Entanglement and Zeeman interaction in diluted magnetic semiconductor quantum dot

A. Hichri a, S. Jaziri b, *

a Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, 7021 Zarzouna, Bizerte, Tunisia
b Département de Physique, Faculté des Sciences de Bizerte, 7021 Zarzouna, Bizerte, Tunisia

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Abstract

We present theoretically the Zeeman coupling and exchange-induced swap action in spin-based quantum dot quantum computer models in the presence of magnetic field. We study the valence and conduction band states in a double quantum dots made in diluted magnetic semiconductor. The latter have been proven to be very useful in building an all-semiconductor platform for spintronics. Due to a strong p–d exchange interaction in diluted magnetic semiconductor (Cd_{0.57}Mn_{0.43}Te), the relative contribution of this component is strongly affected by an external magnetic field, a feature that is absent in nonmagnetic double quantum dots. We determine the energy spectrum as a function of magnetic field within the Hund–Mulliken molecular-orbit approach and by including the Coulomb interaction. Since we show that the ground state of the two carriers confined in a vertically coupled quantum dots provide a possible realization for a gate of a quantum computer, the crossing between the lowest states, caused by the giant spin splitting, can be observed as a pronounced jump in the magnetization of small magnetic field amplitude. Finally, we determine the swap time as a function of magnetic field and the inter dot distance. We estimate quantitatively swap errors caused by the field, establishing that error correction would, in principle, be possible in the presence of nonuniform magnetic field in realistic structures.

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1. Introduction

Modern information technology utilizes the charge degree of freedom of electrons in semi- conductors to process information and spin degree of freedom in magnetic materials to store information. In semiconductor devices, the spin of carriers has played a minor role so far because the most well-established semiconductor devices based on Si and GaAs are nonmagnetic and show only negligible effect of spin. On the other hand, from the physical point of view, the enhanced
spin-related phenomena due to the coexistence of the magnetism and semiconductor properties have been recognized in magnetic semiconductors and diluted magnetic semiconductors (DMSs). DMSs are based on nonmagnetic semiconductors, and are obtained by allowing them with a sizeable amount (a few percents or more) of magnetic elements, such as Mn. In addition, DMSs have been used to inject spin into normal semiconductor, where enormous spin life time and coherence have been demonstrated. The family of magnetic semiconductors have been extensively studied because of their peculiar properties resulting from the coupling between itinerant electrons and localized magnetic spins (s–d exchange interactions). The magnetically doped II–IV ternary semiconductor exhibited spin glass or related disordered magnetic behavior and any ferromagnetism invariably had very low (\( \leq 5 \text{K} \)) transition temperature. In this paper we restrict ourselves in the domain of weak temperature, i.e. around 5 K. We focus the strong carrier’s magnetic ion Zeeman splitting which leads, e.g. to the effect of giant spin splitting of energy bands in the special case of quantum dots (QDs) made of DMSs. We show that this effect is more significant for the hole system in comparison with the electrons. The part of this interest stems from the fact that the presence of the Zeeman splitting gives rise to a unique possibility to control electrical and optical properties of quantum structures by means of an external magnetic field in a range difficult to achieve in other materials.

