Quantum gates between capacitively coupled double quantum dot two-spin qubits

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We study the two-qubit controlled-NOT gate operating on qubits encoded in the spin state of a pair of electrons in a double quantum dot. We assume that the electrons can tunnel between the two quantum dots encoding a single qubit, while tunneling between the quantum dots that belong to different qubits is forbidden. Therefore, the two qubits interact exclusively through the direct Coulomb repulsion of the electrons. We find that entangling two-qubit gates can be performed by the electrical biasing of quantum dots and/or tuning of the tunneling matrix elements between the quantum dots within the qubits. The entangling interaction can be controlled by tuning the bias through the resonance between the singly occupied and doubly occupied singlet ground states of a double quantum dot.

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I. INTRODUCTION

The spin 1/2 of a single electron trapped in a quantum dot (QD) is a promising candidate for a carrier of quantum information in a quantum computer.[1] To perform a quantum computation, we need to have all the unitary operations from some universal set of quantum gates at our disposal.[2] One such universal set consists of all the single-qubit quantum gates and a two-qubit controlled-NOT (CNOT) quantum gate. Quantum computation over the single-spin qubits with the logical states corresponding to the spin orientations $|\uparrow\rangle$ and $|\downarrow\rangle$ can, in principle, be achieved using an external magnetic field or with g-factor engineering for the single-qubit operations and with the time-dependent isotropic exchange interaction $H_{ex}(t)=J(t)\mathbf{S}_1\cdot\mathbf{S}_2$ for manipulating a pair of qubits encoded into spins $\mathbf{S}_1$ and $\mathbf{S}_2$.[1]

Control of electron spins in quantum dots is in the focus of many intense experimental investigations. Manipulation of pairs of electron spins using the tunable isotropic exchange interaction has already been demonstrated in several experiments.[3–5] Such control was used in a study of the QD spin decoherence due to the hyperfine coupling to the surrounding nuclear spins, where the splitting between the singlet states with the total spin $S^{tot}=0$, where $\mathbf{S}^{tot}=\mathbf{S}_1+\mathbf{S}_2$, and the triplet states with $S^{tot}=1$ was used to turn the singlet-triplet mixing caused by the hyperfine interaction on and off. An important result of these studies is that the coherence time of an electron spin in a quantum dot is very long if the decoherence due to the interaction with the nuclear spins can be suppressed. The spin coherence times can be improved by the manipulation of nuclear spins,[6–8] in principle, allowing for elaborate sequences of operations to be performed. Single-spin control is based on the local manipulation of the magnetic field or g factor[1] or on electron-spin-resonance methods[9,10] and has only recently been demonstrated experimentally.[11]

The difficulty of single-spin control has inspired a number of proposals for quantum computation based on the encoding of qubits into more than one spin. These encoding schemes reduce the requirement on the control over electron spins, but have the drawback of introducing so-called leakage errors, in which the state of encoded qubit "leaks" out of the set of computational states. Standard error-correction procedures can be modified to prevent this kind of error.[12] A universal set of quantum gates operating on qubits encoded into states of three quantum dot spins with equal total spin quantum numbers can be implemented through control of the isotropic exchange coupling H_{ex} alone.[13–15] Control over interactions that are symmetric only with respect to rotations about a fixed axis in spin space allows for the construction of a universal set of quantum gates that operate over qubits encoded into a pair of spins. One such encoding is into the orthogonal states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ of two spins 1/2. A universal set of quantum gates over such qubits can, in principle, be performed by the control over H_{ex}, with the anisotropy provided by an external static homogeneous magnetic field and a site-dependent g factor.[16,17]

We consider a variant of the two-spin encoding where the logical zero $|0_L\rangle$ and the logical one $|1_L\rangle$ quantum states are the singlet and the triplet with zero projection of the total spin to the symmetry axis z ($S_z^{tot}=0$); e.g., for lateral QDs, the z axis is the normal to the plane of the heterostructure,

$$|0_L\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$
$$|1_L\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle). \quad (1)$$

These qubits can be manipulated by an axially symmetric interaction to produce a universal set of quantum gates. The interaction with an inhomogeneous Zeeman field and the isotropic exchange,[16,17] the interaction with an inhomogeneous Zeeman field and an anisotropic spin-orbit coupling,[18] and the spin-orbit coupling alone[19] were all proposed as a way of producing a universal set of quantum gates operating on singlet-triplet two-spin qubit [Eq. (1)]. Recently, it was suggested that an architecture based on singlet-triplet qubits individually addressed using the isotropic exchange interaction and inhomogeneous magnetic field and coupled through Coulomb interactions of the electrons is scalable and, in principle, realizable.[20]

In this paper, we study a particular realization of entangling two-qubit gates between singlet-triplet qubits [Eq. (1)], where each qubit is represented by a pair of tunnel-coupled single-electron quantum dots, as proposed in Ref. 20. In this

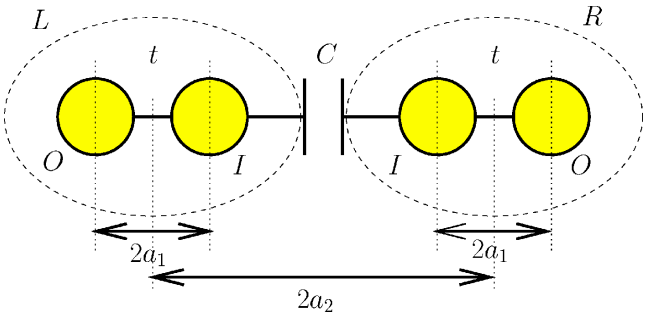

FIG. 1. (Color online) Double-double quantum dot (DDQD) setup. The four single-electron quantum dots are aligned along a fixed direction. The spins of the electrons on two quantum dots, inner (I) and outer (O), separated by a distance $2a_1$ encode a qubit. Two such double quantum dot (DQD) qubits, left (L) and right (R), at the distance $2a_2$ are separated by an impenetrable barrier. The tunneling matrix element t within the DQDs carrying the qubits and the bias ϵ of the inner dots with respect to the outer are equal on both DQDs and can be electrically tuned. The Coulomb interaction between the DQD is represented by the capacitor C.

realization, the double quantum dots are separated by a barrier, which is impenetrable for the electrons, so that the qubits are coupled exclusively through the Coulomb repulsion of electrons, while the exchange terms between electrons on different double quantum dots vanish. The setup of this double-double quantum dot (DDQD) is illustrated in Fig. 1.

The Coulomb interaction is spin independent, leading to an isotropic interaction $J\mathbf{S}_1\cdot\mathbf{S}_2$ between tunnel-coupled spins $\mathbf{S}_1$ and $\mathbf{S}_2$. The anisotropic correction to this interaction is dominated by the spin-orbit coupling induced term $J\boldsymbol{\beta}\cdot(\mathbf{S}_1\times\mathbf{S}_2)+O(|\boldsymbol{\beta}|^2)$. The relative strength of the anisotropic interaction in quantum dot systems is estimated to be $|\boldsymbol{\beta}|\sim 0.1-0.01$.[21,22] The influence of the anisotropic corrections can be reduced in specific implementations of the quantum gates.[23,24] Coupling of singlet and triplet states in a DQD induced by the anisotropy would introduce errors in a quantum gate operation at the rate of approximately $|\boldsymbol{\beta}|^2$ for a generic implementation of the entangling gates and at the rate $|\boldsymbol{\beta}^4|$ if the methods of Ref. 24 are applied. In our study of a two-qubit gate operation, we will only consider the case of isotropic interaction and neglect the weak anisotropy. In this case, transitions between spin-singlet and spin-triplet states on a DQD are forbidden. Due to this spin symmetry, the four-electron Hamiltonian is block diagonal,

$$H=\mathrm{diag}(H_{SS},H_{ST},H_{TS},H_{TT}). \tag{2}$$

The nonzero blocks H_{ab}, where $a,b=S,T$, act on the states in which electron pairs on each DQD are either in the singlet (S) or in a triplet (T) state of the total spin $S^{tot}=0$ or $S^{tot}=1$.

Our main results are the effective low-energy spin interaction and a scheme to perform a two-qubit CNOT gate in an electrically controlled DDQD system. The effective low-energy spin interaction in this setup has the form

$$H=J(\mathbf{S}_{LI}\cdot\mathbf{S}_{LO}+\mathbf{S}_{RI}\cdot\mathbf{S}_{RO})+E_e|SS\rangle\langle SS|. \tag{3}$$

Two pairs of spins, $\mathbf{S}_{LI}$ and $\mathbf{S}_{LO}$ on the left (L) qubit and $\mathbf{S}_{RI}$ and $\mathbf{S}_{RO}$ on the right (R) qubit (see Fig. 1), interact via the isotropic exchange interaction of strength J and the entangling interaction of strength E_e that shifts the energy of the singlet-singlet state. We show how the entangling two-qubit quantum gates for universal quantum computation can be performed through the electrical control of E_e.

