THEORETICAL ISSUES IN SPIN-BASED QUANTUM DOT QUANTUM COMPUTATION

XUEDONG HU AND S. DAS SARMA
Department of Physics, University of Maryland, College Park, MD 20742-4111
E-mail: xdhu@physics.umd.edu, dassarma@physics.umd.edu

We review our recent work addressing various theoretical issues in spin-based quantum dot quantum computation and quantum information processing. In particular, we summarize our calculation of electron exchange interaction in two-electron double quantum dots and multi-electron double dots, and discuss the physical implication of our results. We also discuss possible errors and how they can be corrected in spin-based quantum dot quantum computation. We critically assess the constraints and conditions required for building spin-based solid state quantum dot quantum computers.

1 Introduction

It has long been pointed out that quantum mechanics may provide great advantages over classical physics in physical computation. However, the expeditious growth of research on quantum computation started after the advent of Shor’s factorization algorithm and quantum error correction schemes. Among the many hardwares that were proposed are the ones based on electron spins. Obviously, electron spin provides a perfect candidate for quantum bits (qubits) as the electron spin sub-Hilbert-space is generally well-defined and its decoherence relatively slow. In addition, electron spin can be manipulated by external magnetic fields and by interacting with other spins through exchange or Heisenberg coupling.

Our study of electron-spin-based quantum computers (QC) has focused on the scheme using single electrons trapped in quantum dots. Here the qubit is the spin degrees of freedom of a single electron trapped in a gated semiconductor (GaAs) horizontal quantum dot (QD). Single-qubit operations can be achieved by applying an external magnetic field, while two-qubit operations can be built upon exchange interaction between electrons in neighboring quantum dots when the inter-dot potential barrier is lowered and electron orbital wavefunction is allowed to mix. Final measurement in this scheme requires single spin detection, for which various proposals such as spin filters have been suggested.

A working quantum computer needs to satisfy many stringent conditions. The main requirements include initialization, well-defined Hilbert space, weak decoherence, precise coherent manipulation, unitary evolution, and efficient quantum measurement. In the case of spin-based quantum dot quantum computer, electron spin can be initialized by lowering the sample temperature, and applying an external magnetic field to differentiate the spin up and down directions. Because of the three-dimensional confinement and the fact that GaAs conduction band is mainly formed from S atomic orbitals, the trapped electron has very weak spin-orbit coupling and therefore its spin has a small decoherence rate. The spin Hilbert space of a single quantum dot with one electron is well-defined as long as the Zeeman splitting between the two spin levels is much smaller than the single electron excitation energy associated with the quantum dot confinement potential, which requires a sufficiently small quantum dot. The Hilbert space structure is not as clear cut when two quantum
dots are brought together for two-qubit operations. The exploration of this part of the spin Hilbert space is one major focus of our recent study, and we will review some of our results in the following section. Coherent control of electrons in mesoscopic nanostructures has been under intensive study by many groups for sometime. To reliably manipulate individual electrons and their spins, more precise controlling techniques have to be developed, and various noise effects such as those from offset charge oscillations and other volatile sources have to be eliminated or suppressed. Single spin detection is another difficult proposition for experimentalists. Currently available SQUID (superconducting quantum interference device) can detect a single Bohr magneton but requires a long detection time (in the order of minutes), while proposed spin valve techniques have not yet succeeded in detecting the spin of a single electron. Converting the spin signal to a charge signal and then using single electron transistor based charge measurement techniques to measure the electron spin seems one promising experimental method, but whether this technique (or any other spin measurement technique) can be implemented in microsecond type time scales (the typical low temperature spin coherence time is expected to be microseconds in a practical QC) remains to be seen.

In Section 2 we summarize our work on the theoretical exploration of double dot electron spin Hilbert space, including both two electrons and six electrons in a double dot. In Section 3 we discuss possible errors in a quantum dot quantum computer.

