Tunable Spin-Qubit Coupling Mediated by a Multielectron Quantum Dot

V. Srinivasa,* H. Xu, and J. M. Taylor
Joint Quantum Institute, University of Maryland, College Park, Maryland 20742, USA
and National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA
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We present an approach for entangling electron spin qubits localized on spatially separated impurity atoms or quantum dots via a multielectron, two-level quantum dot. The effective exchange interaction mediated by the dot can be understood as the simplest manifestation of Ruderman-Kittel-Kasuya-Yosida exchange, and can be manipulated through gate voltage control of level splittings and tunneling amplitudes within the system. This provides both a high degree of tunability and a means for realizing high-fidelity two-qubit gates between spatially separated spins, yielding an experimentally accessible method of coupling donor electron spins in silicon via a hybrid impurity-dot system.

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Single spins in solid-state systems represent versatile candidates for scalable quantum bits (qubits) in quantum information processing architectures [1–6]. In many proposals involving single-spin qubits localized on impurity atoms [2,7] and within quantum dots [1,8], two-qubit coupling schemes harness the advantages of tunneling-based nearest-neighbor exchange interactions: exchange gates are rapid, tunable, and protected against multiple types of noise [9–13]. These features have been demonstrated for electron spins in quantum dots [14–18], while a similar demonstration for spins localized on impurity atoms such as phosphorus donors in silicon remains an outstanding experimental challenge [6,19].

Although the exchange interaction originates from the long-range Coulomb interaction, directly coupling two spins via exchange typically has a strength that decays exponentially with distance [8,20]. Many approaches to implementing long-range interactions therefore involve identifying a system that acts as a mediator of the interaction between the qubits, with proposed systems including optical cavities and microwave stripline resonators [21–26], floating metallic [27] and ferromagnetic [28] couplers, the collective modes of spin chains [29–31], superconducting systems [32,33], and multielectron molecular cores [34]. Recently, long-range coupling of electrons located in the two outer quantum dots of a linear triple-dot system has been demonstrated [35,36]. The effective exchange interaction in that system arises from electron cotunneling between the outer dots and exhibits the fourth-order dependence on tunneling amplitudes that is characteristic of superexchange [37], but suffers from a large virtual energy cost from the doubly occupied center dot states. In contrast, a many-electron quantum dot in the center can also couple distant spins via the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, with low-energy intermediate states [38,39], but perhaps at the cost of low fidelity as impurity-Fermi sea correlations become hard to disentangle [40,41].

Here, we show that a multilevel quantum dot containing two electrons can mediate a high-fidelity exchange interaction between two spatially separated single-electron spin qubits. We assume in what follows that the qubit electrons are localized on single-level impurity atoms, but our analysis also maps directly to the case of a triple quantum dot system [35,36] with the same level structure and electron occupation. Our approach suggests an experimentally accessible method for achieving tunable coupling between donor electron spins in silicon [19,42,43].

Hubbard model description.—The minimal model for our approach comprises a two-level quantum dot coupled to two impurities which are chosen to be near their ionization point by appropriate choice of gate voltages. This reduces to a multiorbital Hubbard model for a linear three-site system in the four-electron regime [44,45]. We assume gate voltages can be applied to the system such that the total electron number can be set to be four, while the charge stability diagram prefers the initial configuration of (1, 2, 1). Here, (n_L, n_M, n_R) represents the configuration with n_L (n_R) electrons in impurity orbital L (R) and n_M electrons in the mediator dot (Fig. 1). We work at a point in the charge stability diagram where transitions to charge configurations (0, 3, 1) and (1, 3, 0) are the closest available charge states, with detunings Δ_L, Δ_R [Fig. 1(a)].

