Spin qubits in multielectron quantum dots

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(Received 6 August 2003; revised manuscript received 15 December 2003; published 24 March 2004)

We study the effect of mesoscopic fluctuations on the magnitude of errors that can occur in exchange operations on quantum dot spin qubits. Midsize double quantum dots, with an odd number of electrons in the range of a few tens in each dot, are investigated through the constant interaction model using realistic parameters. It is found that the constraint of having short pulses and small errors implies keeping accurate control, at the few percent level, of several electrode voltages. In practice, the number of independent parameters per dot that one should tune depends on the configuration and ranges from one to four.

DOI: 10.1103/PhysRevB.69.115329 PACS number(s): 73.21.La, 03.67.Lx

I. INTRODUCTION

Since the discovery that quantum algorithms can solve certain computational problems much more efficiently than classical ones,1,2 attention has been devoted to the physical implementation of quantum computation (QC). Among the many proposals, there are those based on the spin of electrons in laterally confined quantum dots (QD’s),3 which may have great potential for scalability and integration with current technologies. For any successful proposal, one must be able to perform single- and double-qubit operations much faster than the decoherence time. In fact, all logical operations required for QC can be realized if these elementary operations are sufficiently error free.

Single-qubit operations involving a single QD will likely require precise engineering of the underlying material or control over local magnetic fields;5 both have yet to be achieved in practice. Two-qubit operations, in contrast, are already within experimental reach. They can be performed by sending electrical pulses to modulate the potential barrier between adjacent QD’s. That permits direct control over the effective, Heisenberg-like, exchange interaction between the qubit spins, which is created by the overlap between the electronic states in multielectron QD’s. The first proposal for a QD spin qubit3 relied on having a single electron in a very small laterally confined QD. One advantage of such a system is that the Hilbert space is nominally two dimensional. Leakage from the computational space involves energies of order of either the charging energy or the single-particle excitation energy, both of which are quite large in practice (~1 meV~10 K). Working adiabatically—such that the inverse of the switching time is much less than the excitation energy— assures minimal leakage. The large excitation energy implies that pulses of tens of picoseconds would be both well within the adiabatic regime and below the dephasing time τφ (which is typically in the nanosecond range since orbital degrees of freedom are involved). However, in practice, it is difficult to fabricate very small tunable devices.6 Moreover, single-electron QD’s may offer little possibility of gate tuning due to their rather featureless wave functions.

Alternatively, a qubit could be formed by the top most “valence” electron in a QD with an odd number of electrons.9 In this case, electrons filling the lower-energy states should comprise an inert shell, leaving as the only relevant degree of freedom the spin orientation of the valence electron. Large QD’s with 100–1000 electrons, while much simpler to fabricate than single-electron QD’s, are unsuitable because the excitation energy is small (~50 μeV ~0.6 K), leading to leakage or excessively slow exchange operations. On the other hand, midsized QD’s, with 10–40 electrons, are sufficiently small to have substantial excitation energies, yet both reasonable to fabricate and tunable through plunger electrodes. For these dots, a careful analysis of errors is necessary.

Perhaps the best example of an exchange operation is the swap of the spin states of the two qubits. For instance, it causes up-down spins to evolve to down-up. Maximum entanglement between qubits occurs when half of a swap pulse takes place—a square-root-of-swap operation. Several authors have treated the problem of swap errors in QD systems.10–14 A primary concern was the occurrence of double occupancy (when both valence electrons move into the same QD) during and after the swap. However, no study so far has considered another intrinsic characteristic of electronic states in multielectron QD’s, namely, their marked dependence on external perturbations such as electrode voltage or magnetic field. This sensitivity gives rise to strong sample-to-sample fluctuations arising from the phase-coherent orbital motion.15 These features can make the precise control of energy levels, wave functions, and interdot couplings a difficult task.