2 Electron Spin-based Quantum Computation

We have studied a double quantum dot (each has one trapped electron) as the basic elementary gate for a quantum computer. This can be considered an artificial double dot quantum molecule with two electrons, analogous to the H₂ molecule with one electron on each dot. In the first order approximation, a Heisenberg exchange Hamiltonian can be written to describe the dynamics of the two electrons trapped in the double dot. However, to establish the operability of such an exchange-based quantum computer, we need to clearly delineate the relation between the two-spin Hilbert space and the complete two-electron Hilbert space. For this purpose, we use a molecular orbital calculation to determine the excitation spectrum of two electrons in two horizontally coupled GaAs quantum dots, and study its dependence on an external magnetic field. In order to provide a more accurate description of the low lying excited states, we include the first excited single particle orbital states (P orbitals of the Fock-Darwin states, which are the eigenstate sequence of a two-dimensional electron in an external perpendicular magnetic field). The resulting spectrum (with an example shown in Fig. 1) confirms the belief that the exchange spin Hamiltonian is sufficient to describe the low energy dynamics of the two electrons.

As shown in Fig. 1, the lowest energy states (one singlet and one triplet) are well-separated from the rest of the excited states. Indeed, the higher energy excited states are separated from the lower energy subspace by the smaller of the single particle excitation energy and the on-site Coulomb repulsion energy (the so-called Coulomb blockade energy) in a single dot. This energy separation is at least 5 meV in our cases, much larger than the GaAs electron Zeeman splitting ($\approx 2.55 \times 10^{-2}$ meV/Tesla) and the energy separation between the ground singlet and triplet states (in the order of 0.1 meV). If the adiabatic condition is satisfied when the exchange gate is turned on, the ground states are essentially isolated from the higher energy excited states. The orbital composition of the ground singlet
Figure 1. A sample energy spectra of a two-electron double quantum dot in GaAs. Here we show the magnetic field dependence of the two-electron energy spectra obtained in a molecular orbital calculation where both S and P single-electron Fock-Darwin orbitals are used. The dot radius is 20 nm, the inter-dot distance is 30 nm, and the central barrier $V_b$ is 30 meV, corresponding to an actual barrier height of 9.61 meV.

and triplet states are basically $\psi_{L0}$ and $\psi_{R0}$, the lowest Fock-Darwin orbitals, which are also the orbital states of the electrons when they are in separate quantum dots. Therefore, throughout the duration of the exchange gate (or the lowering of the inter-dot potential barrier), the electron orbital degrees of freedom are frozen, and a spin Hamiltonian such as the Heisenberg exchange Hamiltonian in this case can describe the complete two-electron adiabatic dynamics.

The low-energy spin subspace of the complete two-electron Hilbert space consists of a singlet and three triplet states (whose degeneracy can be lifted by an external magnetic field). The splitting between the singlet and the unpolarized triplet state is the key parameter that determines the speed of two-qubit operations such as an exact swap of the spin states and controlled NOT (CNOT). In essence, the exchange interaction generates a phase difference between the singlet and the unpolarized triplet states (but not the relative weight) in a general two-spin state, thus changing the density matrix of each individual spin. Our numerical results show the singlet-triplet splitting $J$ (also called exchange con-
stant in this context) to be in the range of 0.01 to 1 meV as we vary the inter-dot distance and the size of the individual dots. Such a magnitude of \( J \) corresponds to reasonably short operating times (in the order of 0.1 to 10 ns after the adiabatic condition is taken into account) compared to the estimated electron spin coherence time (possibly of the order of microseconds at 50-100 mK temperature) in semiconductor heterostructures.\(^4\)\(^5\)\(^6\) Note that low temperature (\( T \)) QD-QC operation is essential in this context: first, \( T \) must be low to obtain a long spin coherence time; and second, \( k_B T \) must be low to satisfy \( \Delta \gg k_B T \) condition, where \( \Delta \) is the separation between the ground and the higher excited orbital levels in the single quantum dot system (\( \Delta > 1 \) meV in small dots), to maintain the integrity of the spin sub-Hilbert space necessary for quantum computation. Thus, the operation (or the manipulation) time for various gates and magnetic field pulses in QD-QC architecture is constrained from below by the adiabaticity requirement (i.e. it cannot be too fast so that adiabaticity is maintained) and from above by the spin coherence requirement (i.e. the operation must be much faster than the spin coherence time). One must realize that in addition to these stringent operational constraints there is also the severe (and as yet experimentally unsolved) constraints of measuring the final spin state (“read out”) which cannot be too slow for successful QD-QC operations.