Moreover, the discovery of new principles of computation based on quantum mechanics has led to the idea of using coupled QDs for quantum computation [1]. The computers based on the principles of quantum mechanics, such as entanglement, promise to deliver results much faster than classical computers in certain tasks such as factoring and searching [2]. A new and powerful algorithm such as the one discovered by Shor [3] and by Grover [4] makes use of the quantum computer’s ability to exist in any superposition of the states of its binary basis. The quantum algorithms perform quantum time evolution for computation: hence the parallelism of quantum computer. The requirement for the quantum bit of information (qubit), which is at the heart of the quantum computer, is that it can exist in any state of a quantum two-level system, i.e. \( |\psi\rangle = \alpha|0\rangle + \beta|1\rangle \), where \( |0\rangle \) and \( |1\rangle \) are the states of the “classical” bit, and \( |\alpha|^2 + |\beta|^2 = 1 \). Apart from this, the qubits must interact with each other in a controlled way but must not interact with the environment to avoid decoherence. Quantum coherence needs to be maintained for a quantum computer to maximize its capability; it has to satisfy stringent requirements [5]. One requirement is that the qubit should have long coherence time (i.e. slow decoherence). Indeed, decoherence can be loosely defined as irreversibly losing information from the operational Hilbert space into the environment, which is the rest of the universe from the perspective of a quantum computer system. In this work, Mn ions in CdMnTe only serve as dopants and never as magnetic impurities, then we can neglect the decoherence due to the coupling to magnetic ions. The impetus for constructing real quantum computer architectures arose from the seminal results [6] establishing that quantum error correction is theoretically possible and therefore decoherence is not an insurmountable barrier as was assumed earlier. It is thus crucial to explore the challenges facing coherent control of qubits in solid state structures, particularly, the issue of possible error corrections in realistic systems. Among various microscopic degrees of freedom that have been considered for the role of qubits in solid state quantum computer, the necessity of weak interaction with the environment makes the entity spin an especially promising candidate. However, the spin \( \frac{1}{2} \) of an electron is a “natural” representation of a qubit since it comprises exactly two levels: there are no additional degrees of freedom into which the system could “leak”.

In the proposed spin-based quantum computer, the exchange energy \( J \) (the energy difference between the two lowest states) and Zeeman coupling to an external magnetic field play a fundamental role of establishing two qubit entanglements [7–10]. In particular, we study the effect of magnetic field on swap actions. In addition, swaps are used to move spin states around [8,10] so that an arbitrary pair of spins can be brought into controlled entanglement, which is
essential to quantum computer. It is therefore important to investigate how Zeeman splitting will affect the swap gate. In this paper, we consider the theoretical issue of controlling the swap operation in the proposed solid state quantum computer involving QD spin entanglement, with externally controlled magnetic field. Our analysis is based on an adaptation of a Hund–Mulliken variational technique to parabolically confined coupled QDs. We calculate the energy of pairs of QDs in which two carriers are vertically coupled via quantum tunneling and are subject to the Coulomb interaction. From the electronic spectrum, we derive the equilibrium magnetization as a function of magnetic field.

2. Model

We consider a system of two vertically coupled QDs containing one carrier each. It is essential that the carriers are allowed to tunnel between the dots, and the total wave function of the coupled system must be anti-symmetric. It is this fact which introduces correlations between the spins via the charge (orbital) degrees of freedom. The Hamiltonian which we use for the description of two electrons or holes confined in vertically coupled QDs is

$$H = \sum_{i=1,2} h_{zi} + C + H_z = H_{\text{orb}} + H_{\text{spin}},$$

$$H_{\text{orb}} = \sum_{i=1,2} h_{zi} + C,$$

$$H_{\text{spin}} = H_z,$$

(1)

where $h_{zi} = (1/2m_{zi})/(p_{zi} - (q_{zi}/e))A(r_{zi})^2 + V_{zi,l}(r_{zi}) + V_{zi,e}(r_{zi})$ is the single particle Hamiltonian for the $i$th electron $(x = c, q_c = -1)$ or hole $(x = h, q_h = +1)$ in three dimensions with coordinate $r_x$ and spin $s^z$. Electrons or holes have effective masses $m_x$ and confinement energies $h_{wx}$. The coupling of the dots $V_z$ along the inter-dot axis is modelled by a double-well potential [11]. For most vertically coupled dot, the vertical confinement is determined by the conduction-band offset between different semiconductor layers; therefore, in principle, a square well potential would be a more accurate description of the real potential than the harmonic double well (note, however, that the required conduction band offsets are not always known exactly). For the lateral confinement we choose the parabolic potential. The Coulomb interaction is included by $C = q^2/(\kappa|z_1 - z_2|)$ with the dielectric constant $\kappa$.

