\bar{Q}\bar{Q}}$, using the observations we made above, we can write $\langle T_0T_0 | \tilde{H}_{AB} | T_+T_- \rangle = \frac{1}{2} \langle T_0T_0 | S_{A,N}^- S_{B,N}^+ | T_+T_- \rangle = -\langle T_+T_- | S_{A,N}^z S_{B,N}^z | T_+T_- \rangle = \chi''$, which proves full agreement with Eq. (11).

3. The structure of $H_{\bar{Q}\bar{Q}}$

The structure of $H_{\bar{Q}\bar{Q}}$ is simple. It is clear that it should be proportional to the identity matrix, as $\tilde{H}_{AB}$ cannot connect $|T_+T_- \rangle$ and $|T_-T_+ \rangle$ because such a process would require two spin flips in each chain. Moreover, since the Hamiltonian does not distinguish between the $\pm \hat{z}$ directions, we should have $\langle T_+T_- | \tilde{H}_{AB} | T_+T_- \rangle = \langle T_-T_+ | \tilde{H}_{AB} | T_-T_+ \rangle = -\chi''$, in agreement with Eq. (11).

APPENDIX D: GENERATING CNOT GATE

Here, we show how to generate a gate *locally equivalent* to CNOT using H_{QQ} in Eq. (11a). We say two two-qubit gates U and U' are locally equivalent if $U' = (L_A \otimes L_B)U(R_A \otimes R_B)$, where L 's and R 's are single-qubit gates acting on qubits A and B. It can be shown that if two two-qubit gates have the same *canonical form* $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ in the *Weyl chamber* $\frac{\pi}{4} \geq \alpha_1 \geq \alpha_2 \geq |\alpha_3| \geq 0$, then they are locally equivalent [57]. There is a standard procedure for finding the canonical form of a two-qubit gate such as U , as follows [57]: (1) Factor out a global phase $U = e^{i\alpha_0} \tilde{U}$ such that $\det(\tilde{U}) = 1$. (2) Form $V = M^\dagger \tilde{U} M$, where

$$M = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{bmatrix}. \quad (D1)$$

(3) Find λ 's, the eigenvalues of $V^T V$. (4) Then the canonical form α is the unique solution of the following set of equations in the Weyl chamber:

$$\lambda_1 = e^{2i(\alpha_1 - \alpha_2 + \alpha_3)}, \quad (D2a)$$

$$\lambda_2 = e^{2i(\alpha_1 + \alpha_2 - \alpha_3)}, \quad (D2b)$$

$$\lambda_3 = e^{-2i(\alpha_1 + \alpha_2 + \alpha_3)}, \quad (D2c)$$

$$\lambda_4 = e^{-2i(\alpha_1 - \alpha_2 - \alpha_3)}. \quad (D2d)$$

The canonical form of CNOT—along with many other common two-qubit gates—is $\alpha_{\text{CNOT}} = (\frac{\pi}{4}, 0, 0)$. Next, we show how to use H_{QQ} in Eq. (11a) to generate a gate with the same canonical form.

1. Arbitrary coupling value J_{AB}

Here we show how to find t_c such that for an arbitrary coupling J_{AB} , $U_{2QQ}(t_c) = e^{-it_c H_{QQ}}(XI)e^{-it_c H_{QQ}}$ has a canonical

form the same as α_{CNOT} . Using the procedure mentioned above, we observe that for any t , the canonical form of $U_{2QQ}(t)$ has the form $\alpha_{2QQ}(t) = (\phi, 0, 0)$, where

$$\sin(\phi) = \text{abs} \left\{ \sin(\omega_1 t) \cos(\omega_2 t) + \frac{\sin(\omega_2 t)}{\omega_2} [\omega_1 \cos(\omega_1 t) + i \Delta \sin(\omega_1 t)] \right\}, \quad (D3a)$$

$$\cos(\phi) = \text{abs} \left\{ \cos(\omega_1 t) \cos(\omega_2 t) + i \frac{\sin(\omega_2 t)}{\omega_2} [\Delta \cos(\omega_1 t) + i \omega_1 \sin(\omega_1 t)] \right\}, \quad (D3b)$$

with $\omega_1 = \chi J_{AB}$, and $\omega_2 = \sqrt{\omega_1^2 + \Delta^2}$. Therefore, to find t_c , one needs to solve $\sin^2[\phi(t_c)] = \cos^2[\phi(t_c)] = \frac{1}{2}$, which can be done numerically, for any given J_{AB} .

2. Special coupling values J_{AB}

It turns out that for a set of special coupling values J_{AB} , one can generate a gate locally equivalent to CNOT by one time application of H_{QQ} in Eq. (11a), as $U_{QQ}(t_c) = e^{-it_c H_{QQ}}$. To see that, we observe that the canonical form of $U_{QQ}(t)$ has the form $\alpha_{QQ}(t) = \frac{1}{2}(\phi_1 + \phi_2, \phi_1 - \phi_2, 0)$, where $\phi_1 = \omega_1 t$, and $\sin(\phi_2) = \frac{\omega_1}{\omega_2} \sin(\omega_2 t)$. Therefore, α_{QQ} can reach at the α_{CNOT} point, if we have $\phi_1 + \phi_2 = \frac{\pi}{2} + m_1 \pi$, and $\phi_1 - \phi_2 = m_2 \pi$, with integer m 's. This implies that $\phi_1 = (2m + 1)\frac{\pi}{4}$, and that $\sin^2(\phi_2) = \frac{1}{2}$. Finding t from ϕ_1 and plugging it in the expression for $\sin(\phi_2)$, we find

$$2 \sin^2 \left[(2m + 1) \frac{\pi}{4} \frac{\omega_2}{\omega_1} \right] = \left(\frac{\omega_2}{\omega_1} \right)^2. \quad (D4)$$

For integers $m > 1$, this equation has a set of solutions for ω_2/ω_1 , from which the special values of J_{AB} for a given Δ can be obtained.

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