Elaboration

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Spin Qubits

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0.1 Motivation

For a long time the speed of calculations doubled every 18 month, according to Gordon Moore [4]. Nevertheless the classical transistor-based computing method reaches its limits in some essential operations. It has been shown that operations based on the non-classical interaction between spins [2] lead to a speed-up in a lot of calculations (an important example is factoring). Quantum computing also gives the

possibility of calculations which are classically too expensive or not even possible (i.e. Deutsch-Josza-Problem, see [3]). In the following I want to give a short overview on one of the most promising techniques in the topic of quantum calculation - the solid state systems. Thereby I will concentrate on systems of spin-qubits.

0.2 Overview

After a short outline, why spin systems are one of major interest in todays research, we will have a look on a concrete implementation. Then the model needed to describe the interaction in this system is introduced. In the second section we will have a closer look on the exchange energy. In the third section we will see how quantum operations can be achieved in our system by controlling the exchange interaction. Last it will be shown how we can implement a quantum gate by using the field-dependence of the exchange energy, calculated in the third section. In the end a short overview of real experiments will be given. Basic knowledge of quantum mechanics presumed. This work closely follows chapter 24 of ref. [1].

1 Introduction

An essential property of an candidate for a quantum-computer is that the coherence time (i.e. the time over which $\alpha |1\rangle + \beta |2\rangle$ is well defined) of the qubit-system is larger than the time which is needed to perform calculation operations. To be sure it is also necessary to have an exact control of the qubits to perform operations. And, to have the possibility of gaining a quantum computer device later on, the system has to be scalable to large numbers of qubits. As so often it is hard to fulfill all of these requirements perfectly with one system. But great expectations are held for solid state systems, because they are well-known and have been well researched over the last century and, for sure, it is much easier to handle solid state systems than ions in a trap or solved molecules. One of the most interesting systems is a spin-1/2-qubit-system. These systems are very well known and can be described by quantum mechanics. Semiconductor systems are one example, in which a 2-dimensional electron gas exists with a very long coherence time, compared to the time needed to perform calculations (i.e. in GaAs around $1\mu s$). The construction of such semiconductor systems requires very exact growth techniques, but it is generally based on todays technology, which makes it very interesting for application. So therefore we will concentrate in the following on spin-1/2-systems.

We now focus on one of the most important spin-1/2-system, namely a quantum dot system in a semiconductor heterostructure as shown in fig. 1.

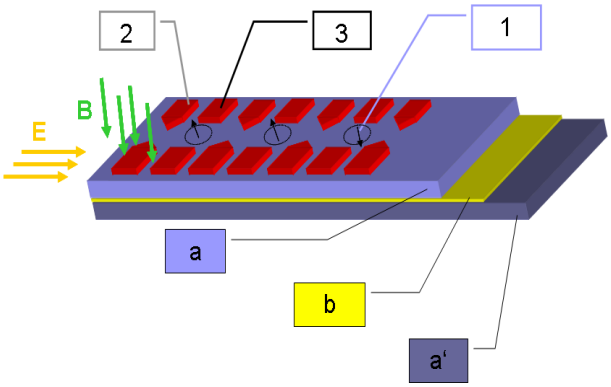

Figure 1: Scheme of quantum dots in a semiconductor heterostructure: between the GaAs-layer (labeled a) and the AlGaAs-Layer (labeled a') exists a 2-dimensional electron gas (b). In a very localized area an electron (labeled 1)is trapped by the use of two gates (2 - split gate, 3 - potential barrier gate). The interaction between two dots is controlled via voltage applied on these gates. Because of a magnetic field perpendicular to the plane there exists a particular direction for the spin.

Two of these quantum dots are interacting by tunnel coupling. Because it has been shown [1] that all essential (and known) operations can be realized with two qubits, only the next neighbour coupling is of interest. To simplify life, we will only look at a system of 2 qubits in the following, which is, as shown above, no restriction for quantum operations. In an 2-qubit-system there exist four different states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)$, $\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$. There is an energy splitting between the singlet and the three triplet states due to the excitation operator, as shown in fig. 2.