Our molecular orbital calculation is based on the effective mass approximation in a single envelope-function approach. Due to the sizable band gap in GaAs and the relatively small inter-band coupling, our single envelope function calculation is valid with quite high accuracy. Indeed, we estimated\(^7\)\(^8\) that the effect of the neglected bands and inter-conduction band coupling amounts to about 1% correction to the single particle wavefunctions. To clearly quantify this correction one would have to employ a more sophisticated multi-band calculation or drop the envelope function approach entirely and adopt an atomistic approach, which would automatically include all valence band effects. However, it is unclear, in principle, whether such a first principle type band theory approach would be a meaningful calculational tool for assessing QD-QC operations since the important energy scales (e.g. \( J \)) in the problem are 1 meV or less, and first principle band calculations cannot achieve 1 meV type accuracies.

Experimentally, it is very difficult to trap one and only one electron in a gated two-dimensional GaAs quantum dot. Thus it has been speculated that perhaps the requirement of single trapped electron per quantum dot as the fundamental qubit may be relaxed in a QD-QC, and that an odd number of electrons in a QD can provide an effective spin-\( 1/2 \) system as a qubit. To explore this possibility, we have recently done a multi-electron calculation where we have three electrons in one quantum dot, thus six electrons in a double dot.\(^9\)\(^:\)\(^2\) We first carry out a Hartree Fock mean field calculation to produce an orthonormal set of single-particle basis states, then employ a restricted configuration interaction (CI) approach to calculate the energy spectrum. Our results show that the low energy dynamics in the multi-electron case is generally much more complicated than the two-electron case because of the single-particle energy level degeneracies in the higher excited Fock Darwin states. This complexity can be alleviated by applying external magnetic fields or deforming the quantum dots, which lift the level degeneracies. Thus we show in Ref.\(^9\)\(^:\)\(^2\) that subject to some constraints spin-based QD-QC architectures are feasible, at least in principle, in multielectron quantum dot arrays.
3 Error correction in quantum dot quantum computer

To evaluate the feasibility of a quantum computer architecture, it is only one of the many steps to study the operating Hilbert space structure. Having a well-defined sub-Hilbert space, as in Fig. 1, is a necessary but by no means a sufficient condition for QC operation. Another important step is to assess the importance of all the possible errors (and how to do the relevant error correction) in this architecture. For spin-based quantum dot quantum computer model, we have explored several kinds of operating error (aside from spin decoherence and errors in single spin measurement). For example, we originally speculated that double occupation in each of the double dot during a two-qubit operation might result in a significant error, the rationale being that one needs to keep tags on all the electrons as each represents a distinct qubit. We now believe that adiabatic operations of these two-qubit gates should effectively erase this problem since adiabaticity will limit the two-electron dynamics within the low-energy two-spin subspace as we discussed in the previous section.

We have done simulations to study the adiabatic condition and the results will be published elsewhere. We no longer believe virtual double occupancy to be a problem.

As the exchange coupling $J$ (the singlet-triplet splitting) is tuned by changing external gate voltage in a QD-QC, thermal fluctuations (or any other types of fluctuations) in the gate voltage will lead to fluctuations in $J$, thus causing phase errors in the exchange-based swap gate which is crucial for two-qubit operations. We have estimated this error by assuming a simple thermal (white) noise. More specifically, we assume $J = f(V)$ where $V$ is the gate voltage that controls the value of $J$. Around any particular value $V_0$, $J$ can be expressed as $J(V) = J(V_0) + f'(V)|_{V_0}(V - V_0)$. During a swap gate between two quantum dots, the phase of the electronic spin wavefunction evolves as $\phi = \int_0^t J(\tau) d\tau / \hbar$. Thus the fluctuation in the phase $\phi$ is

$$\langle \delta \phi^2 \rangle = \langle \phi^2 \rangle - \langle \phi \rangle^2 = \frac{1}{\hbar^2} \int_0^t \int_0^t \langle \delta J(\tau_1) \delta J(\tau_2) \rangle d\tau_1 d\tau_2 \sim \int_0^t \int_0^t \frac{|f'(V)|^2}{\hbar^2} \langle \delta V(\tau_1) \delta V(\tau_2) \rangle d\tau_1 d\tau_2.$$ (1)