As a starting point of our calculation, we consider the orbital part of the Hamiltonian $H$. We use a Hund–Mulliken method [12] of molecular orbits which include the states with double occupation $|\psi^d_{\pm}\rangle = (|0\rangle \pm |1\rangle)(|0\rangle \pm |1\rangle)/(2(1 \pm S))$ and the states with simple occupation $|\psi^s_{\pm}\rangle = \{(|0\rangle \pm |1\rangle)(|0\rangle - |1\rangle) \pm (|0\rangle - |1\rangle)(|0\rangle + |1\rangle)$

$\sqrt{1 - S^2}$, here $|0\rangle$ is the ground state wave function of the one-particle confined in the upper dot of the double-dot system, whereas $|1\rangle$ corresponds to the lower dot. A non-vanishing overlap $S = \langle 0|1 \rangle$ implies that the carrier can tunnel between the dots. If the inter-dot distance is large enough, we may expect the coupling between the dots due to the tunnel effect. At low temperatures where $k_B T \ll h_{wx}$, we can restrict ourselves to the two lowest orbital eigenstates of $H_{\text{orb}}$ [13], one of which is symmetric (singlet state) and the other one is antisymmetric (triplet state). In this reduced (four-dimensional) Hilbert space, $H_{\text{orb}}$ can be replaced by the effective Heisenberg spin Hamiltonian $H_s = J_{s_1 s_2}$ where the exchange energy $J = E_T - E_S$ is the difference between the triplet and singlet energy. The ratio between the Zeeman splitting and the relevant orbital energies is small for all $B$-values of interest here. Thus, we can safely ignore the Zeeman splitting when we discuss the orbital degrees of freedom and include it later into the effective spin Hamiltonian. Zeeman splitting is purely a spin effect while the exchange energy $J$ originates from the Coulomb interaction (due to Pauli principle) and the two interaction terms in the Hamiltonian commute with each other if the magnetic field is homogenous.
3. Zeeman coupling

The main difference between calculations for DMS based and nonmagnetic structures arises from the presence of the carrier-magnetic ion (sp–d) exchange interaction. The s–d exchange interaction can be written in terms of Zeeman-like Hamiltonian

$$H_{s-d} = N_0 zx \langle S \rangle s^e$$

(2)

in the case of the conduction electrons, and the p–d interaction [14],

$$H_{p-d} = \frac{1}{2} N_0 \beta z \langle S \rangle s^h$$

(3)

in the case of the valence band holes. Here $s^e$ and $s^h$ are operators of electrons spin and the total angular momentum of hole, respectively, and $x$ is the molar fraction of magnetic ions. To describe the average value of the component of the localized spins along the applied magnetic field direction $\langle S^j \rangle$, a modified Brillouin function is commonly used [15]:

$$\langle S^j \rangle = S_0 B_j \left( \frac{g \mu_B BS}{k_B(T + T_0)} \right),$$

(4)

where $g = 2$ is the Lande factor of manganese d-electrons, $S = \frac{3}{2}$ is a magnitude of the spin of the magnetic ions, and $\mu_B$ is the Bohr magneton. The remaining two components of average spin vanish in the materials in question $\langle S^x \rangle = \langle S^y \rangle = 0$.

$$B_j(x) = ((2S + 1)/2S) \coth((2S + 1)/2S)x - 1/2S \coth(x/2S)$$

is the Brillouin function. The two phenomenological parameters of this description, the saturation value $S_0$ and the temperature shift $T_0$, have been found to obey the following empirical expressions [16]:

$$S_0(x) = E_x a \exp \left[ \left( \frac{E_x}{b} \right) + c \exp\left( \frac{E_x}{d} \right) + e \right]$$

