Spintronics and Quantum Computing: Switching Mechanisms for Qubits

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Quantum computing and quantum communication are remarkable examples of new information processing technologies that arise from the coherent manipulation of spins in nanostructures. We review our theoretical proposal for using electron spins in quantum-confined nanostructures as qubits. We present single- and two-qubit gate mechanisms in laterally as well as vertically coupled quantum dots and discuss the possibility to couple spins in quantum dots via exchange or superexchange. In addition, we propose a new stationary wave switch, which allows to perform quantum operations with quantum dots or spin-1/2 molecules placed on a 1D or 2D lattice.

1. Introduction

Recent spin-related experiments with electrons\cite{1–6} have attracted much interest since the spin of the electron was shown to reach very long dephasing times of the order of microseconds in quantum-confined nanostructures\cite{2–4}, as well as surprisingly long phase coherence lengths of up to 100 $\mu$m\cite{2}. These achievements provide interesting possibilities for finding novel mechanisms for information processing and information transmission, such as quantum computing\cite{7–9} and spin-based devices for conventional\cite{1} computers. Not only that the fields of quantum computing\cite{7,9} and quantum communication\cite{9,10} could revolutionize computing, but also the performance of quantum electronic devices in conventional computers can be enhanced by the electron spin, e.g. spin-transistors (based on spin-currents and spin injection), non-volatile memories, single spin as the ultimate limit of information storage etc.\cite{11}. In Ref.\cite{8} we have shown that the electron spin is a most natural candidate for a qubit, which, when located in quantum-confined structures such as semiconductor quantum dots, atoms or molecules, satisfy all requirements needed for a scalable quantum computer. In particular, the Heisenberg exchange coupling between spins in neighboring quantum dots creates spin-entanglement which is needed for qubit gates in quantum computers, as well as for producing mobile Einstein-Podolsky-Rosen (EPR) pairs for quantum communication\cite{12}.

In this paper we review our proposals for spin-based switching mechanisms for single-qubit and two-qubit operations on 1D chains or 2D arrays of qubits; in addition we present a new proposal for switching which might be interesting for atomic systems. A more extensive review of our recent work can be found in Ref.\cite{12} and references therein.

2. Quantum Gate Operations with Coupled Quantum Dots

One and two qubit gates are known to be sufficient to carry out any quantum algorithm. For electron spins in nearby coupled quantum dots the desired two qubit coupling is provided by a combination of Coulomb interaction and the Pauli exclusion principle. At zero magnetic field, the ground state of two coupled electrons is a spin singlet, whereas the first excited state in the presence of strong Coulomb repulsion is usually a triplet. The remaining spectrum is separated from these two states by a gap which is either given by the Coulomb repulsion or the single particle confinement. The low-energy physics of such a system can then be described by the Heisenberg spin
Hamiltonian

\[ H_s(t) = J(t) \mathbf{S}_1 \cdot \mathbf{S}_2, \]

(1)

where \( J(t) \) is the exchange coupling between the two spins \( \mathbf{S}_1 \) and \( \mathbf{S}_2 \), and is given by the energy difference between the singlet and triplet states. If we pulse the exchange coupling such that \[ \int dt J(t)/\hbar = J_0 \tau_s / \hbar = \pi \text{ (mod } 2\pi), \] the associated unitary time evolution \( U(t) = T \exp(i \int_0^t H_s(\tau) d\tau / \hbar) \) corresponds to the “swap” operator \( U_{\text{sw}} \) which exchanges the quantum states of qubit 1 and 2. Having an array of dots it is therefore possible to couple any two qubits. Furthermore, the quantum XOR gate, \( U_{\text{XOR}} \), can be constructed by applying an appropriate sequence \( U_{\text{XOR}} \) of “square-root of swap” \( U_{\text{sw}}^{1/2} \) and single-qubit rotations \( \exp(i \pi \mathbf{S}_i^z) \). Since \( U_{\text{XOR}} \) (combined with single-qubit rotations) is proven to be a universal quantum gate, it can be used to assemble any quantum algorithm. The study of universal quantum computation in coupled quantum dots (or atoms etc.) is thus essentially reduced to the study of single qubit rotations and the exchange mechanism, in particular how the exchange coupling \( J(t) \) can be controlled experimentally. Note that the switchable coupling mechanism described below need not be restricted to quantum dots: the same principle can be used in other systems, e.g. coupled atoms in a Bravais lattice, supramolecular structures, or overlapping shallow donors in semiconductors.