In this work we study errors and error rates that can take place during the exchange operation of two spin qubits based in multielectron QD’s. We consider realistic situations by taking into account an extra orbital level and fluctuations in level positions and coupling matrix elements. These lead to
deviations from a preestablished optimal swap operation point, especially when a single-particle level falls too close to the valence electron level. Reasons for such fluctuations can be, for instance, (i) the lack of a sufficient number of tuning parameters (i.e., plunger electrodes), or (ii) the cross talk between the tuning electrodes. Our results set bounds on the amount of acceptable detuning for midsize QD qubits.

This paper is organized as follows. In Sec. II, we introduce and justify the model Hamiltonian. The states involved in the exchange operation are presented in Sec. III, where we also discuss the pulses and the parameters involved in the exchange operations. In Sec. IV we present the results of our numerical simulations. We also discuss the impact of mesoscopic effects on errors and put our analysis in the context of actual experiments. Finally, in Sec. V we draw our conclusions.

II. MODEL SYSTEM

We begin by assuming that the double QD system can be described by the Hamiltonian

\[ H = H_A + H_B + H_{AB}, \]

where

\[ H_A = \sum_{j, \sigma} e_j^{\sigma} n_{a,j,\sigma} + \frac{U_a}{2} \sum_{j, \sigma} n_{a,j,\sigma} \left( \sum_{k, \sigma'} n_{a,k,\sigma'} - 1 \right), \]

\[ H_B = \sum_{k, \sigma} \left( t_{jk} a_{j,\sigma}^\dagger b_{k,\sigma} + \text{H.c.} \right), \]

and

\[ H_{AB} = \sum_{j, k, \sigma} (t_{jk} a_{j,\sigma}^\dagger b_{k,\sigma} + \text{H.c.}). \]

Here, \( n_{a,j,\sigma} = a_{j,\sigma}^\dagger a_{j,\sigma} \) and \( n_{b,k,\sigma} = b_{k,\sigma}^\dagger b_{k,\sigma} \) are the number operators for the single-particle states in the QD’s (named A and B). \( e_j^{\sigma} \) denotes the single-particle energy levels, \( t_{jk} \) are the tunneling amplitudes between the dots, and \( U_a \) is the charging energy (\( \sigma = \uparrow, \downarrow \) and \( j, k \) run over the single-particle states). Typically, for mid- to large-size QD’s, the charging energy is larger than the mean-level spacing.

In the literature of Coulomb blockade phenomena in closed QD’s, the Hamiltonian in Eq. (2) is known as the constant interaction model. It provides an excellent description of many-electron QD’s, being supported by both microscopic calculations and experimental data.\(^{15-19}\) The reasoning behind its success can be understood from two observations. First, mid- to large-size QD’s, with more than ten electrons, behave very much like conventional disordered metals in the diffusive regime. Wavelengths are sufficiently small to resolve irregularities in the confining and background potentials, leading to classical chaos and the absence of shell effects in the energy spectrum. In this case, the single-particle states obey the statistics of random matrices, showing complex interference patterns and resembling a random superposition of plane waves. This is in contrast with the case of small, circularly symmetric, few-electron QD’s, where shell effects are pronounced.\(^{3,20}\)

Second, for realistic electron densities, the QD linear size is larger than the screening length of the Coulomb interaction. In the presence of random plane waves, the screened interaction can then be broken up into a leading electrostatic contribution characterized by the QD capacitance plus weak interparticle residual interactions.\(^{16,19}\) This description becomes more accurate as the number of electrons gets larger since the residual interactions become weaker. The electron bunching is reduced as wave functions become more uniformly extended over the QD. Also, the increase in the number of oscillations in the wave functions leads to a self-averaging of the residual interactions. In this limit, one arrives at the so-called “universal Hamiltonian” for QD’s, containing only single-particle levels, the charging energy, and a mean-field exchange term.\(^{15,16}\) This Hamiltonian can be derived explicitly via a random-phase approximation treatment of the Coulomb interaction and the use of random-matrix wave functions.\(^{16,19}\)