We can write the Hamiltonian as $H_{\mathrm{Hub}} = H_n + H_t$, where

$$H_n = \sum_i \epsilon_i n_i + \frac{U_i}{2} n_i(n_i - 1) + \sum_{i \neq j} \frac{K_{ij}}{2} n_i n_j + J_{12} \sum_{\sigma,\sigma'} c^\dagger_{1,\sigma} c^\dagger_{2,\sigma'} c_{1,\sigma'} c_{2,\sigma}, \quad (1)$$

$$H_t = -\sum_{i=1,2} \sum_\sigma \left(t_{Li} c^\dagger_{i,\sigma} c_{L,\sigma} + t_{Ri} c^\dagger_{i,\sigma} c_{R,\sigma} + \mathrm{H.c.} \right) \quad (2)$$

with $i, j = L, R, 1, 2$ denoting the impurity and dot orbitals shown in Fig. 1(b). H_n is diagonal with respect to the

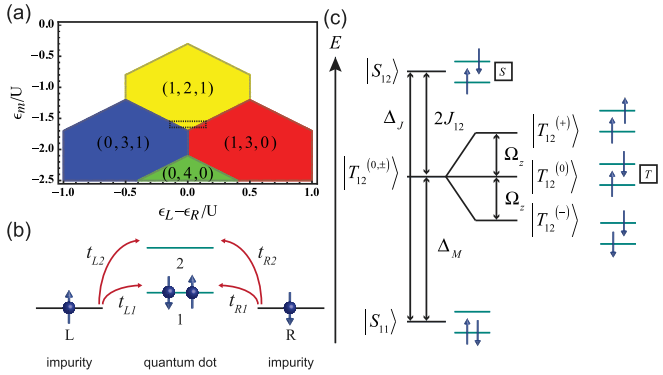

FIG. 1 (color online). (a) Charge stability diagram for the combined impurity-dot three-site model ($U \equiv U_1$, $\epsilon_m \equiv \epsilon_1$), with the operating point indicated. (b) Schematic diagram showing the orbitals of a pair of single-level impurity atoms coupled via a two-level quantum dot. The electron occupation illustrates the initial configuration (1, 2, 1). Arrows depict the tunneling amplitudes defined in Eq. (2). Reversing the direction of an arrow corresponds to taking the complex conjugate of the associated tunneling amplitude. (c) Energy level diagram illustrating the two-spin states of the mediator dot used in our calculation.

charge occupation defined by the set of eigenvalues of the electron number operators $n_i = \sum_\sigma n_{i,\sigma} = \sum_\sigma c^\dagger_{i,\sigma} c_{i,\sigma}$, where $c^\dagger_{i,\sigma}$ creates an electron in orbital i with spin σ. The quantity ϵ_i denotes the on-site energy of orbital i. U_i and K_{ij} are the Coulomb repulsion energies for two electrons in the same orbital i and in different orbitals i and j, respectively, and J_{12} is the exchange energy for electrons in orbitals 1 and 2 of the dot with spins $\sigma, \sigma' = \uparrow, \downarrow$. The tunneling term H_t couples subspaces of fixed charge occupation and is expressed in terms of the complex tunneling amplitudes $t_{Li,Ri}$ between orbitals L, R and orbital i of the dot [Fig. 1(b)].

In the present work, we are interested in a system where we can effectively turn on and off the induced exchange, either by gate voltage (varying the energy difference between different charge sectors) or by tuning tunneling. We consider our low-energy manifold to be the (1, 2, 1) charge configuration with the center dot spins in the lowest-energy singlet. This set of states is gapped (as noted below) from other configurations by an energy that is large compared to typical dilution refrigerator temperatures and provides the starting point for our perturbation theory.

Since we assume at most single occupancy of orbitals L, R, and 2 and a linear geometry for the three sites, we implicitly have set $U_L, U_R \to \infty$ and have neglected U_2 and K_{LR} in Eq. (1). For simplicity, we assume symmetric impurity-dot Coulomb repulsion energies [46] and set $K_{Li} = K_{Ri} \equiv K_i$ for $i = 1, 2$, while we take exchange terms $J_{Ri} = J_{Li} = 0$, appropriate for weak tunneling. Since H_t couples only states with the same total spin $S_{\rm tot}$ and total z component S_z, we can independently consider the two subspaces $(S_{\rm tot} = 0, S_z = 0)$ and $(S_{\rm tot} = 1, S_z = 0)$. Neglecting higher-energy states, the intermediate charge configurations generated by H_t within each spin subspace are (0, 3, 1), (1, 3, 0), and $(1, 2^*, 1)$, where $n_M = 2^*$ denotes an excited two-electron state of the dot with one electron in each orbital (see Fig. 2). Choosing as the energy origin $E_0 = \epsilon_L + \epsilon_R + 2\epsilon_1 + U_1 + 4K_1$, which is the energy of the (1, 2, 1) states in the absence of tunneling, we find that the zeroth-order energies of the (0, 3, 1) [(1, 3, 0)] states are