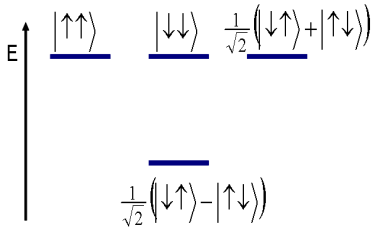

Figure 2: Energy-splitting of the quantum dot in a singlet (ground-) state and a triplet (excited-) state.

If we now want to write down the Hamiltonian for the two qubit-system, we first need the Hamiltonian for one particle, which looks like

$$h(\mathbf{r}_i, \mathbf{p}_i) = \frac{1}{2m_{eff}} \left(\mathbf{p}_i - \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right)^2 + e\mathbf{r}_i \cdot \mathbf{E} + V(\mathbf{r}_i)$$

where $\mathbf{A}(\mathbf{r}_i) \perp \hat{z}$ is the vector potential and $E \parallel \hat{x}$ the electric field and $V(\mathbf{r}_i)$ the potential created by the gates around the two quantum dots, which has the form $V(\mathbf{r}_i) = \frac{m_{eff}\omega_0}{2}\left(\frac{1}{4a}(x^2 - a^2)^2 + y^2\right)$. An example is shown in fig 3.

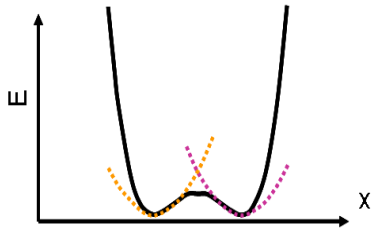

Figure 3: double minima potential created by the gates on top of the GaAs-heterostructure, which restricts the quantum dot to a certain area and gives by the high of the inner well the strength of the interaction between the two dots. It can locally be approximated as an harmonic potential (doted lines).

This double-well-potential can be approximated as a harmonic potential near each of the two minima. The well between those is inversely proportional to the coupling strength of the tunnel coupling between the two dots. To derive the total Hamiltonian we now have to sum over both particles, consider the interaction between both and add another term due to the ZEEMAN coupling (which we have ignored until now) between the spins and the magnetic field from the gates. This leads us to the following Hamiltonian

$$H_{tot} = \sum_{i=}^{2} h(\mathbf{r}_i, \mathbf{p}_i) + \frac{e^2}{\varepsilon \left|\mathbf{r}_1 - \mathbf{r}_2\right|} + \mu_B \sum_{i=1}^{2} g_i \mathbf{B}_i \cdot \mathbf{S}_i$$

where $\frac{e^2}{\varepsilon|\mathbf{r}_1-\mathbf{r}_2|}$comes from the COULOMB-interaction and $\mathbf{B}_i$is the magnetic field on spin $\mathbf{S}_i$. Of course we still have the double-well-potential in each single particle operator. We still have in mind the energy splitting. If we now tune the barrier between the two dots, we can control whether the system is in the singlet or triplet state. This control will be the essential part for applying quantum operations to our system, which will be shown in the following chapter.

2 Implementation of quantum operations

The first step we have to take, is to find an easy description of the interaction between the two spins. As mentioned above it is a tunnel coupling. The most easy description therefore is given by the HEISENBERG model. By the way the question occurs: why we should have a closer look on the spin-spin-interaction while there is no spin-spin-term in our total Hamiltonian (see 1). Bring to mind the description of an H_2-molecule: inderiving the quantummechanical description, one has to pay attention to the indistinguishability of the electron, which then leads to spin-spin-effects. The HEISENBERG Hamiltonian has the form

$$H_{Hei} = \sum_{i,j} J_{ij}(t) \mathbf{S}_i \mathbf{S}_j - \mu_B \sum_k g_k \mathbf{B}_k(\mathbf{r}_k) \cdot \mathbf{S}_k$$

whereby our parameter to tune is now the exchange energy $J_{ij}(t)$which is just the energy-difference between singlet and triplet state: $J_{ij}(t) = E^{ij}_{singlet} - E^{ij}_{triplet}$.