The triplet states with $S_z^{tot}=0,\pm 1$ are degenerate in the absence of a magnetic field. A uniform magnetic field $\mathbf{B}$, pointing along the z axis normal to the plane of QDs, causes a Zeeman splitting $g\mu_B\mathbf{B}\cdot\mathbf{S}$ between the $S_z^{tot}=0$ states and the states with $S^{tot}=1$, $S_z^{tot}=\pm 1$. Our results apply to both the isotropic ($\mathbf{B}=0$) and the anisotropic but axially symmetric ($\mathbf{B}\neq 0$) case if we take the $S_z^{tot}=0$ state to represent the qubit $|1_L\rangle$ state.

A two-qubit quantum gate can, in principle, be performed by adiabatically varying the tunneling amplitude t and the bias ϵ within the DQD. A generic voltage pulse will modify the electrostatic potential in the quantum dots. We use the tunneling amplitude and the bias to describe this potential. In a more general approach, the new potential would be calculated as a solution to the electrostatic problem with external voltages specifying the boundary conditions. However, the wave functions of electrons are well localized at the positions of the quantum dots, and the parameters t and ϵ capture the possible variation of the electron Hamiltonian. In a naive picture, the tunneling and bias are controlled by separate electrodes. Another important issue is independent control over the two parameters. In principle, a change in the gate potentials will modify both parameters. The control will, however, be approximately independent as long as the quantum dots are well separated. In practice, it is much simpler to change the bias ϵ while t remains fixed.[27] The control parameters ϵ and t have to vary slowly on the time scale set by the energy splitting between the states of a given spin configuration. During the gate application, the orbital components of the S and T states are different due to the Pauli principle that forbids the electrons in a spin triplet to share their orbital state (see Fig. 2). As opposed to t and ϵ that are determined by gate voltages and can be changed more or less at will, the Coulomb interaction is set by the geometry of the system and therefore fixed. We show how the control of the parameters t and ϵ, or even ϵ alone, can nevertheless be used to implement entangling two-qubit gates on encoded singlet-triplet qubits through its influence on the Coulomb terms.

When an adiabatic gate is applied, the lowest-energy state in each block H_{ab}, of energy E_{ab}, where $a,b=S,T$ [see Eq. (2)], acquires a phase $\phi_{ab}=\int_{t_i}^{t_f}E_{ab}(t')dt'/\hbar$. The energy E_{ab} becomes time dependent through the time dependence of the parameters t and ϵ in the interval $t_i<t'<t_f$. The resulting interaction is described by an effective four-dimensional two-qubit Hamiltonian acting in the space spanned by the lowest-energy states $|SS\rangle$, $|ST\rangle$, $|TS\rangle$, and $|TT\rangle$ in the corresponding blocks H_{ab}, and has the form of Eq. (3).

In the regime of strong bias, $|\epsilon-U|\gg t$, where U is the on-site Coulomb repulsion, we investigate the DDQD system using perturbation theory. For the case of arbitrary bias ϵ, we numerically diagonalize the Hamiltonian [Eq. (2)]. We show that the two-qubit quantum gate can be operated by tuning the bias ϵ so that the amplitude of the doubly occupied state in the lowest-energy spin singlet becomes appreciable. In

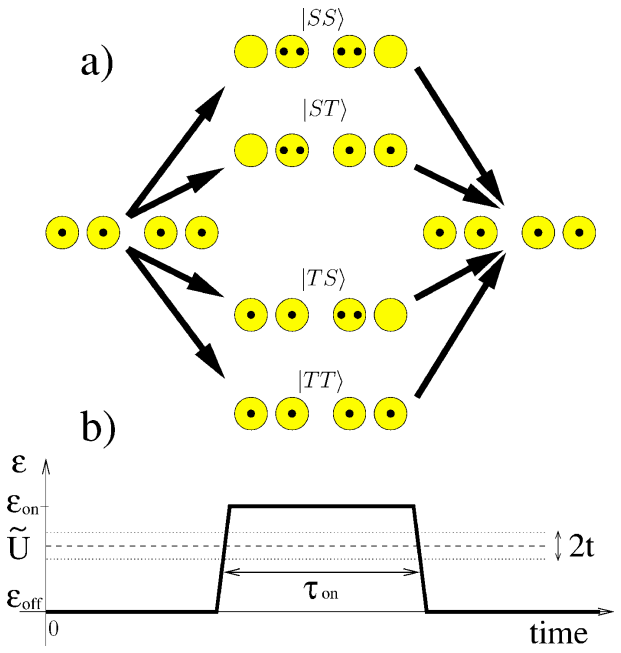

FIG. 2. (Color online) Two-qubit quantum gate. (a) When the inner quantum dots of the two double quantum dots system are strongly biased ($\epsilon > \tilde{U}+t$), the ground state is the doubly occupied inner dot. Due to the Pauli principle, only the spin singlets (S) can tunnel into the doubly occupied states on their DQDs. As the bias ϵ is reduced, the states again become degenerate. (b) A quantum gate is performed by sending a bias pulse $\epsilon(t')$. Each qubit state $|ab\rangle$ acquires a phase $\phi_{ab}=\int_{-\infty}^{\infty}E_{ab}(t')dt'/\hbar$, where $E_{ab}(t')$ is the ground-state energy of the Hamiltonian at time t' reduced to the appropriate spin subspace, resulting in a two-qubit quantum gate.

this "on" state with a large double occupancy amplitude, entanglement is generated between the two-spin qubits. The entanglement generation is suppressed in the "off" regime with weak bias and tunneling. Therefore, the generation of entanglement between the two two-spin qubits encoded into DDQD can be efficiently controlled using the bias ϵ alone. Together with the single-qubit operation, this control is sufficient for universal quantum computing.

This paper is organized as follows. In Sec. II, we introduce our model of the DDQD system, followed by the discussion of the control through voltage pulses. In Sec. III, we focus on the case of the strongly biased ($|\epsilon - U| \gg t$) DDQD system and calculate the interaction between the qubits. The constraint of the strong bias is lifted in Sec. IV, where we numerically find the interaction between the qubits, valid at an arbitrary bias ϵ. In Sec. V, we outline the construction of a CNOT gate based on the resources for the control over a pair of qubits deduced from the results of Secs. III and IV. Our results are summarized in Sec. VI. The technical details of the calculation are collected in the Appendix.

II. MODEL

For the purpose of finding the effective low-energy spin Hamiltonian, the excited orbital states of single quantum dots can be neglected, leading to the Hund-Mulliken (HM) approximation with one orbital per dot.[9,25] In the HM approximation, the state space of the two-electron system in a double quantum dot (DQD) encoding the left ($q=L$) or the right ($q=R$) qubit is spanned by three singlet basis states, $|\bar{S}\rangle$, $|D_I\rangle$, and $|D_O\rangle$, and one triplet basis state, $|T_0\rangle$,

$$|\bar{S}\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{qI\uparrow}c^\dagger_{qO\downarrow} - c^\dagger_{qI\downarrow}c^\dagger_{qO\uparrow})|0\rangle, \tag{4}$$

$$|D_I\rangle = c^\dagger_{qI\uparrow}c^\dagger_{qI\downarrow}|0\rangle, \tag{5}$$

$$|D_O\rangle = c^\dagger_{qO\uparrow}c^\dagger_{qO\downarrow}|0\rangle, \tag{6}$$

$$|T_0\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{qI\uparrow}c^\dagger_{qO\downarrow} + c^\dagger_{qI\downarrow}c^\dagger_{qO\uparrow})|0\rangle, \tag{7}$$

where c_k is the annihilation operator for an electron in the state $k=(q_k,p_k,s_k)$ on the qubit $q_k=L,R$, with position $p_k=I,O$, where I stands for inner and O for outer quantum dot within a qubit, and spin $s_k=\uparrow,\downarrow$. The vacuum $|0\rangle$ is the state of empty QDs.

In the standard notation, the singlet states of a DQD are denoted by $|(n,m)S\rangle$, where n is the number of electrons on the left QD and m is the number of electrons on the right QD. Our singly occupied singlet is then expressed as $|\bar{S}\rangle \equiv |(1,1)S\rangle$. The doubly occupied singlet states on the left, $q=L$, DQD are $|D_I\rangle \equiv |(0,2)S\rangle$ and $|D_O\rangle \equiv |(2,0)S\rangle$. On the right, $q=R$, DQD the definitions are reversed, $|D_I\rangle \equiv |(2,0)S\rangle$ and $|D_O\rangle \equiv |(0,2)S\rangle$.