2.1. Laterally coupled quantum dots

We first discuss a system of two laterally coupled quantum dots defined by depleted regions in a 2DEG containing one (excess) electron each. The electrons are allowed to tunnel between the dots (if the tunnel barrier is low) leading to spin correlations via their charge (orbital) degrees of freedom. We model the coupled system with the Hamiltonian \( H = H_{\text{orb}} + H_Z \), where

\[ H_{\text{orb}} = \sum_{i=1,2} h_i + C \]

\[ h_i = \frac{1}{2m} \left( p_i - \frac{e}{c} A(\mathbf{r}_i) \right)^2 + V(\mathbf{r}_i), \]

\[ C = \frac{e^2}{\kappa |\mathbf{r}_1 - \mathbf{r}_2|}, \]

(2)

Here, \( h_i \) describes the single-electron dynamics in the 2DEG confined to the xy-plane, with \( m \) being the effective electron mass. We allow for a magnetic field \( \mathbf{B} = (0,0,B) \) applied along the z-axis that couples to the electron charge via the vector \( \mathbf{A}(\mathbf{r}) = \frac{B}{2}(y,x,0) \), and to the spin via a Zeeman coupling term \( H_Z \). The single dot confinement as well as the tunnel-coupling is modeled by a quartic potential, \( V(x,y) = \frac{m \omega_0^2}{2} \left( \frac{1}{4\kappa} (x^2 - a^2)^2 + y^2 \right) \), which, in the limit \( a \gg a_B \), separates into two harmonic wells of frequency \( \omega_0 \) where \( 2a \) is the interdot distance and \( a_B = \sqrt{\hbar/m \omega_0} \) is the effective Bohr radius of a dot. This choice for the potential is motivated by the experimental observation that the low-energy spectrum of single dots is well described by a parabolic confinement potential. The (bare) Coulomb interaction between the two electrons is described by \( C \) where \( \kappa \) denotes the dielectric constant of the semiconductor. The screening length \( \lambda \) in almost depleted regions like few-electron quantum dots can be expected to be much larger than the bulk 2DEG screening length (about 40 nm for GaAs). Therefore, \( \lambda \) is large compared to the size of the coupled system, \( \lambda \gg 2a \approx 40 \text{ nm for small dots, and we will consider the limit of unscreened Coulomb interaction } (\lambda/a \gg 1) \). At low temperatures \( kT_B \ll \hbar \omega_0 \).
we are allowed to restrict our analysis to the two lowest orbital eigenstates of $H_{\text{orb}}$, leaving us with a symmetric (spin-singlet) and an antisymmetric (three triplets $T_0$, $T_\pm$) orbital state. In this reduced (four-dimensional) Hilbert space, $H_{\text{orb}}$ can be replaced by the effective Heisenberg spin Hamiltonian $\text{Eq. (1)}$ where the exchange coupling $J = \epsilon_t - \epsilon_s$ is given by the difference between the triplet and singlet energy. We make use of the analogy between atoms and quantum dots (artificial atoms) and calculate $\epsilon_t$ and $\epsilon_s$ with variational methods similar to the ones used in molecular physics. With the Heitler-London approximation using single-dot groundstate orbitals we find for 2D dots $\text{[15]}$.

$$J = \frac{\hbar \omega_0}{\sinh \left( \frac{2d^2}{d^2 + 1} \right)} \left\{ \frac{3}{4b} \left( 1 + bd^2 \right) + c\sqrt{b} \right\} \times \left[ e^{-bd^2} I_0 (bd^2) - e^{d^2(b-1)/b} I_0 \left( d^2 \frac{b - 1}{b} \right) \right],$$

where we introduce the dimensionless distance $d = a/a_B$ and the magnetic compression factor $b = \sqrt{1 + \omega_i^2/\omega_0^2}$, where $\omega_i = eB/2m$ is the Larmor frequency.

