Single-spin readout for buried dopant semiconductor qubits

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(Received 14 August 2003; revised manuscript received 4 February 2004; published 3 June 2004)

For qubits based on donor nuclear or electron spins in the solid state, single-spin detection for readout remains a crucial unsolved problem. We analyze the Kane adiabatic scheme based on spin-dependent electron tunnelling between individual donor atoms, detected electrically using a single electron transistor (SET). Despite stabilization due to the presence of the D^+, the field strengths required place severe constraints on the SET measurement time. We propose a new method based on resonant electron transfer at low field strengths, and discuss various implementation issues.

DOI: 10.1103/PhysRevB.69.233301 PACS number(s): 72.25.−b, 03.67.Lx, 85.75.−d

Solid-state qubit systems where the quantum information is encoded by single donor degrees of freedom have been the subject of intense activity in recent years since the seminal work of Kane.[1] Indeed, advances in single-atom doping of semiconductors[2,3] bring closer to reality the construction of such a quantum computer (QC) device based on single donor spin[1,4] or charge[5] qubits. Solid-state spin qubits are of wide interest because of the nexus to scalable fabrication technology, and the relatively long coherence times of donor nuclear and electron spins. Progress towards the fabrication of such devices is reviewed in Ref. 6. The detection of a single donor electron or nuclear spin remains a crucial problem, and a number of schemes have been proposed.[1,7–9] The direct measurement of a few electron spins in SiO_2 have been reported by Mamin *et al.*[10] A recent scheme proposed by Friesen *et al.*[11] for the resonant spin to orbital conversion for electron spins in asymmetric quantum dots might also be applicable to the buried dopant case with appropriate gating. In this paper we investigate the dynamics of the adiabatic indirect single spin detection proposal,[1] and as a direct consequence we develop a resonant transfer scheme suitable for both electron and nuclear spin readout.

Indirect spin detection involves transfer of the spin information to charge degrees of freedom via a spin-dependent tunnelling process, detected by a single electron transistor (SET) as an ultrasensitive electrometer.[12] A realistic architecture for spin-dependent charge transfer, applicable for electron and nuclear spin readout, is shown in Fig. 1 for the case of phosphorous dopants in silicon. The concept relies on the adiabatic application of a dc electric field F_0 to induce tunnelling of the qubit electron to a secondary (spin polarized) ''SET-donor,'' forming a doubly occupied D^- donor state. The detection of the charge distribution change by the SET is effectively a measurement of the qubit spin state, as the tunnelling event $D^0D^0 \rightarrow D^+D^-$ will be Pauli blocked if the qubit and SET-donor electron spins are parallel.

A potential problem with this scheme is the possible destruction of the qubit through ionization since the D^- state binding energy is only about 1.7 meV. The question is whether the D^- state will tunnel to the conduction band under the application of the dc field destroying the qubit system during the SET measurement. For the small charge levels to be measured ($\Delta q < 0.05e$) single-shot RF SET readout operating near the quantum limit requires measurement times of order $T_{\mathrm{SET}} \approx 1\ \mu$s,[13] and determines the required survival time of the doubly occupied state.

In this paper we address this problem by carrying out detailed simulations of the device shown in Fig. 1. Our starting point is a simple WKB calculation of the critical dc field strength, F_0^*, corresponding to a ''safe'' D^- state dwell time of $T_{D^-} \approx 10\ \mu\mathrm{s} > T_{\mathrm{SET}}$. This serves as the main constraint for the spin-dependent transfer scheme. We then compute the dc field strength F_0^{ad} required for adiabatic spin transfer. Despite stabilization effects from the electron–hole interaction in the D^+D^- system, which can be quite significant, we find F_0^{ad} exceeds F_0^* for all cases by more than an order of magnitude indicating that, even allowing for the crude approximation used in the determination of the critical field strength, the qubit will probably not survive adiabatic spin readout. We then investigate a resonant transfer readout scheme, similar to that implied by Laroniov *et al.*[14] in the context of a D^- based quantum computer proposal. In this work, however, we simulate the device shown in Fig. 1 with a rapidly varying electric field applied to the gates. In this analysis the local dc fields required for addressing individual qubits for readout are shown to be much less than F_0^*. There is real potential for this approach in that resonant transfer may be achieved with state-of-the-art FIR laser technology[15]—a claim supported by the fact that the transition $D^0D^0 \rightarrow D^+D^-$ has been experimentally observed in spectroscopic