The orbital states annihilated by c_k approximate the ground states of the single-particle Hamiltonian,

$$H_1 = \sum_i \frac{1}{2m}\left[\mathbf{p}_i - \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right]^2 + V(\mathbf{r}_i), \tag{8}$$

describing an electron in the magnetic field $\mathbf{B}=\nabla\times\mathbf{A}$ and confined to the system of quantum dots by the electrostatic potential V. The quantum dots form in the minima of this potential, which is locally harmonic with the frequency ω_0. The ground states of H_1 localized in these wells are the translated Fock-Darwin states.[9]

The HM Hamiltonian is of the generic form

$$H = t\sum_{k,l}(\delta_{q_k,q_l}\delta_{s_k,s_l}c^\dagger_{q_kIs_k}c_{q_kOs_k} + \text{H.c.}) - \epsilon\sum_{k,p_k=I} c^\dagger_k c_k + \frac{1}{2}\sum_{klmn}\langle kl|V_C|mn\rangle c^\dagger_k c^\dagger_l c_n c_m. \tag{9}$$

The intra-DQD tunneling term $\propto t$ preserves the electron spin. The bias ϵ of the inner ($p_k=I$) QDs with respect to the outer ($p_k=O$) QDs is taken to be symmetric; i.e., the energy of both inner dots is lowered by the same amount. The two-body Coulomb interaction is denoted by V_C. Near the center of the quantum dot, the electrostatic potential is approximately harmonic and we assume that the wave functions of the electrons annihilated by the operators c_k are well approximated by the orthogonalized Fock-Darwin ground states.

The impenetrable barrier that separates the DQDs imposes the conservation of the number of $L(R)$ electrons, $\hat{n}_{L(R)}=\Sigma_{p=I,O;s=\uparrow,\downarrow}\hat{n}_{L(R)ps}$, where $\hat{n}_{qps}=c^{\dagger}_{qps}c_{qps}$. The $\hat{n}_{L(R)}$ conserving terms, proportional to the interaction matrix elements $\langle kl|V_C|mn\rangle$ in Eq. (9), where the indices k,l,m,n denote the single QD ground states, can be divided into intra-DQD terms where $q_k=q_l=q_m=q_n$ and inter-DQD terms that satisfy $q_k\neq q_l$ and $q_m\neq q_n$. All the other terms, e.g., the ones that annihilate two electrons on the left (L) DQD and create two on the right (R) DQD, violate the conservation of the electron numbers and therefore vanish.

A. Interaction within a double quantum dot

The terms for the interaction within a DQD in Eq. (9) were discussed in Ref. 9. They renormalize the one-body tunneling matrix element $t\rightarrow t_H=t+\langle\bar{S}|V_C|D_{I(O)}\rangle/\sqrt{2}$, introduce the on-site repulsion $U=\langle D_{I(O)}|V_C|D_{I(O)}\rangle$ of two electrons on the same QD, and cause transitions between the two doubly occupied DQD states with the matrix element $X=\langle D_{I(O)}|V_C|D_{O(I)}\rangle$. Also, the Coulomb interaction on a DQD contributes $V_+=\langle\bar{S}|V_C|\bar{S}\rangle$ to the electrostatic energy of the symmetric and $V_-=\langle T_0|V_C|T_0\rangle$ to the antisymmetric singly occupied orbitals of two electrons in a DQD,[9] giving rise to a direct exchange interaction between spins. As a result, the electrons on a DQD are described by an extended Hubbard model with the isotropic exchange interaction,[9]

$$J=V_- - V_+ - \frac{U_H}{2}+\frac{1}{2}\sqrt{U_H^2+16t_H^2}, \tag{10}$$

where $U_H=U-V_++X$ is the effective on-site repulsion.

B. Interaction between the double quantum dots

The Coulomb interaction between the DQDs produces three new classes of direct terms in the Hamiltonian, while the exchange terms between the DQD vanish due to the impenetrable barrier.

In the first class are the terms proportional to the number operators $\hat{n}_{qps}\hat{n}_{\bar{q}p's'}$, describing the electrostatic repulsion of the electrons in states qps and $\bar{q}p's'$, where $\bar{L}=R$ and $\bar{R}=L$. For a pair of identical DQDs, there are three such terms: the interaction of a pair of electrons on the inner QDs, $U_N=\langle qIs,\bar{q}Is'|V_C|qIs,\bar{q}Is'\rangle$, the interaction of an electron on the inner QD of one DQD and an electron in the outer QD of the other DQD, $U_M=\langle qIs,\bar{q}Os|V_C|qIs,\bar{q}Os\rangle$, and the interaction of electrons on the outer QDs, $U_F=\langle qOs,\bar{q}Os|V_C|qOs,\bar{q}Os\rangle$ [Fig. 3(a)].

In the second class are the terms proportional to $\hat{n}_{qps}c^{\dagger}_{\bar{q}p's'}c_{\bar{q}\bar{p}s'}$, where $\bar{I}=O$ and $\bar{O}=I$. These terms describe the spin-independent correction to the tunneling matrix element in the $\bar{q}$ qubit due to the interaction with an electron in the state qps. The two parameters that determine the tunneling corrections are $T_{p'}=\langle qps,\bar{q}p's'|V_C|q\bar{p}s,\bar{q}p's'\rangle$, and are due to the interaction with an electron in the $p'=I,O$ orbital in the other DQD [Fig. 3(b)].

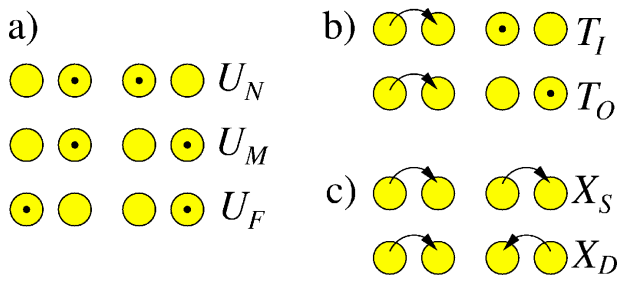

FIG. 3. (Color online) Effects of the direct Coulomb interaction between double quantum dots (DQDs). All the exchange terms between the DQDs vanish due to the impenetrable barrier. (a) The Coulomb repulsion between the electrons on different double quantum dots contributes to the energy of the system. In the case of identical DQDs separated by an impenetrable barrier, there are three such contributions, coming from the electrons in orbitals that are near (U_N), at a medium distance (U_M), or far apart (U_F). (b) The tunneling matrix elements within a DQD are renormalized by T_I or T_O due to the interaction with an electron on the inner or the outer dot of the other DQD. (c) The interaction enables the correlated hopping processes in which electrons simultaneously tunnel in both DQDs. In one such process, the electrons tunnel to the same side (either left or right) with the matrix element X_S. In the other correlated hopping process, electrons simultaneously tunnel into the inner or outer quantum dots of their double quantum dots with the matrix element X_D.

The terms in the third class are proportional to $c^{\dagger}_{qps}c_{q\bar{p}s}c^{\dagger}_{\bar{q}p's'}c_{\bar{q}\bar{p}s'}$ and describe the processes in which electrons in both DQD tunnel simultaneously [Fig. 3(c)]. The two independent matrix elements for these processes are $X_S=\langle qps,\bar{q}ps'|V_C|q\bar{p}s,\bar{q}\bar{p}s'\rangle$, describing the tunneling from the inner to the outer orbital in one DQD and from the outer to the inner in the other, and $X_D=\langle qps,\bar{q}\bar{p}s'|V_C|q\bar{p}s,\bar{q}ps'\rangle$, describing the simultaneous tunneling into inner or outer orbitals in both DQDs. For the system in zero magnetic field, these two matrix elements are equal, $X_S=X_D$.

C. Control of the interaction

In order to describe the influence of the intra-DQD tunneling t and the bias ϵ on the spectrum of the DDQD, we have to model the dependence of the Hamiltonian on these external parameters. In an experiment, both t and ϵ are controlled by applying voltages to the electrodes that define the quantum dots. The exact form of the voltage-dependent DDQD binding potential was studied using the Schrödinger-Poisson equation,[26] but here we do not attempt to calculate the dependence of the Hamiltonian [Eq. (2)] on ϵ and t from first principles.