$$\Delta_{L(R)} = \epsilon_2 - \epsilon_{L(R)} + W, \tag{3}$$

where $W \equiv -2K_1 + K_2 + 2K_{12} - J_{12}$. The energies of the $(1, 2^*, 1)$ states depend on the two-spin state of the center dot electrons: for the triplet and singlet states, the energies [Fig. 1(c)] are, respectively,

$$\Delta_M = \epsilon_2 - \epsilon_1 + W - U_1 + K_2 - K_{12}, \tag{4}$$

$$\Delta_J = \Delta_M + 2J_{12}. \tag{5}$$

Typical values for the energies $\Delta_L, \Delta_R, \Delta_M, \Delta_J$ in practice range from ~20–500 μeV, while the tunneling amplitudes $t_{Li,Ri}$ in Eq. (2) are ~1–10 μeV. Thus, H_t can be regarded as a perturbation to H_n.

Within our toy model, the effective exchange coupling is given by the energy splitting between the states $|(1, 2, 1); S_{LR}, S_{11}\rangle$ and $|(1, 2, 1); T^{(0)}_{LR}, S_{11}\rangle$ in the presence of the tunneling term H_t. Here, $|S_{ij}\rangle$ and $|T^{(m)}_{ij}\rangle$ represent two-electron singlet and triplet spin states of the electrons in orbitals i, j and $m = 0, \pm$ indicates the spin magnetic quantum number of the triplet state. Details of the fourth-order perturbation theory analysis used to determine the energy shifts are given in the Supplemental Material [47]. We find that the first-order and third-order corrections to the energy vanish, while the second-order shifts are

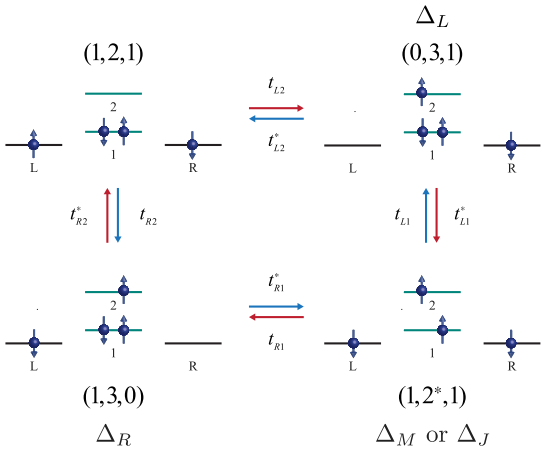

FIG. 2 (color online). Schematic illustration of virtual tunneling processes which give rise to the effective exchange interaction in Eq. (6). The red (blue) arrows correspond to the process in which the electron in orbital L (R) tunnels to the center dot in the first step. Each step is labeled with the tunnel coupling for the associated hopping term in H_t [Eq. (2)], and the zeroth-order energies of the charge configurations [Eqs. (3)–(5)] are indicated.

identical for both states. The fourth-order shifts $\delta E_S^{(4)}$ and $\delta E_T^{(4)}$ are therefore the lowest-order corrections that give rise to an energy splitting. The difference $\delta E_T^{(4)} - \delta E_S^{(4)}$ is the Heisenberg exchange coupling J, which we find to be given by

$$J = -2\left(\frac{t_{R2}^* t_{R1} t_{L1}^* t_{L2}}{\Delta_R \Delta_M \Delta_L} + \text{c.c.}\right). \quad (6)$$

This is the central result of our paper: using an initial singlet configuration yields an RKKY-like interaction [48], including both small-energy intermediate states (Δ_M being small compared to the dot charging energy) and nontrivial interference terms (J depends on the phases of the tunneling terms in the presence of the magnetic fields typically present in experiments).