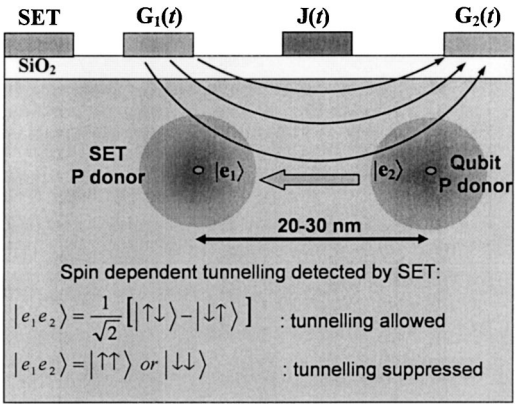

FIG. 1. Spin-dependent charge transfer scheme for single-spin readout based on dopant atoms in semiconductors.

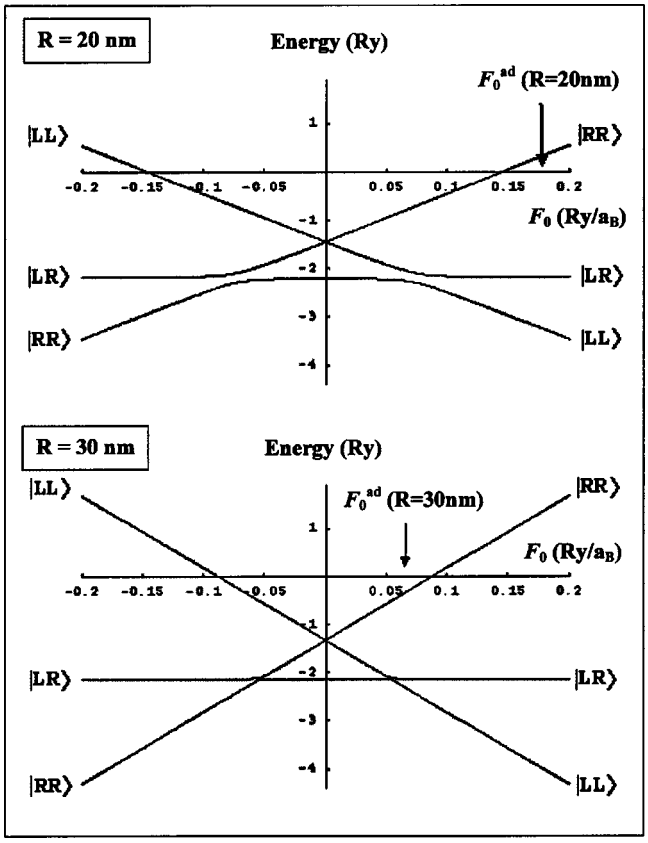

FIG. 2. Energy level diagrams for separations $R=20$ and 30 nm as a function of the dc field strength, F_0.

studies[16] of bulk-doped Si:P. Finally, we analyze the resonant readout scheme for the case of nuclear spin readout involving a pre-readout preparation stage, where the nuclear spin information is transferred to the electron spin.

When a dc field F_0 is applied to the shallow D^- one of the electrons can tunnel to the conduction band through the relatively low barrier formed. The field tunnelling dwell time $T_{D^-}(F_0)$ for such states is notoriously sensitive to the field strength F_0, indicating the difficulty in calculating this quantity. To set a reference scale for this initial analysis, we use a straightforward estimate for tunnelling through a Coulomb potential in the standard one-dimensional 1-D WKB approximation.[17] At 100 mK we solve the condition $T_{D^-}(F_0^*)=10\ \mu$s in the device configuration shown and obtain $F_0^*[D^-]=0.00037$ Ry/a_B. In itself this is a small value, and would seem at first sight to be very discouraging. However, in the case of the D^+D^- system there will be stabilization due to the electron–hole interaction. In order to compute F_0^* for the D^+D^- system and compare with the field strength F_0^{ad} for adiabatic transfer, we must solve the nontrivial donor molecular problem[18] in the presence of an electric field for the process $D^0D^0 \rightarrow D^+D^-$.