According to these arguments, interaction effects beyond the charging energy term are omitted in Eq. (2). In addition, the intradot exchange interaction, which tends to spin polarize the QD, is also neglected. The reason for that is the following. One can show that the intradot exchange term only affect states where there is double occupancy of a level. Thus, the exchange interaction constant always appears side-by-side with the charging energy. But in multielectron dots, the exchange energy (which is, at most, of order of the mean-level separation) is much smaller than the charging energy. Thus, intradot exchange effects are strongly suppressed by the charging energy. We have verified that their inclusion does not modify appreciably our final results. We expect the exchange interaction to become important for two-qubit operations only in the case of small QD’s with only a few electrons, when all energy scales (including the mean-level spacing) are of the same order.

Thus, the simple picture where single-particle states are filled according to the Pauli principle up to the top most level is an appropriate description of multielectron dots.\(^{15-19}\) In order to define the spin-\(\frac{1}{2}\) qubits, both QD’s should contain an odd number of electrons (say, \(2N_A - 1 \) and \( 2N_B - 1 \)). The QD spin properties are then dictated by the lone, valence electron occupying the highest level. The remaining electrons form an inert core, provided that operations are kept sufficiently slow so as not to cause particle-hole excitations to other levels.

Experimentally, the two-qubit exchange operations also require the capability of isolating the QD’s from each other, so that a direct product state can be prepared, such as

\[ |i\rangle = |N_A \cdot \uparrow\rangle_A \otimes |N_B \cdot \downarrow\rangle_B, \]

where the kets represent only the spin of the valence electron on each QD.

III. ERRORS IN EXCHANGE OPERATIONS

We focus our study on errors that appear after a full swap operation (which should result in no entanglement). Although it could, in principle, seem more sensible to look at the square-root-of-swap operation (which creates entanglement and is therefore a building block of logical gates), error magnitudes for the latter are straightforwardly related to
FIG. 1. Schematic disposition of energy levels of a system of two QD spin qubits (only levels close to the top occupied state are shown). The dashed lines indicate the most probable transitions that can occur during the exchange operation.

those of the full swap operation, as we will show. We leave the discussion of the square root of swap to Sec. IV.

The ideal full swap operation exchanges the valence electrons of the QD system. For instance, it takes the product state \( |\psi\rangle \) into

\[
|\psi\rangle = |A\rangle_A \otimes |B\rangle_B. 
\]

Physically, the full swap can be implemented by starting with isolated QD’s, turning on the interdot coupling for a time \( T \) (the pulse duration), and then turning it off, isolating the QD’s again. For weakly coupled QD’s (\( |t| \ll U, \Delta \)), one finds \( T = (\pi/4) U/|t|^2 \), where \( t \) and \( U \) here represent typical values for the coupling matrix element and the charging energy, respectively (throughout we assume \( \hbar = 1 \)). To quantify the amount of error that takes place during the operation, we use the probability of not reaching \( |\psi\rangle \) asymptotically, namely,

\[
e = 1 - |\langle \psi | \psi (\pm \infty) \rangle|^2. 
\]

We solved numerically the time-dependent Schrödinger equation that derives from Eq. (1) for the particular but nevertheless realistic case shown in Fig. 1. We assumed that voltage tuning allows one to place the top most electron of QD \( A \) into an isolated single-particle state of energy \( e_{N_A} = 0 \) aligned with the energy of the top most electron in QD \( B \), \( e_{N_B} = 0 \). However, limited tuning ability leaves an adjacent empty state close in energy in QD \( B \): \( e_{N_B + 1} = \Delta \). Therefore, while we can approximately neglect all levels but one in QD \( A \), for QD \( B \) we needed to take two levels into account, having hopping matrix elements denoted by \( t_1 = t_{N_A N_B} \) and \( t_2 = t_{N_A N_B + 1} \). To facilitate the analysis, we assumed that the dots have the same capacitance, \( C \), so that \( U_A = U_B = U = e^2/C \).