So we need to calculate this energy difference. Therefor we use the so called HEITLER - LONDON-approach [1] which was originally developed in 1927 for the calculation of H_2-molecules and is a good approximation for weak spin-spin interactions (for example for large distances

between quantum dots) and is easy to calculate. We now have to make several approximations. First, we will focus on ground states from now on. An we consider the COULOMB interaction so strong that the electrons do not come near each other, which essentially means we have only one electron per dot. And we will neglect the spin-field coupling from now on. Then we arrive at reduced Hamiltonian:

$$H_{red} = \sum_{i=1}^{2} h(\mathbf{r}_i, \mathbf{p}_i) + \frac{e^2}{\varepsilon \left|\mathbf{r}_1 - \mathbf{r}_2\right|}$$

With this Hamiltonian it is much easier to calculate the wave function which fulfills the SCHRÖDINGER-equation. We will skip the detailed calculation, which results in

$$|\psi_\pm\rangle = \frac{|12\rangle \pm |21\rangle}{\sqrt{2(1 \pm U^2)}}$$

where $U = \langle 2|1\rangle$ is the overlap of the wave-functions. Because we now only have the ground state, we do not have any energy-splitting. But we consider our reduced solution as a good approximation for the true wave function and therefore calculate the energies for singlet- and triplet-state with these wave functions $|\psi_\pm\rangle$ and our total Hamiltonian from above (1). Then the energies are

$$\begin{aligned} E_{singlet} &= \langle\psi_-| H_{tot} |\psi_-\rangle \\ E_{triplet} &= \langle\psi_+| H_{tot} |\psi_+\rangle \end{aligned}$$

The difference is then the searched for exchange-energy.

If we now calculate this expression explicitly, we gain information about the dependencies of J_{ij}. Despite this term being rather nasty, we will have a closer look at it. The exchange energy is given by

$$J = A\big(c\sqrt{b}\left(I_0(bd^2)e^{-bd^2} - I_0(d^2b - \frac{d^2}{b})e^{d^2(b-\frac{1}{b})}\right) + \frac{3}{4b}\left(1 + bd^2\right)\big)$$

where $A \sim \frac{1}{sinh(2d^2(2b-\frac{1}{b}))}$, c is the ratio of the COULOMB-energy to the confining energy and I_0 is the first BESSEL-function, d the distance, normalized with the BOHR-radius and b the normalized frequency, which depends on the applied magnetic field. We will now discuss the last three terms in detail. Obviously the BESSEL-term occurs because of the interference between the wave-functions of the two particles. The normalized distance occurs due to the fact that the interaction between the two dots strongly depends on their distance and therefore gives us one possibility to control the interaction. The frequency, normalized by the LARMOR-frequency, depends on the applied magnetic field and therefore gives us another possibility of control. Of course it is much easier to control an external magnetic field, than a distance in a solid. Because of this we will focus on the field-dependency of the exchange interaction in the following. The graph in fig.4 shows the curve.

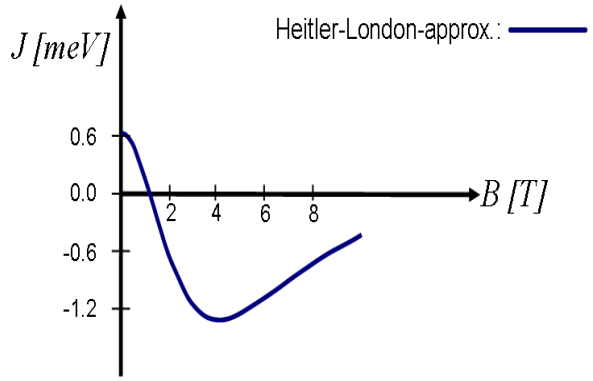

Figure 4: the dependency of the exchange energy on the external magnetic field. In terms of magnetism the coupling goes from a antiferromagnetic regime to a ferromagnetic regime, whereby there exists a zero-coupling despite the finite barrier between the dots.