For the typical donor separations we will be considering ($R>20$ nm), the natural choice for a basis of states in the singlet sector are $\{|\psi_i\rangle\}=\{|LL\rangle,|LR\rangle,|RR\rangle\}$ (where L and R refer to the position of the electrons on left and right donors, respectively). The system is initially in the $|LR\rangle=|D^0D^0\rangle$ state. A first-order quantitative analysis of the adiabatic readout scheme is most easily carried out in the envelope approximation. Further improvements using a Bloch structure of the donor electron wave functions are possible, however, to illustrate the basic principles, our approach is quite adequate. We use the following wave functions to describe this basis:

$$\phi_{LL}(r_1,r_2)=N_{LL}(e^{-\alpha r_1}e^{-\beta r_2}+e^{-\beta r_1}e^{-\alpha r_2})(1+\lambda r_{12}),$$

$$\phi_{LR}(r_1,r_2)=N_{LR}(e^{-r_1}e^{-|r_2-R|}+e^{-|r_1-R|}e^{-r_2}),$$

$$\phi_{RR}(r_1,r_2)=N_{RR}(e^{-\alpha|r_1-R|}e^{-\beta|r_2-R|}+e^{-\beta|r_1-R|}e^{-\alpha|r_2-R|})\times(1+\lambda r_{12}),$$

where the N_{ij} are normalization constants. For the case of the doubly occupied states we have taken the Chandrashakar wave function—well known to give a good account of the H^- ion—where α, β, and λ are variational parameters (λ controls the electron correlation strength). The wave functions are evaluated with standard parameters appropriate for donors in Si, i.e., $a_B=2$ nm, and $m_{\rm eff}=0.2m_e$ (the scheme can be readily reworked for other substrate:dopant systems), and we scale the Rydberg energy to the D^0 ground state: 1 Ry=45.5 meV.

The ungated two-donor Hamiltonian in the $\{|LL\rangle,|LR\rangle,|RR\rangle\}$ basis is formed by computing overlap integrals for various donor separations. For large donor separations the eigenstates are $|\phi_1\rangle\approx|LR\rangle,|\phi_{2,3}\rangle\approx[|LL\rangle \pm|RR\rangle]/\sqrt{2}$. An electric field is included along the interdonor axis of the form $F(t)=F_0+F_1\sin\omega t$. To investigate adiabatic transfer we set $F(t)=F_0$ and compute the energy level diagram as a function of F_0 for donor separations $R=20$ nm and 30 nm (Fig. 2). As R is increased, several observations can be made: the level crossing point $F_0^c(R)$ between the ground and excited states moves to lower values of F_0, the gap at the crossing narrows, and the binding energy of the D^0D^0 state at zero field decreases. For $F_0<F_0^c$, the energy gap $\Delta E=E_2-E_1$ decreases with increasing F_0 as expected and has residual R dependence in its slope.

The single electron binding energy is computed by subtracting $E_{D^+D^-}$ from the single electron state energy $E_{D^+D^0}$, giving the effective barrier height for the WKB tunnelling analysis. The results for the various critical field strengths are summarized in Table 1. As a measure of the adiabatic field required we define F_0^{ad}, where the transition $|LR\rangle\rightarrow|LL\rangle$ has occurred with Prob$[|LL\rangle]>0.99$ in the final (ground) state. The results, albeit for a different parameter set, agree qualitatively with the calculations of Fang *et al.*[18] for the adiabatic transition. Clearly, in comparison to the isolated

TABLE I. The dc field strengths: corresponding to the level crossing (F_0^c), adiabatic transition $D^0D^0\rightarrow D^+D^-$ (F_0^{ad}), and 10 μs D^+D^- dwell time (F_0^*). All values are quoted in Ry/a_B.