The Hamiltonian of Eq. (1) conserves total spin. Assuming that filled inner levels in both QDS are inert (forming the “vacuum” state \( |0\rangle \)), we can span the \( S_z = 0 \) Hilbert subspace with nine two-electron basis states. According to their transformation properties, they can be divided into “singlet”

\[
|S_{1}\rangle = \frac{1}{\sqrt{2}} (|b_{N_B + t - 1} \rangle a_{N_A}^\dagger |b_{N_B + t - 1} \rangle |a_{N_A} \rangle |0\rangle,
\]

and “triplet”

\[
|T_{1}\rangle = \frac{1}{\sqrt{2}} (|b_{N_B + t - 1} \rangle a_{N_A}^\dagger |b_{N_B + t - 1} \rangle |a_{N_A} \rangle |0\rangle,
\]

and “triplet”

\[
|T_{2}\rangle = \frac{1}{\sqrt{2}} (|b_{N_B + t - 1} \rangle a_{N_A}^\dagger |b_{N_B + t - 1} \rangle |a_{N_A} \rangle |0\rangle,
\]

classes, with \( l = 1,2 \).

The final states that correspond to an error have either double occupancy \((|D_{1}\rangle, k = 1, \ldots, 5)\), or an electron in the \((N_B + 1)\) level of QD \( B \) \((|S_{2}\rangle) \). In addition, a return to the initial state is also considered an error. It is worth noticing the difference between our treatment of the problem and that of Ref. 13. In our case, errors come mainly from either ending in the excited single-particle state after the operation is over (i.e., states \(|S_{2}\rangle \) and \(|T_{2}\rangle \)), or from “no-go” defective operations. In Ref. 13, errors come from having double occupancy in the final state. Double occupancy errors can be exponentially suppressed by adiabatically switching the pulse on and off on time scales larger than the inverse charging energy.\(^ {3,11,12} \) Making pulses adiabatic on the time scale of the inverse mean-level spacing for multielectron quantum dots is more challenging, especially because the spacings fluctuate strongly both from quantum dot to quantum dot and upon variation of any external parameter (mesoscopic fluctuations). Therefore, multielectron quantum dots require extra tunability to get around such problems.

Very small errors, below \( 10^{-6} - 10^{-4} \), can, in principal, be fixed by the use of error correction algorithms.\(^ {23} \) The pulses, therefore, should be sufficiently adiabatic for errors to remain below this threshold. We adopted the following pulse shape:

\[
v(t) = \frac{1}{2} \left( \frac{\tanh \left( \frac{t + T/2}{2\tau} \right)}{\tanh \left( \frac{t - T/2}{2\tau} \right)} \right),
\]

where \( \tau \) is the switching time. The pulse will remain both well defined and adiabatic provided that \( T \gg \tau \gg \max \{ \Delta^{-1}, U^{-1} \} \). Note that this pulse is equivalent to that adopted in Ref. 13 up to exponential accuracy, \( O(e^{-T/\tau}) \), with \( T \gg \tau \). There is no particular reason to believe that either performs better than the other; our choice was dictated by technical convenience.

IV. RESULTS

We used a standard numerical method, the so-called Richardson extrapolation,\(^ {24} \) to solve the Schrödinger equation for \(|\psi(t)\rangle\). The first step in our analysis was to find the
optimal value of $T$ which minimized the full swap error, as defined in Eq. (6), for a given set of parameters $U$, $t_1$, and $\tau$ (we used $\Delta=1$ and took $t_2=t_1$). The second step was to study how this minimal error depends on $\tau$. There is actually an optimal interval for $\tau$, since small switching times spoil adiabaticity, while large ones compromise the pulse shape (when $T$ is relatively short). Empirically, we find that errors related to switching times become negligible once $\tau$ reaches values of about $\tau_0=4 \max\{\Delta^{-1},U^{-1}\}$, provided that $\tau \ll T$. In what follows, we fix $\tau= \tau_0$.