Using Nyquist theorem $\langle \delta V(\tau_1) \delta V(\tau_2) \rangle = 4Rk_B T \delta(\tau_1 - \tau_2)$, we obtain the approximate expression for the phase fluctuation:

$$\langle \delta \phi^2 \rangle \sim 4Rk_B T \alpha^2 t / \hbar^2,$$ (2)

where $\alpha$ is the upper bound of $|f'(V)|$. Assuming the swap gate is performed at 1 K (since $J$ is in the order of 0.1 meV $\sim$ 1 K, the experimental temperature can only be lower than 1 K), and the transmission line connecting the gate to the surrounding bath of cryogenic temperature has an impedance of 50 ohm, the rate for phase fluctuation $\langle \delta \phi^2 \rangle / t$ is about 3.2 MHz. The phase error accrued during a swap gate is then about 0.06%. This is quite a small error which is the same order of magnitude as the theoretical tolerance of the currently available quantum error correction codes. To further lower this error rate, one can go to lower experimental temperature and turn up $J$ more gently (which requires longer time but produces smaller $\alpha$) in the QD-QC operation.

Another possible error in the two-qubit operations of the architecture we studied is caused by inhomogeneous magnetic fields. Such a field may come from magnetic impurities or unwanted currents away from the structure. Magnetic field affects both orbital and spin
part of the electron wavefunction. The orbital effect is accounted for by adjusted exchange coupling $J$, while the spin effect is accounted for through Zeeman coupling terms:

$$H_s = J(B) \mathbf{S}_1 \cdot \mathbf{S}_2 + \gamma_1 S_{1z} + \gamma_2 S_{2z},$$

where $\mathbf{S}_1$ and $\mathbf{S}_2$ refer to the spins of the two electrons; $J(B)$ is the exchange coupling (singlet-triplet splitting); $\gamma_1$ and $\gamma_2$ are the effective strength of the Zeeman coupling in the two quantum dots. In an inhomogeneous field, $\gamma_1 \neq \gamma_2$, so that the Zeeman terms do not commute with the exchange term in the Hamiltonian (3). We have done a detailed analysis on how to achieve swap with such a Hamiltonian, and found that there is at the minimum an error proportional to the square of field inhomogeneity in the swap. For example, if the initial state of the two electron spin is $|\phi(0)\rangle = |\uparrow\downarrow\rangle$, the density matrix of the first spin after the optimal swap is

$$\rho_1|e^{i\theta}=-1 = \frac{1}{1+x^2} |\downarrow\rangle \langle \downarrow| + \frac{x^2}{1+x^2} |\uparrow\rangle \langle \uparrow|,$$

where $x = \delta/(2J) = (\gamma_1 - \gamma_2)/2J$. In other words, the first spin can never exactly acquire the state (|\downarrow\rangle) of the second spin. Its state will remain mixed and the smallest error from an exact swap is $1/\sqrt{1+x^2}$, which needs to be corrected. We have estimated that in GaAs a Bohr magneton can lead to an error in the order of $10^{-6}$, which is within the capability of currently available quantum error correction schemes.

4 Conclusion

In this paper we have reviewed some of our recent results in our study of electron-spin-based quantum dot quantum computation. We discuss various issues regarding the Hilbert space structure of a double quantum dot artificial molecule. We also describe possible errors in a spin-based QC. Our tentative conclusion is that building a practical GaAs electron-spin-based QD-QC, while being certainly possible in principle, will be extremely difficult in practice (even assuming a working temperature of 100 mK or less) because of severe constraints and limitations arising from the spin coherence time, the adiabatic condition, the magnitude of exchange coupling, the error correction requirement, and the unsolved experimental problem of a reasonably fast (in less than a microsecond) measurement of a single Bohr magneton.

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