and

$$T_0(E_x) = \frac{f E_x}{1 + g E_x}$$

with $E_x = 1563x$ where $a = 0.4595$, $b = 36.06$, $c = 1.272$, $d = 252.5$, $e = 0.01258$, $f = 0.02263$, and $g = 0.001761$ [17]. The corresponding exchange constants $N_02x$ for the conduction band states and $N_0\beta$ for the valence band states in majority of II–VI DMS are usually of opposite signs [18]. Usually also, the absolute value of $N_0\beta$ is considerably greater than $N_02x$. For example, in Cd$_{1-x}$Mn$_x$Te $N_02x = 220$ meV and $N_0\beta = -880$ meV [19] thus the giant spin splitting of excitonic states in DMSs is mainly determined by the spin splitting of the hole states. The negative exchange constant $N_0\beta$ is several times greater in magnitude than the positive $N_02x$, even a small admixture of $\Gamma_8$ states to $\Gamma_6$ state can reduce significantly (up to 30% in the case of quantum wells) the value of total effective exchange constant of the conduction electrons [20]. For QDs this reduction of the conduction band exchange constant is expected to be even more significant.

The magnetic field $B$ also couples to the carrier spin via the Zeeman term, hence to take it into account means to introduce an additional parameter into the equations, describing splitting of spin levels in the magnetic field. According to this notation, the Hamiltonian describing the electrons and holes in DMS QD takes the form

$$H_z = \sum_i h_i + C + N_02x \langle S \rangle s^e_i - g_e \mu_B B s^e_i,$$

(5)

$$H_x = \sum_i h_i + C + \frac{1}{2} N_0 \beta z \langle S \rangle s^h_i - g_h \mu_B B s^h_i,$$

(6)

where $g_e, g_h$ are the Lande factor, correspondingly, for $\pm \frac{1}{2}$ electrons in the conduction band and $\pm \frac{1}{2}$ heavy holes in the valence band.

For the sake of simplicity, to describe s–d and p–d exchange interactions, we use in this paper the values of these constants equal to their values in the bulk. This simplification becomes invalid only in very small QDs (with radius smaller than about 30 Å). Admittedly, for small quantum dots one should replace bulk by the values of p–d exchange constants, calculated in Ref. [21]. This does not change, of course, the qualitative results obtained in this work. Throughout this paper, we have evaluated our results for two vertically equal large Cd$_{0.57}$Mn$_{0.43}$Te QDs with 125 Å in diameter and 70 Å high. Calculations are performed using the following parameters $\kappa = 8.5$, $T = 1.7$ K, for holes, $m_0 = 0.14$, $m_\perp = 0.48$, $g_e = 0.15$, for conduction electrons, $m_0 = 0.095$, $g_e = -5$ [22]. We plot in Fig. 1 the energy spectrum as a function of
magnetic field. The inter-dot distance $a = 225\, \text{Å}$ for holes and $a = 85\, \text{Å}$ for electrons system. We see immediately that the character of the hole ground state via the Zeeman splitting differ strongly by an applied magnetic field than the electron spectrum. Since the crossing between the two lowest ground states is depicted at a field of few $T$ for holes, this makes the hole system in DMSs QD more practical for the experiments manipulation than electrons.

For using now coupled QDs as quantum gates for quantum computation, we can determine the measurement of the carrier spin (qubit) with the magnetization’s measurement. The magnetization of the system is given by $M = -\partial E_g/\partial B$ where $E_g$ is the ground state energy of the double QDs. Due to the crossing between the lowest states, the magnetization spectrum (Fig. 2) shows a jump which marks the phase transition. It is also found that the magnetization has a linear relation with the magnetic field in the low-field region and at $T = 1.7\, \text{K}$. In the limit of weak magnetic field, it is elementary to show that the magnetization of two-carriers is in proportion to the magnetic field [23],

$$M \approx -x B, \quad x = \left\langle \psi_g \left| \frac{\hbar^2}{2m_0} \left( |r_1|^2 + |r_2|^2 \right) \right| \psi_g \right\rangle,$$

where $\psi_g$ is the ground state of the two-carriers. It is straightforward to see that $x$ also measures the extension of the ground state. When we study the temperature effect on the magnetization, we must include all the highest states.