$I_0$ denotes the zeroth Bessel function. The first term in Eq. (3) comes from the confinement potential. The terms proportional to $c = \sqrt{\pi/2}(e^2/\alpha a_B)/\hbar \omega_0$ are due to the Coulomb interaction $C$, where the exchange term appears with a minus sign. Note that typically $|J/\hbar \omega_0| \ll 1$ which makes the exclusive use of ground-state single-dot orbitals in the Heitler-London ansatz a self-consistent approach. The most remarkable feature of $J(B)$ is the change of sign from positive (ferromagnetic) to negative (antiferromagnetic), which occurs at some finite $B$ over a wide range of parameters $c$ and $a$. This singlet-triplet crossing is caused by the long-range Coulomb interaction and is therefore absent in the standard Hubbard model that takes only into account short range interaction and, in the limit $t/U \ll 1$, is given by $J = 4t^2/U > 0$. Large magnetic fields ($b \gg 1$) and/or large interdot distances ($d \gg 1$) reduce the overlap between the dot orbitals leading to an exponential decay of $J$ contained in the $1/\sinh$ prefactor in Eq. (3). This exponential suppression is partly compensated by the exponentially growing exchange term $\propto \exp(2d^2(b - 1/b))$. As a consequence, $J$ decays exponentially as $\exp(-2d^2b)$ for large $b$ or $d$. Thus, $J$ can be tuned through zero and then exponentially suppressed to zero by a magnetic field in a very efficient way (exponential switching is highly desirable to minimize gate errors). Further, working around the singlet-triplet crossing provides a smooth exchange switching, requiring only small local magnetic fields. Qualitatively similar results are obtained $\text{[15]}$ when we extend the Heitler-London result by taking into account higher levels and double occupancy of the dots (using a Hund-Mullikan approach). In the absence of tunneling ($J = 0$) direct Coulomb interaction between the electron charges can still be present. However the spins (qubit) remain unaffected provided the spin-orbit coupling is sufficiently small, which is the case for $s$-wave electrons in GaAs structures with unbroken inversion symmetry. Finally, we note that a spin coupling can also be achieved on a long distance scale by using a cavity-QED scheme $\text{[16]}$ or superconducting leads to which the quantum dots are attached $\text{[17]}$.

### 2.2. Vertically coupled quantum dots

We also investigated vertically coupled Quantum dots $\text{[13]}$. This kind of coupling can be implemented with multilayer self-assembled quantum dots $\text{[19]}$ as well as with etched mesa heterostructures $\text{[20]}$.

We model the vertical coupled dot system by a potential $V = V_l + V_r$ where $V_l$ describes the parabolic lateral confinement and $V_r$ models the vertical dot coupling assumed to be a quartic potential similar to the one introduced above for the lateral coupling. We allow for different dot sizes $a_{B\pm} = \sqrt{\hbar /m a_{\pm} \omega_z}$ with $\omega_z$ being the vertical confinement, implying an effective Bohr radius $a_B = \sqrt{\hbar /m \omega_z}$ and a dimensionless interdot distance $2d = 2a/a_B$. By applying an in-plane electric field $E_{\parallel}$ an interesting new switching mechanism arises. The dots are shifted parallel to the field by $\Delta x_\pm = E_{\parallel}/E_0 a_{\pm}^2$, where $E_0 = \hbar \omega_z/ea_B$. Thus, the larger dot is shifted a greater distance $\Delta x_- > \Delta x_+$ and so the mean distance between the electrons grows as $d' = \sqrt{d^2 + A^2(E_{\parallel}/E_0)^2}$,

...
taking \( A = (\alpha^2_0^+ - \alpha^2_0^-)/2\alpha^2_0^+\alpha^2_0^- \). Since the exchange coupling \( J \) is exponentially sensitive to the interdot distance \( d' \) (see Eq. (3)) we have another exponential switching mechanism for quantum gate operations at hand.