Instead, we adopt a quartic double-well model for the potential of a DQD centered at $(\pm a_2,0)$ of the form[9]

$$V(x,y)=\frac{m\omega_0^2}{2}\left\{\frac{1}{4a_1^2}[(x\mp a_2)^2-a_1^2]^2+y^2\right\}, \tag{11}$$

where m is the electron effective mass, $2a_1$ is the distance between the approximately harmonic wells in a DQD, and $2a_2$ is the distance between the DQD double-well minima. In

the limit of well separated dots, $a_{1,2} \gg a_B$, where a_B is the QD Bohr radius given by $a_B^2 = \hbar/m\omega_0$, and near the local minima of the quartic potential well at $(\pm a_2 \pm a_1, 0)$, the potential is approximately harmonic with the frequency ω_0. The Fock-Darwin ground-state wave functions in this harmonic potential centered at $(x_c, 0)$ and in the magnetic field B normal to the plane of the dots, described in the symmetric gauge by the vector potential $\mathbf{A} = B(-y, x, 0)/2$, are

$$\phi_{x_c}(x,y) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-m\omega[(x-x_c)^2+y^2]/2\hbar + im\omega_L x_c y/\hbar}, \qquad (12)$$

where $\omega_L = eB/2mc$ is the electron Larmor frequency and $\omega = \sqrt{\omega_0^2 + \omega_L^2}$ is the resulting confinement frequency with both electrostatic and magnetic contributions. We will use the magnetic compression factor $b = \omega/\omega_0$ to measure the strength of the magnetic field, consistent with the notation in Ref. 9.

The translated single-electron Fock-Darwin states $\phi_{\pm a_2 \pm a_1}(x,y)$ define the state space of the variational HM approximation for a DDQD. The tunneling matrix element between the Fock-Darwin ground states in the local minima of the potential [Eq. (11)] is our control parameter t,[9]

$$t \equiv \langle \phi_{\pm a_2 + a_1} | H_1 | \phi_{\pm a_2 - a_1} \rangle = \frac{3}{8} \frac{S}{1+S^2} \left(\frac{a_1^2}{a_B^2} + \frac{1}{b} \right), \qquad (13)$$

where $S = \langle \phi_{\pm a_2 + a_1} | \phi_{\pm a_2 - a_1} \rangle = \exp[-d_1^2(2b - 1/b)]$ is the overlap between the Fock-Darwin ground states in a DQD and $d_1 = a_1/a_B$ is the distance between the QDs within the DQD in the units of the QD Bohr radius.

As t is changed by external voltages, we assume that the overlap S between the oscillator states remains consistent with the relation in Eq. (13), which is valid for the double-well potential V. All the Coulomb matrix elements can be expressed in terms of S so that after solving Eq. (13) for the overlap, they become functions of t (see the Appendix). The bias ϵ is modeled as an energy shift of the orbitals, so that the inner $p_k = I$ orbitals have their energy reduced by ϵ.

The two-qubit gates are applied by time-dependent tuning of the tunneling matrix element t and/or the bias ϵ in the DQDs using voltage pulses. In a typical experiment, the control of the QD energies through ϵ is much easier to achieve than the control over tunneling matrix element t.[27] The reason behind this is that the energy bias is linear in applied voltage, while the tunneling is typically exponential.

The structure of the energy levels is particularly simple in the limit of zero tunneling $t = 0$. In this limit, the eigenstates are the Hund-Mulliken basis states [Eqs. (4)–(7)]. Their energies are determined by the bias ϵ, the external magnetic field B, and the direct Coulomb interaction that is set by the device geometry. A drastic change in the structure of the DDQD spectrum as a function of bias ϵ appears at the crossings of the lowest-energy singlet states within a DQD. Each of the singlet states $|\bar{S}\rangle$, $|D_I\rangle$, and $|D_O\rangle$ is lowest in energy for some values of the bias ϵ (Fig. 4). A crossing occurs when either the positive bias overcomes the effective on-site repulsion $\tilde{U}$, making the state with both electrons in an inner dot $|D_I\rangle$ the lowest in energy, or the negative bias makes $|D_O\rangle$ the lowest in energy (see Fig. 5). We use the effective on-site repulsion $\tilde{U}$ to emphasize the fact that it includes not only the repulsion of two electrons in the same dot, denoted by U, but also the energy of the interaction with the electrons on the other DQD. We will also use two special values of the effective on-site repulsion, $U_\pm$. Due to the dependence of the effective on-site repulsion on the state of the other DQD, the lowest-energy singlet-singlet DDQD state can consist of dif-

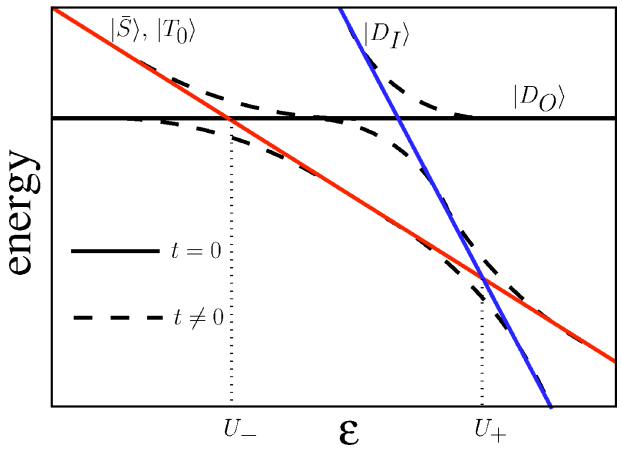

FIG. 4. (Color online) Illustration of the double quantum dot energy levels as a function of the bias ϵ. The energy of the singlet state with doubly occupied outer quantum dot, $|D_O\rangle$, is independent of the bias. The energies of the singly occupied singlet, $|\bar{S}\rangle$, and the singly occupied triplet, $|T_0\rangle$, state are lowered with the increasing bias as they have a contribution of -2ϵ from the biased inner quantum dots. The energy of the singlet with doubly occupied inner quantum dots, $|D_I\rangle$, is lowered with the increasing bias faster than the energy of $|\bar{S}\rangle$ and $|T_0\rangle$ state due to the bias contribution of -4ϵ. When the tunneling t is zero, the lowest-energy levels cross at the bias $U_\pm$, leading to a drastic change of the effective spin interaction. For nonzero tunneling, the levels anticross, but the effective spin interaction still changes significantly when we tune the system from one side of the anticrossing to the other.

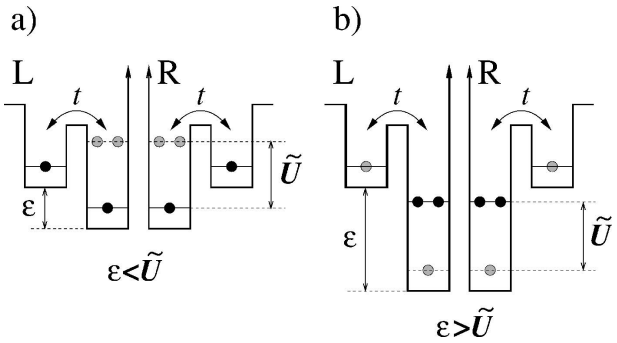

FIG. 5. Bias dependence of the double-double quantum dot (DDQD) ground state. (a) When the bias ϵ of the inner quantum dots with respect to the outer ones is weaker than the effective on-site Coulomb repulsion $\tilde{U}$, the charge configurations of the lowest-energy singlet and triplet states consists of singly occupied orbitals. (b) When $\epsilon > \tilde{U}$, the lowest-energy singlet has a doubly occupied inner quantum dot, while the orbital state of the lowest-energy triplet remains unchanged.

ferent singlets on the two dots, as in $|\bar{S},D_I\rangle$ and $|D_I,\bar{S}\rangle$. In the strong-bias regions, the lowest-energy singlets are doubly occupied states. For $\epsilon - U_+ \gg t$, the lowest-energy singlet is $|D_I D_I\rangle$, and for $U_- - \epsilon \gg t$, the lowest-energy singlet is $|D_O D_O\rangle$. The second doubly occupied singlet state is separated by an energy gap $\approx |2\epsilon|$ from the lowest-energy state.

III. STRONG BIAS

To develop an intuitive picture of the operation of an entangling two-qubit gate and the mechanisms for its control, we consider the simple case of strong bias. We show how the switching between the strong-bias regime ($\epsilon - U_+ \gg t$) and the weak-bias regime, in which the dominant interaction is the on-site repulsion, provides us with control over the entangling interaction E_e. The boundary of the strong-bias regime considered here is set by $U_+ = (3U_N - 2U_M - U_F - 2V_- + 2U)/2$. A similar strong-bias regime with the lowest-energy singlet $|D_O, D_O\rangle$ exists for $U_- - \epsilon \gg t$, where $U_- = (3U_F - 2U_M - U_N - 2V_- + 2U)/2$, but we do not consider it here in detail. In both of these regimes, a wide energy gap $\approx 2|\epsilon|$ to the second doubly occupied state allows us to neglect that state. This approximation reduces the dimensions of the Hamiltonian blocks H_{ab} [Eq. (2)] and allows for a perturbative solution.