The magnetization must be calculated as the following expression:

$$M = -\partial F/\partial B,$$
where \( F = -k_B T \ln(Z) \) is the free energy, \( Z = \sum_i \exp(-E_i/k_B T) \) is the partition function and \( k_B \) is the Boltzmann constant. It is found that the temperature decreases the magnitude of the magnetization, and until a certain temperature no crossing can occur and the curves is smooth. The magnetization reveals the nature of the ground state of the coupled QD. Direct measurement of the magnetization \( M \) as a function of magnetic field and temperature is plotted in Fig. 2.

4. Swap action

We assume, in the following, that the electron orbital degrees of freedom are frozen, so that an effective spin Hamiltonian quite faithfully describes the two electron spin system [9].

\[
H_s = J_s \mathbf{S}_1 \cdot \mathbf{S}_2 + \left( \langle \uparrow | N_0 \mathbf{S}_1 \mathbf{S}_2 - g_e \mu_B B \downarrow \rangle \right) \mathbf{S}_1^0
\]

\[
+ \left( \langle \downarrow | N_0 \mathbf{S}_1 \mathbf{S}_2 - g_e \mu_B B \uparrow \rangle \right) \mathbf{S}_2^0
\]

\[
= J_s \mathbf{S}_1 \cdot \mathbf{S}_2 + \gamma_1 \mathbf{S}_1^0 + \gamma_1 \mathbf{S}_2^0.
\]  (9)

Here, we have implicitly assumed, based on the small inter-dot wave function overlap, that the two spins are distinguishable, with spin 1 on the upper dot and spin 2 on the lower dot. We have also assumed that the field is entirely along the \( z \) direction.

Hamiltonian (9) can be expressed on the basis of four two-spin states \( |\uparrow \uparrow \rangle, |\downarrow \downarrow \rangle, |\uparrow \downarrow \rangle \) and \( |\downarrow \uparrow \rangle \) and its eigenstates can be easily obtained. The two polarized states are decouples from the other two, which are mixtures of singlet and triplet states: \( |\psi_1 \rangle = |\uparrow \uparrow \rangle, |\psi_2 \rangle = |\downarrow \downarrow \rangle, |\psi_3 \rangle = \frac{1}{\sqrt{2}}(|\uparrow \downarrow \rangle + |\downarrow \uparrow \rangle) \) and \( |\psi_4 \rangle = \frac{1}{\sqrt{2}}(|\uparrow \downarrow \rangle - |\downarrow \uparrow \rangle) \). The energies are \( E_1 = (2J + \Delta)/4, \ E_2 = (2J - \Delta)/4, \ E_3 = J/4 \) and \( E_4 = -3J/4 \), where \( \Delta = \gamma_1 + \gamma_2 \) represents the average magnetic field. An important question here is whether these mixtures and shifts will cause any error in quantum computation in the schemes based on the exchange energy. After all, the swap action in these models depends on the perfect phase matching in the evolution of singlet and triplet states, as we will show later. Since swap operation is an essential component of the spin-based quantum dot quantum computer and several other architectures, we need to precisely quantify the effects of mixtures in singlet and triplet states on the swap action.

To determine whether swap is affected, we explore whether a product state of spins 1 and 2 will evolve into a product state (pure states for both spins) again. Our strategy here is to calculate the concurrence \( C \), which varies from \( C = 0 \) for an unentangled state (in the usual sense that they are factorized into single particle states) to \( C = 1 \) for a maximally entangled state. The most general pure states in the case of the two-qubit model can be written as \( |\psi \rangle = a_1 |\uparrow \rangle + a_2 |\downarrow \rangle + a_3 |\uparrow \rangle + a_4 |\downarrow \rangle \) where \( \sum_{i=1}^{4} |a_i|^2 = 1 \). The concurrence of the pure state is simply given by [24] \( C(|\psi \rangle) = 2|a_2a_3 - a_1a_4|/\sqrt{2} \), thus, the pure state is entangled if and only if \( a_1a_4 \neq a_2a_3 \). We can then find out whether this pure state corresponds to a swapped state. We consider that the initial state is an unentangled state given by \( |\phi(0) \rangle = (a_1 |\uparrow \rangle + a_2 |\downarrow \rangle)(b_1 |\uparrow \rangle + b_2 |\downarrow \rangle) \).