2.3. Coupling two spins by superexchange

There is a principal problem if one wants to couple two “extended” dots whose energy levels are closely spaced (i.e. smaller than \( k_B T \)), as would be the case if there is a sizable distance between the two confined qubits before the barrier is lowered. In this case, the singlet-triplet splitting becomes vanishingly small, and it would not take much excitation energy to get states which are not entangled at all. In other words, the adiabatic switching time\([5]\) which is proportional to the inverse level spacing becomes arbitrarily large. A better scenario for coupling the two spin-qubits is to make use of a superexchange mechanism to obtain a Heisenberg interaction\([8,21]\). Consider three aligned quantum dots where the middle dot is empty and so small that only its lowest levels will be occupied by 1 or 2 electrons in a virtual hopping process. The left and right dots can be much larger but still small enough such that the Coulomb charging energies \( U_L \approx U_R \) are high enough (compared to \( k_B T \)) to suppress any double occupancy. Let us assume now that the middle dot has energy levels higher than the ground states of right and left dots, assumed to be approximately the same. These levels include single particle energy (set to zero) and Coulomb charging energy \( N^2e^2/2C \), with \( N \) the number of electrons and \( C \) the capacitance of the middle dot, and thus the ground state energy of the middle dot is 0 when empty, \( \epsilon = e^2/2C \) for one electron, and \( 4\epsilon \) for 2 electrons. The tunnel coupling between the dots is denoted by \( t_0 \). Now, there are two types of virtual processes possible which couple the spins but only one is dominant. First, the electron of the left (right) dot hops on the middle dot, and then the electron from the right (left) dot hops on the same level on the middle dot, and thus, due to the Pauli principle, the two electrons on the middle dot form a singlet, giving the desired entanglement. And then they hop off again into the left and right dots, respectively. (Note that \( U \) must be larger than \( k_B T \), otherwise real processes involving 2 electrons in the left or right dot will be allowed). It is not difficult to see that this virtual process leads to an effective Heisenberg exchange interaction with exchange constant \( J = 4t_0^4/4\epsilon^3 \), where the virtual energy denomina-
tors follow the sequence $1/\epsilon \rightarrow 1/4\epsilon \rightarrow 1/\epsilon$.

In the second type of virtual process the left (right) electron hops via the middle dot into the right (left) dot and forms there a singlet, giving $J = 4t^2_0/U_R\epsilon^2$. However, this process has vanishing weight because there are also many nearby states available in the outer dots for which there is no spin correlation required by the Pauli principle. Thus, most of the virtual processes, for which we have 2 electrons in the left (right) dot, do not produce spin correlations, and thus we can neglect these virtual processes of the second type altogether.

3. Single-Spin Rotations

In order to perform one qubit gates single-spin rotations are required. This is done by exposing a single spin to a time-varying Zeeman coupling $(g\mu_B \mathbf{S} \cdot \mathbf{B}(t))$, which can be controlled through both the magnetic field $\mathbf{B}$ and/or the g-factor $g$. We have proposed a number of possible implementations for spin-rotations: Since only relative phases between qubits are relevant we can apply a homogeneous $\mathbf{B}$-field rotating all spins at once. A local change of the Zeeman coupling is then possible by changing the Larmor frequency $\omega_L = g\mu_B B/\hbar$. The equilibrium position of an electron can be changed through electrical gating, therefore if the electron wavefunction is pushed into a region with different magnetic field strength or different (effective) g-factor, the relative phase of such an electron then becomes $\phi = (g'\mu_B' B - g\mu_B)\tau/2\hbar$. Regions with an increased magnetic field can be provided by a magnetic (dot) material while an effective magnetic field can be produced e.g. with dynamically polarized nuclear spins (Overhauser effect).