J_{ij} starts at a positive value (which means, in case of magnetism, an antiferromagnetic coupling), then goes to zero at about 1.2 T and has a minimum at about 4 T. Afterwards it goes asymptotically to zero. What happens is very interesting, because at about 1.2T we have no coupling between the spins despite the finite barrier in between (remember that this is a kind of tunnel coupling, which in the zero field case has a finite tunneling-possibility through a finite barrier). In fig. 4 we also see why we do not have a quantum computer available at the local computer store - the minimum of the exchange energy lies around 1.3 meV, which is small compared to the thermal energy at room temperature (around 26 meV). Therefore such devices currently only work at very low temperatures. But it is very important to point out that we can decouple the dots. Starting from this we can turn on the coupling for a certain time and thereby apply an operation.

But how will the curve look, if we take a different approach. We only looked at groundstates. We will now also look at higher energy states, which means in the sense of molecule physics, where these methods were originally developed, at higher orbitals. This approximation is called sp-hybridization. We will not derive the formula for the exchange energy in detail, but only look at the results. The dependency of J on the magnetic field is shown in fig. 5

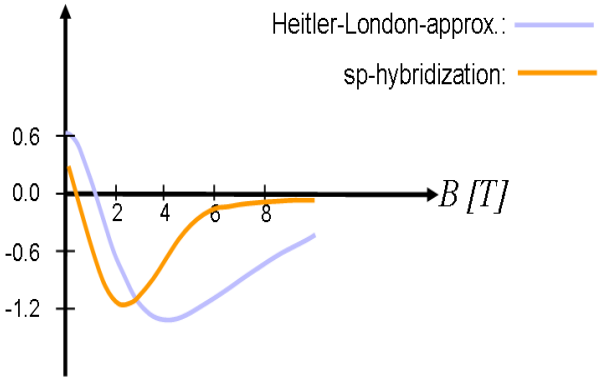

Figure 5: the dependency of the exchange energy on the external magnetic field. The light blue line is the same as above, thereby we only had a look a the groundstates of the wavefunction. The orange graph shows the dependency of the exchange energy on the magnetic field considering also higher energy levels.

Fortunately we have a very similar curve, only the position an value of the zero-coupling changed. This means we also can hope to find a sequence of time dependent changes in the coupling which leads to bit-operations.

But first we will look at what changes if we now also allow two electrons per dot, which is a realistic case. Therefore we will have to expand our HILBERT-space to four instead of two dimensions [1]. This approximation was first done by HUND and MULLIKEN and is based on the advanced HUBBARD-model . We will also not dicuss this in detail, but just compare the curve to the others, as done in fig. 6

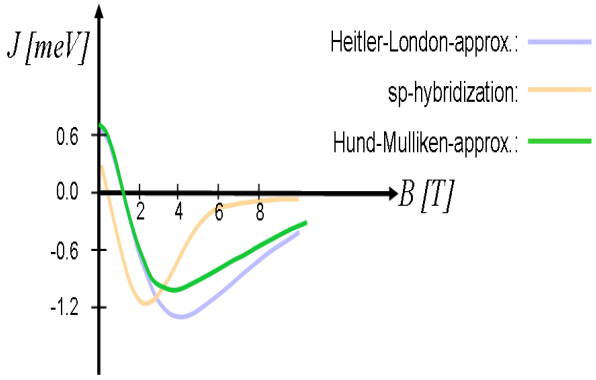

Figure 6: the dependency of the exchange energy on the external magnetic field. The light blue curve as well as the orange curve are the same as above.The green graph shows the dependency of the exchange energy on the magnetic field using the Hund-Mulliken-approach.