Examining Eq. (6), we first remark that Δ_J, which differs from Δ_M by the intradot exchange splitting $2J_{12}$, does not appear in this expression. From the dependence of Eq. (6) on Δ_L, Δ_R, and Δ_M, we see that J is inversely proportional to the energy detunings $\epsilon_2 - \epsilon_L$ and $\epsilon_2 - \epsilon_R$ between orbital 2 of the quantum dot and the impurity orbitals as well as to the on-site energy difference $\epsilon_2 - \epsilon_1$ between the two levels of the quantum dot. As the detunings can be controlled via the voltages applied to the dot and have a lower limit set only by the tunnel coupling and magnetic field magnitudes, the strength of the exchange coupling mediated by the two-level dot is highly tunable. In contrast to cotunneling [35,36], this tunability is not limited by the fixed charging energy associated with virtual double occupation of the center dot. Tuning the gate voltages applied to the impurities in order to shift the impurity orbital levels away from their ionization point effectively suppresses tunneling between the impurities and the dot, enabling the exchange coupling to be switched off. Alternatively, the coupling may be turned off by initially transferring the qubit states from the electron spins to the nuclear spins of the donors [2,49] and subsequently ionizing the donors via the applied gate voltages.

We now turn to the phase dependence in Eq. (6). The terms correspond to two alternative pathways for the electrons which give rise to the effective coupling J (Fig. 2); thus, the interaction can have interference between these pathways, and their nontrivial relative phase for finite magnetic fields leads to an interaction strength that depends on the tunneling phase factors [48]. This provides a glimpse of the beginning of the expected sign fluctuations in exchange for a true RKKY interaction, where the finite Fermi wave vector k_F of the two-electron Fermi "sea" matters. For phosphorus donor electrons in silicon, the tunneling amplitudes also oscillate rapidly with the donor positions due to interference between electronic states associated with different degenerate minima, or valleys, existing in the conduction band [50,51]. In the context of our approach, this can be seen by taking $t_{ij} \propto \langle \psi_i | \psi_j \rangle$ for $i = L, R$ and $j = 1, 2$, where $\psi_{i,j}$ are superpositions of orbital wave functions associated with each valley. The oscillatory tunneling amplitudes lead to a spatial dependence of the terms in Eq. (6) that requires control of the dot center relative to the donor positions with precision on the scale of the lattice constant in order to achieve a particular coupling strength [52]. We note, however, that the simplified model we use here does not take into account interfacial disorder present in realistic silicon quantum dot devices, which mixes valley eigenstates having different phases [53–55] and may thus suppress valley interference effects for dot-mediated donor coupling.

Charge noise and exchange gate fidelity.—Fluctuating electric fields introduce variations in the parameters determining the effective exchange J in Eq. (6) and consequently affect the operation of exchange-based gates [1,56–58]. Here, we consider the effects of classical charge noise on the detuning parameters Δ_α for $\alpha = L, M, R$ and calculate the fidelity of the exchange gate $\hat{U}(\tau) = \exp(-iH_{\text{exch}}\tau)$, where $H_{\text{exch}} = -J|S_{LR}, S_{11}\rangle\langle S_{LR}, S_{11}|$ and $|S_{LR}, S_{11}\rangle$ is the corrected state after elimination of states outside the (1, 2, 1) subspace (note that we suppress the charge state in this notation, since the effective Hamiltonian acts only in this subspace). Letting $\Delta_\alpha \to \Delta_\alpha + \delta_\alpha$, where δ_α represents small fluctuations about the average detuning Δ_α, and expanding to first order in δ_α gives $J \to J' = J(1 - \sum_\alpha \delta_\alpha/\Delta_\alpha)$. We assume that the fluctuations δ_α are independent and described by Gaussian distributions $\rho_\alpha(\delta_\alpha) = e^{-\delta_\alpha^2/2\sigma_\alpha^2}/\sqrt{2\pi}\sigma_\alpha$ with charge noise standard deviations σ_α [58]. The exchange gate in the presence of these fluctuations is then given by $\hat{U}'(\tau) = \mathbf{1} + (e^{iJ'\tau} - 1)|S_{LR}, S_{11}\rangle\langle S_{LR}, S_{11}|$.