### A. Mesoscopic effects

Figure 2 shows the full swap error as a function of $\Delta$ when $T$ is fixed to its optimal value for $\Delta=1$. Such a situation would arise experimentally if the pulse is optimized for a certain configuration, but a fluctuation in level spacing occurs. Note the sharp increase in error as $\Delta$ decreases. While increasing $\tau$ reduces this error (by making the switching more adiabatic), very small level spacings would be problematic, since $\tau$ cannot be larger than $T$ without sacrificing pulse shape and effectiveness. In order to make space for an adiabatic switching time for small $\Delta$, one would also have to increase pulse duration. This is clear in the case of $U=1$ (see Fig. 2): Even moderate couplings, $t_{1,2}=0.2$, lead to larger errors, which can then be suppressed by decreasing $t_{1,2}$ by a factor of two; however, that causes a fourfold increase in pulse width which may be problematic in terms of decoherence.

The dependence of errors on fluctuations in the coupling amplitude $t_2$ is shown in Fig. 3. Again, the pulse duration used is the optimal value obtained when $t_2=t_1=0.2$. As expected, the error grows as $t_2$ increases. Errors related to large values of $t_2$ can also be minimized by increasing the switching time, but the same issues raised above appear.

Figure 4 presents the error for two situations involving pulses with duration of about $T/2$, corresponding to the square-root-of-swap operation. The cases shown are (i) one, and (ii) two consecutive square-root-of-swap pulses. For comparison, the curve corresponding to a full swap pulse is also shown. The error for the square-root-of-swap operation is given by Eq. (6) with $|f|$ replaced by $|f'| = \frac{1-i}{2} |S_1| + \frac{1+i}{2} |T_1|$.

One can observe from Fig. 4 that error rates are nearly the same after a full swap operation and after two consecutive square-root-of-swap operations. This insensitivity of the error to the pulse duration led us to concentrate our effort on the full swap operations.

In order to establish an upper bound for QD tuning accuracy, we have performed simulations where both $\Delta$ and $t_2$ were allowed to vary. The spacing between the levels in QD $B$ was taken from a Gaussian distribution centered at $\bar{\Delta}=1$, with standard deviation $\sigma_\Delta$ ($\epsilon_{N_b}=0$ was kept fixed). For the coupling amplitude, we generated Gaussian distributed level widths $\Gamma_2=2 \pi \bar{t}_2^2/\bar{\Delta}$, with average $\bar{\Gamma}_2=2 \pi \bar{t}_2^2/\bar{\Delta}$ and standard deviation $\sigma_{\Gamma_2}$. The pulses had their widths optimized for the typical case where $\Delta=\bar{\Delta}=1$, $U=4$, $t_{1,2}=0.2$, and $\tau=6$. For fixed values of $\bar{\Delta}$, $\sigma_\Delta$, $\bar{\Gamma}_2$, and $\sigma_{\Gamma_2}$, we generated 10 000 realizations of $\Delta$ and $\Gamma_2$ and each time calculated the error after the application of the full swap pulse. In Fig. 5 we show how the probability of having an error larger than the $10^{-4}$ threshold depends on the energy level accuracy, $\sigma_\Delta$. Two cases are considered, namely, plain and limited control of the interdot coupling constant ($\sigma_{\Gamma_2}$).
large level-position detuning: $s_D$

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mesoscopic fluctuations more generally affect a collection of degree.26 While these numbers are yet too small to have an effect on the total number of states from which a single pulse can be generated. For times of $100 ps$, these numbers match those used in Fig. 5. For this case, switching times of $100 ps$ would be long enough to operate in the adiabatic regime and also provide an efficient and well-defined pulse shape. Thus, the combined times should allow for 8–10 consecutive full swap gates before running into dephasing effects related to orbital degrees of freedom.26 While these numbers are yet too small for large-scale quantum computation, they could be sufficient for the demonstration of QD spin qubits. Based on Fig. 5, we find that accuracies in $\Gamma_2$ of about 10% would make operations only limited by dephasing, and not by fluctuation-induced errors. However, as shown in the inset, even for small QD’s (typically having small $U/\Delta$ ratios), the occurrence of large errors is quite frequent when level detuning is large.