Since the only available DQD states in the strong-bias regime are the triplet, $|T_0\rangle$, and two singlets, $|\bar{S}\rangle$ and $|D_I\rangle$, the H_{TT} block of Eq. (2) is one dimensional, H_{ST} and H_{TS} are two dimensional, and H_{SS} is four dimensional. For the present discussion of the strong-bias regime, we choose the zero of the energy scale at $4\hbar\omega - 2\epsilon + U + 2V_+ + U_N + 2U_M + U_F$, setting the expectation value of the energy of four singly occupied QDs with the DQDs in the electron singlet states to zero, $\langle \bar{S},\bar{S}|H|\bar{S},\bar{S}\rangle = 0$. Using the expressions for the Hamiltonian matrix elements given in the Appendix, we find the matrices of the H_{ab} blocks $(a,b = S,T)$. The energy of the $|TT\rangle$ state is then

$$E_{TT} = 2(V_- - V_+). \tag{14}$$

The two-dimensional blocks H_{TS} and H_{ST} are related by the symmetry under exchange of the double quantum dots $L \leftrightarrow R$ and in the bases $\{|\bar{S},T_0\rangle, |D_I,T_0\rangle\}$ and $\{|T_0,\bar{S}\rangle, |T_0,D_I\rangle\}$, and have the identical matrix form

$$H_{TS} = H_{ST} = V_- - V_+ + \begin{pmatrix} 0 & \sqrt{2}t_S \\ \sqrt{2}t_S & V_D - \epsilon \end{pmatrix}, \tag{15}$$

where $t_S = -t_H + T_S$ is the renormalized hopping matrix element and $V_D = U - V_+ + U_N - U_F$ is the electrostatic energy cost of doubly occupying the $p_k = I$ state in the presence of the triplet DQD. With our choice of the zero of the energy scale, the ground-state energies of H_{ST} and H_{TS} are

$$E_{ST} = E_{TS} = V_- - V_+ + \frac{1}{2}(V_D - \epsilon) - \frac{1}{2}\sqrt{(V_D - \epsilon)^2 + 8t_S^2}. \tag{16}$$

From the energies E_{ST} and E_{TS}, we extract the isotropic exchange part of the low-energy four-spin Hamiltonian [Eq. (3)] as

$$J = E_{TT} - E_{ST} = E_{TT} - E_{TS}. \tag{17}$$

The resulting exchange interaction strength is

$$J = V_- - V_+ - \frac{1}{2}(V_D - \epsilon) + \frac{1}{2}\sqrt{(V_D - \epsilon)^2 + 8t_S^2}. \tag{18}$$

Comparing this result with the case of an unbiased isolated double quantum dot [Eq. (10)], we see that the effect of the strong bias ϵ and the presence of another DQD behind the impenetrable barrier is the change of the effective on-site repulsion to the value $V_D - \epsilon$ and a reduction of the effective tunneling matrix element because of the large gap to the excited doubly occupied state. As a consequence of this gap, the isotropic exchange in the limit of noninteracting DQDs and weak tunneling is $J = V_- - V_+ + 2t_H^2/(U - V_+ - \epsilon)$, with the hopping contribution reduced to half of the result expected from the standard Hubbard model in the unbiased case, $4t_H^2/U_H$.[9]

The four-dimensional block H_{SS} in the basis $\{|\bar{S},\bar{S}\rangle, (|\bar{S},D_I\rangle + |D_I,\bar{S}\rangle)/\sqrt{2}, |D_I,D_I\rangle, (|\bar{S},D_I\rangle - |D_I,\bar{S}\rangle)/\sqrt{2},\}$ is

$$H_{SS} = \begin{pmatrix} 0 & 2t_S & 2X_D & 0 \\ 2t_S & V_D - \epsilon + 2X_S & 2t_I & 0 \\ 2X_D & 2t_I & E_{DD} & 0 \\ 0 & 0 & 0 & V_D - \epsilon - 2X_S \end{pmatrix}, \tag{19}$$

where t_I is the tunneling matrix element renormalized by the spectator DQD in the doubly occupied state, and

$$E_{DD} = 2U + 3U_N - 2U_M - U_F - 2V_+ - 2\epsilon \tag{20}$$

accounts for the repulsion energy of four electrons in the $p_k = I$ orbitals and the bias ϵ (see the Appendix). Due to the symmetry with respect to exchange of the DQDs, $L \leftrightarrow R$, the antisymmetric state $(|\bar{S},D_I\rangle - |D_I,\bar{S}\rangle)/\sqrt{2}$ decouples from the other, symmetric, states.

In the limit of large and positive bias, $|\epsilon - V_D| \gg t_{S/I}, X_{S/D}$, all the tunneling and correlated hopping terms in the Hamiltonian H_{SS} can be taken to be small. The unperturbed Hamiltonian is then diagonal and the ground-state energy is E_{DD}. This situation is relevant because all the small terms are proportional to the overlap S of the localized states in the quantum dots, which is small for weakly tunnel-coupled QDs, and we can reach this regime by applying external voltage to make $|\epsilon - V_D|$ large enough.

Operating the system in the strong-bias regime causes a qualitative change to the effective low-energy Hamiltonian by turning on the entanglement generating term E_e in Eq. (3),

$$E_e = E_{TT} - 2E_{ST} + E_{SS}. \tag{21}$$

For a weak bias and in the absence of tunneling, the entanglement generating E_e term is zero, as can be checked from the energies of the states $|\bar{S},\bar{S}\rangle$, $|T_0,\bar{S}\rangle$, and $|T_0,T_0\rangle$,

given in the Appendix. This is not true in the case of a strong bias, where the entangling interaction of the strength $E_e = U_N - 2U_M + U_F \neq 0$ is present even if the tunneling terms are zero. In the strong-bias regime, the conditions for $E_e=0$ are $t_I=t_S$, $X_S=X_D$, and $E_{DD}=2(V_D-\epsilon)$. While the first two conditions are satisfied when there is no tunneling, the third is independent of the tunneling. It is only satisfied in the limit of long distance between DQDs, $a_2 \gg a_1$ (see Fig. 1). The tunneling causes a second-order correction to E_{SS},

$$E_{SS} = E_{DD} + \frac{4t_I^2}{E_{DD} - (V_D - \epsilon)} + \frac{4X_D^2}{E_{DD}}, \tag{22}$$

and the corresponding correction to E_e.[28] Since the basic control mechanism relies on turning the entangling interaction on and off in the $E_e \neq 0$ and $E_e=0$ regimes, the control is robust against small imperfections. For example, if the quantum dots are not identical or the distances between the QDs within two DQDs are different, the value of E_e would change, but it could still be turned on and off using external voltages.

We have calculated the matrix elements of the Coulomb interaction using the basis of single-electron Wannier states obtained by orthogonalizing the Fock-Darwin ground states centered at the quantum dot positions, following Ref. 9. The resulting matrix elements can all be expressed in terms of the distances between the quantum dots and the tunneling matrix element t between QD in DQD. These results are summarized in the Appendix. Together with Eqs. (3), (18), and (22), they provide a model of the low-energy Hamiltonian of a pair of qubits realized on a DDQD in the strong-bias regime. This model can describe a two-qubit quantum gate realized by adiabatically switching the value of the control parameter ϵ so that the qubit goes from the weak-bias regime to the strong-bias regime and back.

In an array of DQDs, where each encodes a qubit, a quantum gate can be applied by bringing the pairs of neighboring qubits that we would like to entangle into the $E_e \neq 0$ regime, while keeping $E_e=0$ for all the other pairs. Each QD can play the role of either an inner or an outer QD, depending on the neighbor with which the entanglement is created. The Hamiltonian [Eq. (3)] and the gates generated by it are invariant under the interchange of the inner and outer QDs within a qubit.

In summary, the interaction of the DQDs causes a change in the parameters of the extended Hubbard model coupling strength [Eq. (10)] so that the energies and hopping matrix elements on one DQD depend on the state of the other. Also, the processes in which the hopping of electrons on the two DQDs is correlated and mediated by the direct Coulomb interaction become possible (see Fig. 3). The coupling between the DQDs causes an effective spin interaction that deviates from the form of exchange-coupled qubits, adding the entangling term E_e to Eq. (3). This deviation creates the entanglement between the two qubits. The generation of entanglement can be efficiently controlled by changing the bias ϵ.