We define the minimum gate fidelity as $F_{\min}(\tau) = e^{-\tau^2/T_2^{*2}}\langle |\langle \psi_0 | \hat{U}_0^\dagger(\tau)\hat{U}'(\tau)|\psi_0\rangle|^2 \rangle$ [59], where $\hat{U}_0(\tau) = \mathbf{1} + (e^{iJ\tau} - 1)|S_{LR}, S_{11}\rangle\langle S_{LR}, S_{11}|$ is the ideal gate, $|\psi_0\rangle = (|T_{LR}^{(0)}, S_{11}\rangle + |S_{LR}, S_{11}\rangle)/\sqrt{2} = |\uparrow_L\downarrow_R, S_{11}\rangle$ is a state for which the exchange gate error is maximized, and the average is taken over the charge noise distributions. The envelope $e^{-\tau^2/T_2^{*2}}$ accounts for additional decay characterized by a time T_2^* over the gate duration τ [60,61]. Evaluation of $F_{\min}$ involves the terms $\langle e^{\pm iJ'\tau}\rangle = e^{-(J^2\tau^2/2)\sum_\alpha \sigma_\alpha^2/\Delta_\alpha^2} e^{\pm iJ\tau}$. Note that the amplitude of $\langle e^{\pm iJ'\tau}\rangle$ describes Gaussian decay of the form $e^{-\tau^2/T_d^2}$ with a decay time $T_d = (1/J)\sqrt{2/\sum_\alpha \sigma_\alpha^2/\Delta_\alpha^2}$ [58]. Using the expressions for $\langle e^{\pm iJ'\tau}\rangle$, we find

$$F_{\min}(\tau) = \frac{e^{-\tau^2/T_2^{*2}}}{2}\left(1 + e^{-(1/2)J^2\tau^2\sum_\alpha(\sigma_\alpha^2/\Delta_\alpha^2)}\right). \quad (7)$$

We plot this fidelity for the square-root-of-swap entangling gate $U_{\text{sw}}^{1/2} \equiv \hat{U}(\pi/2J)$ [1] as a function of the effective quantum dot level splitting Δ_M and symmetric effective impurity-dot detunings $\Delta_L = \Delta_R \equiv \Delta_I$ in Fig. 3. For $\Delta_M = 90$ μeV, $\Delta_I = 60$ μeV, and a tunnel

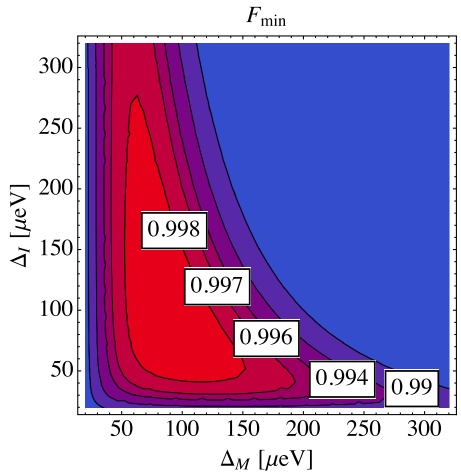

FIG. 3 (color online). Minimum fidelity [Eq. (7)] of the square-root-of-swap exchange gate $U_{\mathrm{sw}}^{1/2} \equiv \hat{U}(\pi/2J)$ as a function of the quantum-dot level splitting Δ_M and impurity-dot detunings $\Delta_L = \Delta_R \equiv \Delta_I$ for $\sigma_L = \sigma_R = \sigma_M = 2$ μeV, $T_2^* = 1$ ms [61,62], and $|t_{Li}| = |t_{Ri}| = t = 2$ μeV [63].

coupling $|t_{Li}| = |t_{Ri}| = t = 2$ μeV, which is relevant for phosphorus donors in silicon [42,43,63], we find $J = 4t^4/\Delta_R\Delta_M\Delta_L = 0.2$ neV. This exchange coupling strength corresponds to a gate time $\tau_{\mathrm{gate}} = \pi/2J \approx 5$ μs and gate fidelity $F_{\min} \approx 0.998$. Thus, setting the quantum dot level splitting and impurity-dot detunings to values within an optimal range in principle enables high-fidelity exchange gates. By contrast, the optimization of fidelity for gates implemented via indirect exchange between the outer electron spins of a triple quantum dot in the (1,1,1) regime is more challenging [64]. We also note that a maximum fidelity of 0.99 was obtained for $U_{\mathrm{sw}}^{1/2}$ implemented using an indirect exchange coupling strength $\gtrsim 10$ μeV in the effective (1, 1, 1) regime of the molecular system considered in Ref. [34]. We therefore find that, for the approach we describe, a smaller effective exchange coupling strength does not fundamentally limit the exchange gate fidelity.