Alternatively one can use electron-spin-resonance (ESR) techniques to perform single-spin rotations, e.g. if we want to flip a certain qubit (say from $|\uparrow\rangle$ to $|\downarrow\rangle$) we apply an ac-magnetic field perpendicular to the $\uparrow\downarrow$ axis that matches the Larmor frequency of that particular electron. Due to paramagnetic resonance the spin can flip.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{(a) 1D chain (b) 2D array of quantum dots sandwiched by two (a) 1D chains (b) 2D arrays of gates, which can be contacted (a) laterally (b) along the axis perpendicular to the $xy$-plane (not shown). The $B$-fields and magnetized/high-g layers can be used for single-qubit switching (see text).}
\end{figure}

4. 1D and 2D Stationary Wave Switch

In this section we propose a new method to perform one- and two-qubit operations on a 1D linear chain and a 2D array of quantum dots, which promises to be extendable to spin-1/2 molecules or even atoms. We define the 2DEG to lie in the $xy$-plane. The initial configuration (IC) of the $D$ lattice of quantum dots $(D = 1D, 2D)$, in which all the isotropic exchange couplings $J_{pq}$ between sites $p$ and $b$ are zero, is represented by a $D$ stationary wave (DSW). The 1DSW refers to the sinusoidal arrangement of the 1D chain of quantum dots controlled by lateral gates on either side of the chain in the $xy$-plane as shown in Fig. 3 (a), whereas the 2DSW denotes the 2D potential (see Fig. 3 (b)) produced by the front and back gates that are positioned above and below the 2D quan-
tum dot array (see Fig. 3), in which the dots are trapped. In this way no split gates are needed. Instead of using gates, it should be possible to produce the DSW by means of, say, x-ray lasers[22], which would confine electrostatically the quantum dots in the IC. X-ray lasers could also be used to distort a D crystal lattice made of spin-1/2 molecules or atoms in order to obtain the IC. As these molecules are neutral in charge, the stationary electrostatic fields produce locally electric dipoles within these molecules, leading to a periodic displacement of the electron spin (qubit) of interest.

In order to perform qubit operations, the DSW must be varied. For operations on a single quantum dot in 1D or 2D the corresponding extremum at which the quantum dot is located must be enhanced such that the qubit is displaced into the magnetized or high-$g$ layer above or below the 2D quantum dot array (see Fig. 3 and the previous section). The coupling between two quantum dots is achieved by reducing the corresponding two pair of gates, which in 1D decreases the distance $a$ between the two quantum dots, and in 2D locally suppresses the extrema of the two quantum dots. $J(d)$ is given by Eq. (3) because two nearby quantum dots of the DSW shown in Fig. 3 can be modelled by a quartic potential of the form $V(x, y) = \frac{ma_2}{2} \left( \frac{1}{a_2} (x^2 - a^2)^2 + y^2 \right)$. While in 1D the distance $a$ is changed (see Sec. 2.1), in 2D the potential height of $V(x, y)$ is altered, which corresponds to a change of the harmonic oscillator frequency $\omega_0$. This in turn results in a variation of the Bohr radius $a_B = \sqrt{\hbar/m\omega_0}$. For small magnetic fields $B \ll 2m\omega_0/e$, i.e. $b = 1$, the magnetic compression factor $b$ is nearly independent of $\omega_0$. Then $J(d)$ in Eq. (3) becomes a function of $d(a)$ in 1D or a function of $d(a_B)$ in 2D (see Fig. 3). Thus, by varying $a$ or $\omega_0$ the exchange $J$ can be switched on or off, see Fig. 3.

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