R (nm)	F_0^c	F_0^{ad}	F_0^*
20	0.0737	0.1740	0.0087
30	0.0540	0.0630	0.0058

case $F_0^*[D^-]=0.000\,37\ \mathrm{Ry}/a_B$, the D^+ stabilizes the system to a large extent against field-induced tunnelling (stabilization of the D^+D^0 state was also taken into account). Near the avoided level crossing, $F_0>0.040\ \mathrm{Ry}/a_B$, the D^+D^- state dwell time decreases to less than 10^{-6} μs. Although larger separations seem to be favored, the requirement $F_0^{\mathrm{ad}}<F_0^*$ for qubit survival of the adiabatic transfer process is clearly not satisfied.

Of course, these conclusions depend on not only the veracity of the WKB calculation of F_0^*, which will receive corrections from transverse momenta,[19] but also the extent to which electron–hole stabilization leads to $F_0^*[D^+D^-] \gg F_0^*[D^-]$. This statement is dependent on the complexities of the molecular description of the two-donor system. However, given the order of magnitude difference in $F_0^*[D^+D^-]$ and F_0^{ad}, it would seem unlikely that improvements in the calculations will change the overall picture that adiabatic single spin readout, at the very least, severely tests the realm of current SET technology.

As an alternative we turn our attention to indirect spin detection through resonant electron transfer, and switch on the ac component F_1 with a small dc offset $F_0<F_0^*$. If the oscillating field is set resonant with the gap $\Delta E(F_0)$ Rabi oscillations $|LR\rangle \leftrightarrow |LL\rangle$ occur over a time scale controlled by the field amplitude F_1. After the Rabi time T_{Rabi} the $|LR\rangle$ component goes to zero and the ac component of the field is switched off, leaving on the dc component. Since the offset dc field merely allows for qubit selection, the value of F_0 can be quite small, giving rise to a long enough D^- state dwell time for SET measurement to take place.

The parameter regime for the process $D^0D^0 \rightarrow D^+D^-$ is shown in Fig. 3. The energy gap for the process has been calculated as a function of dc field strength F_0 for two donor separations and plotted with respect to the single donor levels. The $1s$-$2p_0$ and $1s$-$2p_\pm$ transitions with a nonzero dipole matrix element (solid horizontal lines) serve as natural boundaries for the resonant charge transfer process. For $R=20$ nm the transition is mainly below the $1s$-$2p_0$ line, while for $R=30$ nm it occurs almost entirely in the $2p_0$-$2p_\pm$ gap.

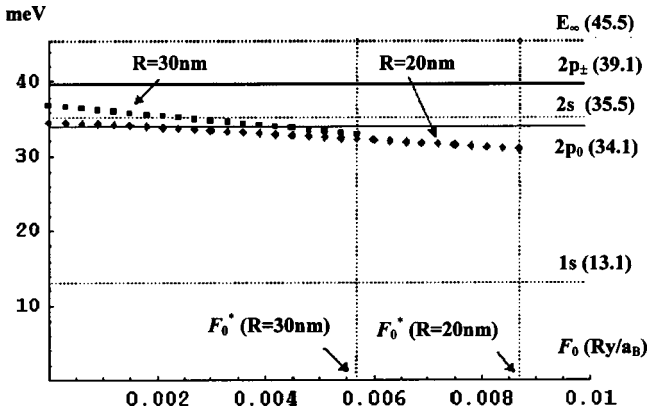

FIG. 3. Energy level diagram (relative to the donor ground state) showing the $D^0D^0 \rightarrow D^+D^-$ ($|LR\rangle \rightarrow |LL\rangle$) transition energy as a function of F_0 for $R=20$ nm (diamonds) and $R=30$ nm (squares) and low-lying single donor levels (horizontal lines).