Finally, studies of exchange in multielectron quantum dots [65–67] suggest that exchange coupling of the type discussed in the present Letter, which is derived from tunneling via an excited orbital of a multilevel quantum dot with lower-energy orbitals filled by electron pairs, may exhibit increased robustness against fluctuations caused by charge noise due to screening of the Coulomb interaction by the paired core electrons already present in the dot. Varying the number of electrons in the dot changes the spacing between the outermost levels [3] and consequently Δ_M, so that J may be tuned in discrete steps. Provided this discrete level description remains valid (i.e., for dot orbital splittings large compared to the thermal energy k_BT), the larger sizes associated with multielectron dots may also enable longer-range coupling.

Effects of inhomogeneous g factors.—While extensions of our model to a large parallel magnetic field cause no changes for homogeneous g factors, a difference in the g factors of the impurities and the quantum dot [68] couples the $S_{\mathrm{tot}} = 0$ and $S_{\mathrm{tot}} = 1$ subspaces. To investigate the form of this coupling, we assume an applied magnetic field $\mathbf{B} = B_z\hat{\mathbf{z}}$ and add a magnetic gradient term of the form

$$H_Z = \frac{\Omega_z}{2}\sum_{i=1,2}(n_{i,\uparrow} - n_{i,\downarrow}) \tag{8}$$

to the Hubbard Hamiltonian [Eqs. (1) and (2)], where $\Omega_z \equiv \Delta g_z \mu_B B_z$ is the magnetic field splitting due to a g-factor gradient Δg_z parallel to the external field [see Fig. 1(c)]. We transform to a basis which diagonalizes $H_0 \equiv H_n + H_Z$ and treat H_t as a perturbation to H_0. Keeping terms up to second order in the tunneling amplitudes and up to linear order in Ω_z, we find that the correction to the effective exchange Hamiltonian H_{exch} is given by $H_g = f_g(|T_{LR}^{(0)}, S_{11}\rangle\langle S_{LR}, S_{11}| + |S_{LR}, S_{11}\rangle\langle T_{LR}^{(0)}, S_{11}|)$, where

$$f_g = \frac{\Omega_z}{2}\left(\frac{|t_{L2}|^2}{\Delta_L^2} - \frac{|t_{R2}|^2}{\Delta_R^2}\right). \tag{9}$$

From this expression, we see that the effects of the g-factor inhomogeneity described by Eq. (8) can be eliminated up to first order in Ω_z and second order in the tunneling amplitudes by choosing t_{L2}, t_{R2}, Δ_L and Δ_R such that the constraint $\Delta_L^2/\Delta_R^2 = |t_{L2}|^2/|t_{R2}|^2$ is satisfied. Note that the preceding analysis assumes $\Omega_z < \Delta_{M,L,R}$, which sets an upper bound on J [see Eq. (6)]. For impurity atoms with nonzero nuclear spin, hyperfine coupling represents an additional source of magnetic gradients between the impurity and dot electrons that may prove useful for alternative coupling schemes. Indeed, for direct exchange coupling between two donor electron spins in silicon, recent work [69] shows that a difference in the hyperfine coupling between the donors enables two distinct methods for realizing high-fidelity two-qubit gates.

The validity of the model considered in the present Letter is limited by the validity of the two-level approximation for the mediator quantum dot in the presence of the Coulomb interaction among the four electrons. Future work should consider a detailed calculation of the effective exchange interaction mediated by the two-level quantum dot in terms of the general form of the pairwise Coulomb interaction and explore how this analysis may be extended to gain insight into the form of the coupling mediated by a quantum dot with more than two levels.

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*vsriniv@umd.edu

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