IV. GENERAL BIAS

The study of a DDQD system in the strong-bias regime presented in Sec. III allows for a simple perturbative solution and offers an insight into the mechanism of entanglement generation. However, it lacks sufficient predictive power for a general analysis of a realistic two-qubit quantum gate: When switching on and off the entangling interaction, a continuous voltage pulse is applied, and the system undergoes a smooth transition from the strong-bias regime to the unbiased (or merely biased) regime and vice versa. During this transition, the system has to pass through an intermediate weak-bias regime where the perturbative expansion [Eq. (22)] breaks down.

In this section, we calculate the full HM Hamiltonian of the four quantum dots, including both $|D_I\rangle$ and $|D_O\rangle$ states. This calculation allows us to predict the quantum gate generated by an arbitrarily shaped adiabatic pulse of the control parameters t and ϵ. The main difference in the system's description is that now we take into account both doubly occupied states $|D_I\rangle$ and $|D_O\rangle$ in each DQD. Therefore, we are working in the entire Hilbert space of the HM approximation, and the strong-bias requirement is not important. Now, H_{TT} is one dimensional, H_{ST} and H_{TS} are three dimensional, and H_{SS} is nine dimensional.

Following the discussion of Sec. III, the effective low-energy spin Hamiltonian H [Eq. (3)] is determined by the energies E_{ab}, where $a,b=S,T$, of the lowest-energy states of a given spin configuration. Due to the $L \leftrightarrow R$ symmetry, H is the sum of the isotropic exchange terms and the entangling term. We proceed by calculating the matrix elements of the Hamiltonian as a function of the tunneling matrix element t and the bias ϵ. The results of this calculation are given in the Appendix. Numerical diagonalization of the resulting Hamiltonian gives the energies E_{ab} for each of the blocks H_{ab}, where $a,b=S,T$. Finally, we extract the effective low-energy Hamiltonian parameters J and E_e using Eqs. (17) and (21).

The dependence of the isotropic exchange coupling on the bias $J(\epsilon)$ is illustrated in Fig. 6. In the zero-tunneling limit, we can identify three regions of qualitatively different behaviors of $J(\epsilon)$. For strong and negative bias, $\epsilon < U_-$, corresponding to the $|D_O D_O\rangle$ lowest-energy singlet state, the isotropic exchange coupling is decreasing linearly with the bias. In the intermediate region, $U_- < \epsilon < U_+$, the exchange coupling is absent. For strong and positive bias, $U_+ < \epsilon$, the exchange coupling grows linearly with ϵ. The asymmetric placement of the $J=0$ plateau is a consequence of the different repulsion energies of the electrons in the inner and outer QDs. As the tunneling is turned on, the isotropic exchange couplings become larger due to the mixing of the doubly occupied states in the plateau region. For a zero magnetic field, the coupling J is positive. In a finite field, there is a region with negative J, consistent with the analysis of Ref. 9 and the experimental findings of Ref. 29.

A plot of the entanglement generating interaction E_e is given in Fig. 7. The zero-tunneling value of E_e shows a structure determined by the Coulomb energies of the basis states [Eqs. (4)–(7)]. In a wide plateau of small bias, the entangling interaction vanishes because all of the lowest-energy states of definite spin are products of $|\bar{S}\rangle$ and $|T_0\rangle$. Since the direct exchange interaction $V_- - V_+$ is zero in the absence of tunneling, those two states are equal in energy. When the bias overcomes the on-site repulsion, the lowest-

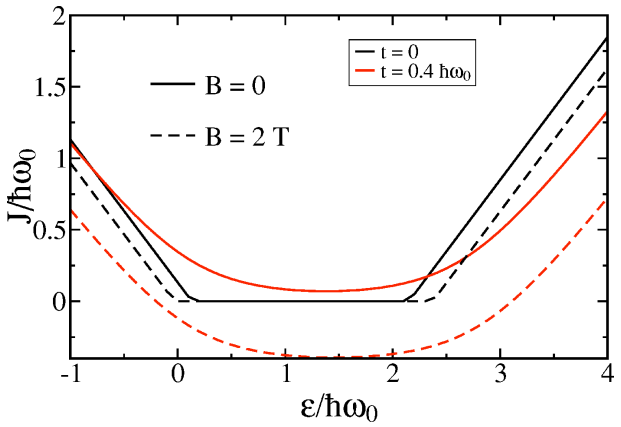

FIG. 6. (Color online) Isotropic exchange coupling J as a function of the bias ϵ. In the regions of strong positive and negative bias, the exchange coupling is approximately linear $J \propto |\epsilon|$. In the intermediate region, the exchange is zero in the zero-tunneling limit and becomes nonzero as the tunneling is turned on. The coupling J is always positive in the absence of a magnetic field. The external magnetic field drives J to negative values in a relatively wide range of values of the tunneling matrix element and bias. The confinement energy of the quantum dots is chosen to be $\hbar\omega_0 = 3$ meV, which corresponds to a quantum dot Bohr radius $a_B = 20$ nm in GaAs. The distances between the dots are chosen to be $2a_1 = 1.6a_B$ and $2a_2 = 3a_B$.

energy states of H_{SS}, H_{ST}, and H_{TS} change. The degenerate lowest-energy states of H_{SS} are either $|\bar{S}D_I\rangle$ and $|D_I\bar{S}\rangle$, in the region of large bias on the right of the plateau, or $|\bar{S}D_O\rangle$ and $|D_O\bar{S}\rangle$, in the region of smaller bias to the left of the plateau. Simultaneously, the analogous states with $|\bar{S}\rangle$ replaced by $|T_0\rangle$ become the lowest-energy states in H_{ST} and H_{TS}. In these two regions, E_e is a linear function of ϵ, $E_e = U_N - U_F - U - \epsilon$ on the left and $E_e = -U_N + U_F - U + \epsilon$ on the right of the plateau. When the absolute value of the bias is even higher, the lowest-energy state in H_{SS} is $|D_I D_I\rangle$ for a very strong and positive bias and $|D_O D_O\rangle$ for a very strong and negative bias. These regions are characterized by an ϵ-independent $E_e = U_N - 2U_M + U_F$ for large $|\epsilon|$. The values $U_\pm$ for the bias ϵ at which the changes in zero-tunneling lowest-energy states occur depend on the geometry of the device, described by the distances $2a_1$ and $2a_2$ (Fig. 1) and the quantization energy $\hbar\omega_0$, and correspond to the changes in behavior of the exchange coupling strength J.

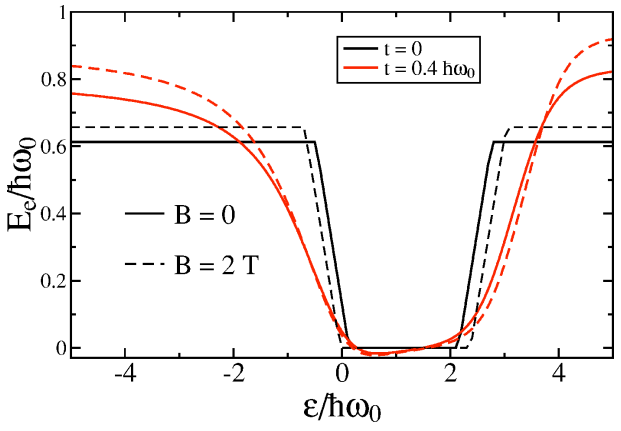

FIG. 7. (Color online) Entangling interaction E_e as a function of bias. The plots correspond to different values of the tunneling matrix elements t within the double quantum dots in the absence of a magnetic field and in an external magnetic field of $B = 2$ T. The $t = 0$ plot indicates the regions of different lowest-energy singlets and the positions of crossings. The strength of the entangling interaction E_e can be changed significantly by tuning the bias ϵ at a fixed tunneling matrix element t. Parameters used in this plot are the same as in Fig. 6.

The zero-tunneling case shows a desirable feature in that E_e, the quantity that determines the entanglement between the qubits, can be switched on and off by tuning ϵ. However, the regions of different E_e cannot be reached by adiabatic pulses in the $t \to 0$ limit. Turning on the tunneling t between the QDs will introduce transitions between previously disconnected regions, and the adiabatic gates become possible. The simple $t = 0$ picture of the entanglement generated by a difference in Coulomb energies is perturbed by the transitions. It is no longer possible to turn off E_e throughout the plateau region by a change in ϵ alone. In the plateau region, E_e is generically nonzero, but small. Therefore, in order to turn off the entangling interaction when t is kept constant, it is desirable to keep t small and to tune ϵ to a value where $E_e = 0$.