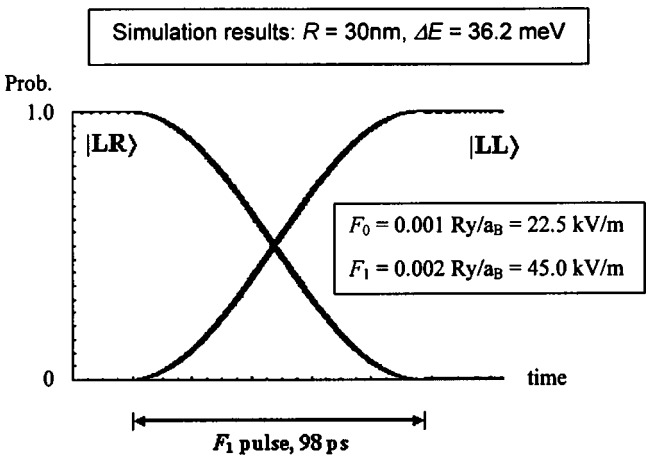

FIG. 4. Simulation results for the time-dependent state probabilities during resonant transfer between donors.

In Fig. 4 we show the results of a time-dependent calculation, in this case an example of the transition $|LR\rangle \rightarrow |LL\rangle$ for $R=30$ nm, occurring in the $2p_0$-$2p_\pm$ band. The local dc field was kept well below F_0^* at $F_0=0.001\ \mathrm{Ry}/a_B$. At $t=20$ ps the ac component was pulsed to $F_1=0.002\ \mathrm{Ry}/a_B$ and held at that value over $T_{\mathrm{Rabi}}=98$ ps during which the transition $|LR\rangle \rightarrow |LL\rangle$ takes place. Similar results were found for $R=20$ nm, although in avoiding the single donor levels, slightly higher dc field strengths are required.

Single dopant implantation technology has a reached the stage where the device shown in Fig. 1 can be fabricated[6] with a twin rf SET capability allowing for signal correlation and noise rejection.[13] Unfortunately, the ac-gated version of readout based on resonant transfer is probably not experimentally viable as it requires voltage pulse timing at frequencies $\approx$10 THz. However, this analysis does contain all the essential ingredients for an optically based resonant transfer scheme where individual qubits are brought into resonance with a field tuned to the gap $\Delta E(F_0,R)$ using the local dc gates, and thus selectively read out. Advances in FIR technology are bringing this wavelength regime into reach.[15] Observations of the $D^0D^0 \rightarrow D^+D^-$ transition for bulk doped Si:P ($1.7\times10^{17}\ \mathrm{cm}^{-3}$) shows a broad IR absorption peak at about 30 meV,[16] which agrees with our results for $F_0=0$ given that the mean donor separation for that dopant density is about 10 nm. Photoionization, over a time scale T_{Photo} can be neglected by selecting F_1 to ensure $T_{\mathrm{Photo}} \gg T_{\mathrm{Rabi}}$.

Finally, we consider the preparation stage for the case of nuclear spin readout, wherein the transfer of nuclear spin information to electrons takes place using the exchange interaction controlled by the J gate. The original Kane proposal calls for the ability to adiabatically increase the exchange interaction between qubit and SET donors above $J_c=0.058$ meV.[20] The two-donor spin system exhibits energy level crossings of a number of eigenstates at J_c. When J is increased adiabatically through J_c anti level-crossing behavior maps the system eigenstates $|e_1e_2\rangle \otimes |n_1n_2\rangle$ as follows: $|\downarrow\downarrow\rangle|11\rangle \rightarrow |\downarrow\downarrow\rangle|11\rangle$, $|\downarrow\downarrow\rangle|10\rangle \rightarrow |\downarrow\downarrow\rangle|s_n\rangle$, $|\downarrow\downarrow\rangle|01\rangle \rightarrow |a_e\rangle|11\rangle$, $|\downarrow\downarrow\rangle|00\rangle \rightarrow |a_e\rangle|a_n\rangle$. Here $|s\rangle$ and $|a\rangle$ refer to