If the two electrons are located in two well-separated QDs in the beginning, the above product state does not violate the anti-symmetry requirement of a two fermions state. This state can be expanded on the basis of the eigenstates of Hamiltonian (9). The two-spin state at time \( t \) takes the form

\[
|\phi(t) \rangle = a_1b_1e^{-iE_1t/\hbar}|\uparrow \uparrow \rangle + a_2b_2e^{-iE_2t/\hbar}|\downarrow \downarrow \rangle
\]

\[
+ (e^{-iE_1t/\hbar} - e^{-iE_2t/\hbar})a_1b_2|\uparrow \downarrow \rangle + a_2b_1|\downarrow \uparrow \rangle
\]

\[
+ e^{-iE_3t/\hbar}(a_1b_2 - a_2b_1)|\uparrow \downarrow \rangle /2
\]

\[
+ e^{-iE_4t/\hbar}(a_1b_2 + a_2b_1)|\downarrow \uparrow \rangle + e^{-iE_3t/\hbar}(a_2b_2 - a_1b_1)|\downarrow \downarrow \rangle /2
\]

to have a pure state means that the concurrence must be equal to zero \( C = 2[|\langle a_1b_2 - a_2b_1 \rangle e^{-i\theta} - (a_1b_2 - a_2b_1)e^{i\theta} \rangle - 4a_1a_2b_1b_2e^{-i\theta}]^2 = 0 \). The solution here are \( e^{i\theta} = \pm 1 \), where \( \theta = Jt/\hbar \). When \( e^{i\theta} = -1 \), \( |\phi_1(t) \rangle = |\uparrow \downarrow \rangle + b_2e^{i\Delta/2\hbar}|\downarrow \uparrow \rangle \), the state of the first spin returns to its initial state with a phase shift between the two coefficients, the swap time \( t_{\text{swap}} = \pi \hbar /J \). When \( e^{i\theta} = 1 \), \( |\phi_1(t) \rangle = (a_1 |\uparrow \rangle + a_2 |\downarrow \rangle)(b_1 |\uparrow \rangle + b_2 e^{i\Delta/2\hbar} |\downarrow \rangle) \), the swap is achieved with the exception of an additional phase that can be corrected easily with a single qubit operation. In Fig. 3, we plot the swap time as a function of...
magnetic field and the QD separation for both Cd$_{0.57}$Mn$_{0.43}$Te QD and for a nonsemi-magnetic GaAs QD. We use for the GaAs QDs the same geometry as described below. The difference between the two spectrum is due especially to the semiconductor’s material.

Physically, a uniform field means that the Zeeman coupling couples to the total spin (including both electron spins), so that the Zeeman term commutes with the exchange term in Hamiltonian (9), and therefore does not change the eigenstates. The shifts in the energy levels of

Fig. 3. Half of the swap time as a function of the magnetic field and a quantum dot separation. The swap time depends only on the exchange energy but does not depend on the spins.
the polarized states cause additional phase shift, but can be corrected by applying an opposite magnetic field with the same pulse shape, magnitude and length.

5. Conclusion

In summary, using the Hund–Mulliken approach, we have calculated the energy as a function of magnetic field for carriers confined in a pair of vertically coupled QDs, and have compared the two-hole spectra to the two-electron spectra. For two-hole filling in the presence of a magnetic field, the ground-state crossing occurs at fields of a few $T$, depending on the strength of the confinement, the distance coupling, and the dots size. The detailed information on the nature of the ground state of the double QDs may be obtained by measurement of the magnetization. The swap time given by $t_{\text{swap}} = \pi \hbar / J$ takes a bit to flip from a state $|\uparrow\rangle$ to an orthogonal state $|\downarrow\rangle$. An external uniform magnetic field does not qualitatively change the proposed quantum computer algorithm logistically, but it makes the quantum computer operation more difficult because of the necessary correction pulses.

References