V. QUANTUM GATE OPERATION

For a quantum gate applied by the time-dependent Hamiltonian [Eq. (2)], with the parameters t and ϵ changing adiabatically on the time scale set by the energy gap between the states within the blocks H_{ab}, the applied gate is determined by the splittings between the lowest-lying states in each of the subspaces of the definite spin. If the energies of the lowest-energy states in singlet-singlet, singlet-triplet, triplet-singlet, and triplet-triplet subspaces are $E_{SS}(t)$, $E_{ST}(t) = E_{TS}(t)$, and $E_{TT}(t)$, respectively, the gate applied by an adiabatic pulse starting at the time t_i and finishing at t_f will be $\mathcal{U} = \mathrm{diag}(\phi_{SS}, \phi_{ST}, \phi_{TS}, \phi_{TT})$, with the phases

$$\phi_{ab} = \exp -\frac{i}{\hbar}\int_{t_i}^{t_f} E_{ab}(t)dt. \tag{23}$$

With the ability to turn the entangling interaction on and off and perform single-qubit gates, it is possible to perform a CNOT gate on a pair of qubits encoded into spin states of DQD. We consider a quantum gate implemented by first adiabatically turning on the entangling interaction for a period τ_{on}, and then again adiabatically switching to the Hamiltonian with the entangling interaction off for the time interval τ_{off}. The lowest-energy states in each of the *SS*, *ST*, *TS*, and *TT* subspaces will acquire a phase dependent on the control parameters ϵ and t and the pulse durations. In the *on* state, the Hamiltonian that describes the ground states in all

the spin subspaces is, up to a constant, $H_{\rm on}=\mathrm{diag}(E_e,J_{\rm on},J_{\rm on},2J_{\rm on})$, where E_e is the strength of the entangling interaction in the *on* regime and $J_{\rm on}$ is the corresponding exchange coupling. After the DDQD was in the on state for the time $\tau_{\rm on}$, the applied gate is

$$\mathcal{U}_{\rm on}=\exp-i\frac{\tau_{\rm on}}{\hbar}H_{\rm on}. \tag{24}$$

Similarly, during the subsequent period of duration $\tau_{\rm off}$ when the entangling interaction is set to zero, the applied gate is

$$\mathcal{U}_{\rm off}=\exp-i\frac{\tau_{\rm off}}{\hbar}H_{\rm off}, \tag{25}$$

where $H_{\rm off}=\mathrm{diag}(0,J_{\rm off},J_{\rm off},2J_{\rm off})$ in analogy with the on regime. The resulting gate is

$$\mathcal{U}=\mathcal{U}_{\rm off}\mathcal{U}_{\rm on}=\exp-i\begin{pmatrix}\phi & 0 & 0 & 0\\ 0 & \lambda & 0 & 0\\ 0 & 0 & \lambda & 0\\ 0 & 0 & 0 & 2\lambda\end{pmatrix}, \tag{26}$$

where $\hbar\lambda=J_{\rm on}\tau_{\rm on}+J_{\rm off}\tau_{\rm off}$ is the integrated strength of the exchange coupling in DQD and $\hbar\phi=E_{\rm on}\tau_{\rm on}$ is the integrated strength of the entangling interaction.

The CPHASE gate, which is equivalent to CNOT up to single-qubit rotations, is obtained when the gate parameters satisfy $\phi=m\pi$ and $\lambda=n\pi$, for an odd integer m and an arbitrary integer n. In order to complete a CNOT, we follow a pulse of on-state Hamiltonian of the duration $\tau_{\rm on}=m\pi\hbar/E_e$ by a pulse of the off-state Hamiltonian with the duration $\tau_{\rm off}=\hbar(n\pi-J_{\rm on}\tau_{\rm on}/\hbar)/J_{\rm off}$. The resulting gate is $\mathrm{diag}(-1,-1,-1,1)=-$CPHASE, for odd n and $\mathrm{diag}(-1,1,1,1)$, which is equal to CPHASE with the X gate applied to both qubits before and after $\mathcal{U}$. For any integer n,

$$\text{CPHASE}\sim(\xi\otimes\xi)\mathcal{U}(\xi\otimes\xi), \tag{27}$$

where $\xi=\exp[i\pi[1+(-1)^n]\sigma_x/4]$. In order to complete the CNOT, we apply the one-qubit Haddamard gates $H=(X+Z)/\sqrt{2}$ to the target qubit both before and after the entangling gate $\mathcal{U}$. The entire construction can be represented as

$$\text{CNOT}=(\mathbf{1}\otimes H)(\xi\otimes\xi)\mathcal{U}(\xi\otimes\xi)(\mathbf{1}\otimes H). \tag{28}$$

Note that the CNOT construction necessarily involves the single-qubit rotations about pseudospin axes different from z. Such operations can be performed using the asymmetric bias within a DQD that encodes the qubit in an inhomogeneous external magnetic field.[27] The entangling part of a CNOT gate can be performed by pulsing the bias ϵ only and keeping the tunneling t constant. Therefore, control over the bias ϵ and the availability of an inhomogeneous magnetic field are sufficient for the universal quantum computing with two-spin qubits.

VI. CONCLUSION

We have analyzed two-qubit gates in a pair of qubits, each encoded into singlet and triplet states of a DQD and coupled by Coulomb repulsion. A two-qubit CNOT gate, which together with the single-qubit rotations forms a universal set of quantum gates, can be performed by tuning the bias of the inner dots with respect to the outer ones. We identify the entangling interaction strength E_e as a quantity that has to be controlled in order to implement a CNOT with the aid of single-qubit rotations.

The dependence of E_e on the externally controllable bias ϵ and the tunneling matrix element t shows that it can, in principle, be turned on and off by changing ϵ alone, if sufficiently low values of t are available.

The largest change in E_e comes from a tuning of the system through the resonance between the singly occupied state and the doubly occupied state on a DQD. At the side of the resonance with a singly occupied ground state, and far from the resonance, the entangling interaction E_e is caused by inter-DQD correlation and is small. On the other side of the resonance, with a doubly occupied DQD ground state, the entangling interaction is caused by the direct Coulomb repulsion and it is much stronger. Two-qubit gates necessary for a universal set of gates can be performed by switching between the strong and weak entanglement generation regimes using voltage pulses.

ACKNOWLEDGMENTS

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APPENDIX: HUND-MULLIKEN 16×16 HAMILTONIAN

The full Hund-Mulliken Hamiltonian is block diagonal due to the symmetry of the interactions with respect to arbitrary rotations in spin space. In reality, this symmetry is broken by the weak spin-orbit coupling interaction that we have neglected. The blocks are the one-dimensional H_{TT}, the two three-dimensional H_{TS} and H_{ST}, and the nine-dimensional H_{SS}, where T stands for a triplet and S for a singlet state on a DQD. In this appendix, we present the matrices of these blocks as functions of the system geometry and the control parameters.

There is only one TT state and its energy is

$$H_{TT}=E_{TT}=2V_-+U_N+2U_M+U_F-2\epsilon. \tag{A1}$$

The three-dimensional blocks H_{TS} and H_{ST} are related by the symmetry operation of exchanging the DQD, and if we choose the basis $\{|T_0,\bar{S}\rangle,|T_0,D_I\rangle,|T_0,D_O\rangle\}$ for the TS and $\{|\bar{S},T_0\rangle,|D_I,T_0\rangle,|D_O,T_0\rangle\}$ for the ST subspace, they can both be represented by the matrix

$$H_{TS}=H_{ST}=\begin{pmatrix}C_{TS} & \sqrt{2}t_S & \sqrt{2}t_S\\ \sqrt{2}t_S & C_{TI} & X\\ \sqrt{2}t_S & X & C_{TO}\end{pmatrix}. \tag{A2}$$

The nine-dimensional block of singlet states, in the direct product basis composed out of the two-electron states [Eq. (4)–(6)], is

$$H_{SS} = \begin{pmatrix} C_{SS} & \sqrt{2}t_S & \sqrt{2}t_S & \sqrt{2}t_S & 2X_D & 2X_S & \sqrt{2}t_S & 2X_S & 2X_D \\ \sqrt{2}t_S & C_{SI} & X & 2X_S & \sqrt{2}t_I & 0 & 2X_D & \sqrt{2}t_I & 0 \\ \sqrt{2}t_S & X & C_{SO} & 2X_D & 0 & \sqrt{2}t_O & 2X_S & 0 & \sqrt{2}t_O \\ \sqrt{2}t_S & 2X_S & 2X_D & C_{IS} & \sqrt{2}t_I & \sqrt{2}t_I & X & 0 & 0 \\ 2X_D & \sqrt{2}t_I & 0 & \sqrt{2}t_I & C_{II} & X & 0 & X & 0 \\ 2X_S & 0 & \sqrt{2}t_O & \sqrt{2}t_I & X & C_{IO} & 0 & 0 & X \\ \sqrt{2}t_S & 2X_D & 2X_S & X & 0 & 0 & C_{OS} & \sqrt{2}t_O & \sqrt{2}t_O \\ 2X_S & \sqrt{2}t_I & 0 & 0 & X & 0 & \sqrt{2}t_O & C_{OI} & X \\ 2X_D & 0 & \sqrt{2}t_O & 0 & 0 & X & \sqrt{2}t_O & X & C_{OO} \end{pmatrix}. \tag{A3}$$