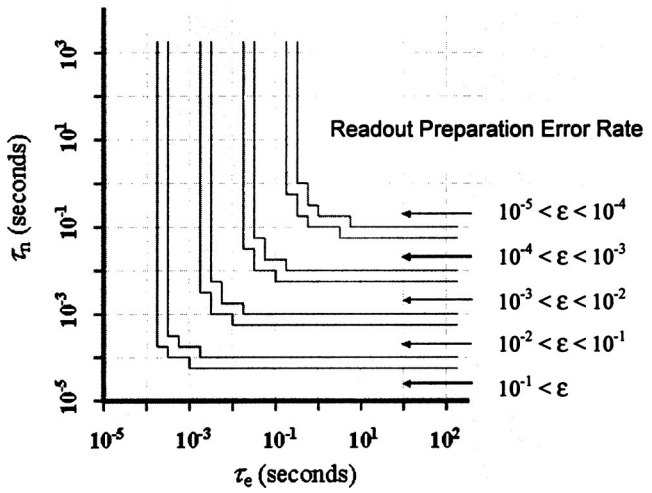

FIG. 5. Fidelity of adiabatically transferring nuclear spin information to the electrons of a two-donor system for a range of dephasing times τ_n, τ_e.

symmetric and antisymmetric states, respectively. Note that if $|n_1\rangle$ is in the $|1\rangle \equiv |\downarrow\rangle$ state the electrons remain spin down, whereas if $|n_1\rangle = |0\rangle$ the two-electron state is mapped to $|a_e\rangle$. The final $|e_1 e_2\rangle$ state is thus dependent on the state of $|n_1\rangle$ and readout of this spin proceeds according to the spin-dependent tunnelling scheme. In order to determine the feasibility and fidelity of the preparation stage, time-dependent simulations of this process were carried out with the dephasing time of the nuclei (τ_n) and electrons (τ_e) included in a similar manner to previous simulations of the nuclear spin CNOT gate.[21] Assuming J can be varied from 0.054 to 0.063 meV over 12 μs, Fig. 5 shows the fidelity of the readout preparation operation as a function of τ_n and τ_e dephasing times. Given that $\tau_n \gg \tau_e$, the electron dephasing dominates the fidelity of the process. Recent measurements[22] in isotopically pure ^{28}Si give $\tau_e > 60$ ms at 7 K.

A calculation of the exchange coupling J using Kohn–Luttinger-type wave functions deformed by a surface bias applied to a J-gate was carried out in Ref. 23. For a bias of 1.0 V applied to a surface gate above donors in the geometry of Fig. 1, the exchange coupling was found to be 0.030 meV for $R = 20$ nm. At face value, this would be insufficient to access the desired level crossing, however, the voltage-dependent exchange coupling calculation is the subject of ongoing work by a number of groups, and we would not claim this to be the last word. We note here also that the relevant spin information could be transferred using nuclear spin-dependent Rabi flipping of the donor electron. Let $E_{Z\uparrow}$ ($E_{Z\downarrow}$) denote the Zeeman energy of the donor electron when the nuclear spin is up (down). The magnetic field frequency resonant with the $E_{Z\downarrow}$ transition and the maximum field strength such that $E_{Z\uparrow}$ is off resonance can be calculated from $E_{Z\downarrow} \cong 0.116$ meV and $E_{Z\uparrow} - E_{Z\downarrow} = 4A$ (where $A \cong 1.2 \times 10^{-4}$ meV is the nucleus–electron hyperfine interaction energy). For a rf field of magnitude $|B_{\mathrm{ac}}| \cong 10^{-4}$ T, we obtain a relatively fast electron flipping time of 0.17 μs.

In summary, we have analyzed the adiabatic single spin readout scheme and found that within the approximations employed the condition for qubit survival $F_0^{\mathrm{ad}} < F_0^*$ is not satisfied for typical donor separations. However, the resonant scheme was found to be a viable alternative involving dc field strengths much less than the critical field.

ACKNOWLEDGMENTS

This work was supported by the Australian Research Council, the Army Research Office under Contract DAAD19-01-1-0653, and the Victorian Partnership for Advanced Computing. The authors would like to acknowledge discussions with R. Scholten, M. Testolin, A. Hamilton, A. Greentree, and J. McCallum.

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