An important issue for multielectron QD’s is their strong mesoscopic, sample-to-sample fluctuations in energy level position and wave function amplitudes. Our results so far indicate how big an effect a given change in energy or wave function will produce; now we go further and discuss how mesoscopic fluctuations more generally affect a collection of qubits.

In experiments, several electrodes are placed around the QD surroundings and their voltages are used to adjust the lateral confining potential, the interdot coupling, and the coupling between QD’s and leads. These voltages are external parameters that can be used to mitigate the effects of mesoscopic fluctuations by tuning energy levels and wave functions to desired values. Having that in mind, our results indicate two different scenarios for QD qubit implementations.

First, if one is willing to characterize each QD pair separately and have them operate one by one, mesoscopic fluctuations will be irrelevant. It will be possible, with a single parameter per QD, say, to isolate and align energy levels reasonably well. Errors can be further minimized by decreasing the inter-dot coupling (thus increasing $T$). But since QD’s are not microscopically identical, each pair of QD’s will require a different pulse shape and duration. Multi-electron QD’s are tunable enough, easy to couple, and much easier to fabricate than single-electron dots; therefore, multi-electron QD’s are most appropriate for this case.

Second, if the goal is to achieve genuine scalability, one has to operate qubits in a similar and uniform way, utilizing a single-pulse source. In this case, $T$ and $\tau$ should be the same for all QD pairs. Based on our results above, one should strive to maximally separate the top most occupied state from all other states, occupied or empty, so as to reduce the possibility of leakage during operations with a fixed duration. At the same time, it is important to reduce interpair cross-talk induced by capacitive coupling between electrodes, as well as all interdot couplings except between the top most states of each QD. One should bear in mind that not all electrodes act independently—in most cases a search in a multidimensional parameter space has to be carried out. Thus, four tuning parameters per QD may be necessary to achieve the following goals: (i) find isolated, single-occupied energy level (two parameters); (ii) align this level with the corresponding level in an adjacent QD (one parameter); (iii) control the interdot coupling (one parameter). For parameters involved in (i) and (ii), an accuracy of a few percent will likely be required. Finally, control over the interdot coupling parameter, (iii), must allow for the application of smooth pulse shapes in the picosecond range. Our simulations also show that the pulse width must be controlled within at least 0.5% accuracy. Although these requirements seem quite stringent, recent experiments indicate that they could be met.27

V. CONCLUSIONS

In summary, our analysis indicates that midsize QD’s, with ten to a few tens of electrons, while not allowing for extremely fast gates, are still good candidates for spin qubits. They offer the advantage of being simpler to fabricate and manipulate, but at the same time require accurate, simultaneous control of several parameters. Errors related to detuning and sample-to-sample fluctuations can be large, but can be kept a secondary concern with respect to dephasing effects provided that a sufficient number of independent electrodes or tuning parameters exists.
ACKNOWLEDGMENTS

We thank D. P. DiVincenzo, C. M. Marcus, and G. Usaj for useful discussions. This work was supported in part by the National Security Agency and the Advanced Research and Development Activity under ARO Contract No. DAAD19-02-1-0079. Partial support in Brazil was provided by Instituto do Milênio de Nanociência, CNPq, FAPERJ, and PRONEX.

8 C.M. Marcus, private communication.
21 Though we assume time-reversal symmetry (real $t_1$ and $t_2$), we have checked that its violation does not modify our results.
22 While such states can lead to the full spin swap (with probability equal to 1/2), they will induce severe detuning errors in subsequent operations.