We do not antisymmetrize with respect to the permutations of electrons that belong to different quantum dots and have nonoverlapping orbital wave functions. The matrix elements of the Hamiltonian that describe the Coulomb interaction within a DQD (intra-DQD terms), U, t, X, V_+, and V_-, were analyzed in Ref. 9. The inter-DQD elements depend on the following matrix elements of the Coulomb interaction between the product states of the $|qps\rangle$ electrons localized in the qubit q and the quantum dot p and having a spin s:

$$X_S = \langle LIs, RIs' | V_C | LOs, ROs' \rangle, \tag{A4}$$

$$X_D = \langle LIs, ROs' | V_C | LOs, RIs' \rangle, \tag{A5}$$

$$T_O = \langle LOs, ROs' | V_C | LIs, ROs' \rangle, \tag{A6}$$

$$T_I = \langle LIs, RIs' | V_C | LIs, ROs' \rangle. \tag{A7}$$

In zero magnetic field, we find that $X_S = X_D$.

The off-diagonal elements are determined by

$$t_S = T_O + T_I - t_H, \tag{A8}$$

$$t_I = 2T_I - t_H, \tag{A9}$$

$$t_O = 2T_O - t_H, \tag{A10}$$

and the diagonal elements are given by

$$C_{TT} = 2V_- + U_N + 2U_M + U_F - 2\epsilon, \tag{A11}$$

$$C_{TS} = V_+ + V_- + U_N + 2U_M + U_F - 2\epsilon, \tag{A12}$$

$$C_{TI} = V_- + U + 2U_N + 2U_M - 3\epsilon, \tag{A13}$$

$$C_{TO} = V_- + U + 2U_M + 2U_F - \epsilon, \tag{A14}$$

$$C_{SS} = U_N + 2U_M + U_F + 2V_+ - 2\epsilon, \tag{A15}$$

$$C_{SI} = 2U_M + 2U_F + U + V_+ - 3\epsilon, \tag{A16}$$

$$C_{SO} = 2U_M + 2U_F + U + V_+ - \epsilon, \tag{A17}$$

$$C_{II} = 4U_N + 2U - 4\epsilon, \tag{A18}$$

$$C_{IO} = 4U_M + 2U - 2\epsilon, \tag{A19}$$

$$C_{OO} = 4U_F + 2U, \tag{A20}$$

where the symmetry with respect to exchange of the DQDs leads to $C_{AB} = C_{BA}$, where $A, B \in \{T, S, I, O\}$.

To represent the matrix elements in terms of the system parameters, the single QD quantization energy $\hbar\omega_0$, tunneling matrix element within an isolated DQD t, the bias ϵ, and the interdot distances a_1 and a_2, we have to adopt a model for the binding potential of a DQD and the orbitals of Hund-Mulliken approximation. We assume that the QD orbitals are Wannier functions obtained by orthogonalization of the Fock-Darwin ground states centered at the positions of the QDs within a DQD, $(a_2 \pm a_1, 0)$ and $(-a_2 \pm a_1, 0)$. The Wannier orbitals are of the generic form

$$|W_{q,I}\rangle = N(|\phi_{q,I}\rangle - g|\phi_{q,O}\rangle), \tag{A21}$$

$$|W_{q,O}\rangle = N(-g|\phi_{q,I}\rangle + |\phi_{q,O}\rangle), \tag{A22}$$

where $|\phi_{q,I(O)}\rangle$ is the Fock-Darwin ground state on the dot belonging to the qubit $q = L, R$ and the inner (I) or outer (O) QD [Eq. (12)]. The Wannier orbitals are determined by the overlap of these wave functions, $S = \langle \phi_{q,I} | \phi_{q,O} \rangle = \exp[-d_1^2(2b - 1/b)]$, through the mixing $g = (1 - \sqrt{1 - S^2})/S$ and normalization constant $N = 1/\sqrt{1 - 2gS + g^2}$.

The Coulomb interaction matrix elements for the DQD centered at $\pm a_2 = \pm d_2 a_B$ and QDs within a DQD displaced by $\pm a_1 = \pm d_1 a_B$ from the center of the DQD are then expressed as

$$\begin{aligned} U_N = cN^4 \Big\{ & f(d_2 - d_1, 0) + 2g^2(1 + S^2) f(d_2, 0) \\ & + g^4 f(d_1 + d_2, 0) + 2S^2 g^2 f(d_2, d_1) \\ & - 4gS \left[f\left(d_2 - \frac{d_1}{2}, \frac{d_1}{2}\right) + g^2 f\left(d_2 + \frac{d_1}{2}, \frac{d_1}{2}\right) \right] \Big\}, \end{aligned} \tag{A23}$$

$$U_F = cN^4\Big\{ f(d_2+d_1,0) + 2g^2(1+S^2)f(d_2,0) + g^4 f(d_2-d_1,0) + 2S^2 g^2 f(d_2,d_1) - 4gS\left[f\left(d_2+\frac{d_1}{2},\frac{d_1}{2}\right) + g^2 f\left(d_2-\frac{d_1}{2},\frac{d_1}{2}\right)\right]\Big\}, \tag{A24}$$

$$U_M = cN^4\Big\{ (1+g^4)f(d_2,0) + g^2\{f(d_1+d_2,0) + f(d_1-d_2,0) + 2S^2[f(d_2,0)+f(d_2,d_1)]\} - 2gS(1+g^2)\left[f\left(d_2+\frac{d_1}{2},\frac{d_1}{2}\right) + f\left(d_2-\frac{d_1}{2},\frac{d_1}{2}\right)\right]\Big\}, \tag{A25}$$

$$T_O = cN^4\Big\{ S\Big[(1+3g^2)f\left(d_2+\frac{d_1}{2},\frac{d_1}{2}\right) + (g^4+3g^2)f\left(d_2-\frac{d_1}{2},\frac{d_1}{2}\right)\Big] - (g+g^3)[(1+S^2)f(d_2,0) + S^2 f(d_2,d_1)] - gf(d_2+d_1,0) - g^3 f(d_2-d_1,0)\Big\}, \tag{A26}$$

$$T_I = cN^4\Big\{ S\Big[(1+3g^2)f\left(d_2-\frac{d_1}{2},\frac{d_1}{2}\right) + (g^4+3g^2)f\left(d_2+\frac{d_1}{2},\frac{d_1}{2}\right)\Big] - (g+g^3)[(1+S^2)f(d_2,0) + S^2 f(d_2,d_1)] - gf(d_2-d_1,0) - g^3 f(d_2+d_1,0)\Big\}, \tag{A27}$$

$$X_S = cN^4\Big\{ (S^2+2g^2+g^4S^2)f(d_2,0) + g^2[f(d_1+d_2,0) + f(d_1-d_2,0) + 2S^2 f(d_2,d_1)] - 2S(g+g^3)\left[f\left(d_2+\frac{d_1}{2},\frac{d_1}{2}\right) + f\left(d_2-\frac{d_1}{2},\frac{d_1}{2}\right)\right]\Big\}, \tag{A28}$$

$$X_D = cN^4\Big\{ S^2(1+g^4)f(d_2,d_1) + g^2[f(d_1+d_2,0) + f(d_2-d_1,0) + 2(1+S^2)f(d_2,0)] - 2S(g+g^3) \times\left[f\left(d_2+\frac{d_1}{2},\frac{d_1}{2}\right) + f\left(d_2-\frac{d_1}{2},\frac{d_1}{2}\right)\right]\Big\}, \tag{A29}$$

in terms of the overlaps of the harmonic oscillator wave functions S, the mixing factor g, and the function

$$f(d,l) = \sqrt{b}\,\exp[-\alpha(d,l)]I_0(\alpha(d,l)), \tag{A30}$$

where $\alpha(d,l)=bd^2-(b-1/b)l^2$. We use the contraction factor $b=\omega/\omega_0$ to measure the magnetic field strength. The overall strength of the Coulomb interaction is set by $c=\sqrt{\pi/2}e^2/\kappa\hbar\omega_0 a_B$, where e is the electron charge, κ is the dielectric constant, and $\hbar\omega_0$ is the single isolated QD quantization energy.[9]

To model the dependence of the matrix elements on the externally controllable tunneling matrix element t, we use the connection between the tunneling and the overlap $S=S(t)$ that holds for the quartic double well, Eq. (13) and assume that it holds throughout the gate operation.

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