And again we see the zero coupling at nearly the same field as in the Heitler-London approach and also a minimum beneath it. That means that we can be hopeful that we can achieve such a non-coupling-regime. But now the next step is to use that fact for producing an operation in our system.

3 Operations

Operations on our qubit can, as mentioned above, now be implemented by applying a time dependent magnetic field to have a controlled interaction. Lets consider such a magnetic pulse. We are starting from no coupling, which means $J_{ij} = 0$, which is achievable, as shown above. An operation takes place, if $J_{ij} \neq 0$. So a pulse with

$$exp\left(\frac{i}{\hbar}S_iS_j\int J_{ij}(t)dt\right) = exp\left(\frac{-i\pi}{\hbar}S_iS_j\right)$$

creates a spin-flip, which means the spin is turned around an angle of π. The graph of this pulse is shown on fig. 7. This is called SWAP-operator and it is equivalent to the classical one.

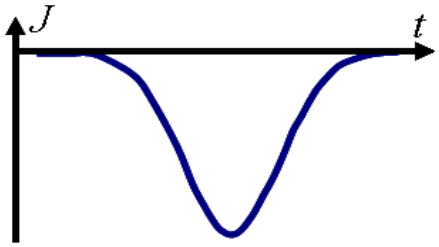

Figure 7: Pulses of such type (the area under the graph is $-\pi$) create spin-flips.

But if this is a classical operation, how can quantum calculations be performed with it? The answer is they can not. What we need for quantum computation are non-classical operations. But it is easy to consider how to achieve a shape which produces such an operation. If the area under the pulse is equal to $\frac{-\pi}{2}$ the operation will be the square root of the previous one:

$$\begin{aligned} exp\left(\frac{i}{\hbar}S_iS_j\int J_{ij}(t)dt\right) & \\ &= exp\left(\frac{-i}{\hbar}\frac{\pi}{2}S_iS_j\right) \\ &= \sqrt{exp\left(\frac{-i\pi}{\hbar}S_iS_j\right)} := S \end{aligned}$$

But $\sqrt{SWAP}$ is a real quantum operation and thus has no classical equivalent. From now on we call this operation S. It has been shown in previous publications ([1] and references therein), that it is possible to create the controlled NOT-operator (CNOT) out of sequence with $\sqrt{SWAP}$ and some single qubit operations and a basic transformation. The CNOT-operator then is

$$U_{CNOT} = V\left[e^{i\frac{\pi}{2}S_1^z}e^{-i\frac{\pi}{2}S_2^z}Se^{i\pi S_{1^z}}S\right]V^\dagger$$

where V and $V^\dagger$ perform the basic transformation. While one can imagine one quantum state as one point on a BLOCH-sphere it would be wrong to imagine n qubits as n points on a BLOCH-sphere. Therefore it is not possible to show this sequence as a simple trajectory on a BLOCH-sphere. Therefore one has to have a close look at the matrix-representation. In its diagonal form, the sequence looks exactly like the CNOT-gate, as it can be seen in many books on quantum information theory (i.e. [3]). One really important aspect of the achievement of a CNOT-gate, is that all operations for computations can be derived from it .The interesting question, now that we have seen that it is theoretically possible to perform quantum operations on a semiconductor heterostructure, is how the experiments are going and we will have a look at examples for the implementation of an 2-qubit-device.

4 Examples for Implementations

The most interesting question is, if implementations of 2-qubit-devices work. The first and promising answer is yes, it is possible to implement such a device and it has already been done in several laboratories ([1] and references therein). The design of the metallic gates on the top of the GaAs-structure is unfortunately not as simple as shown in graphic 1. Figure 8 shows how a design looks like in todays laboratories. The expectations on this technology are very high and a lot of research is being performed, both by national and commercial research institutes. Nevertheless the goal to realize a pair of qubits in such a system at roomtemperature has not been achieved yet. But hope lies in further investigations to find materials with high exchange energies (higher than $k_B T$).

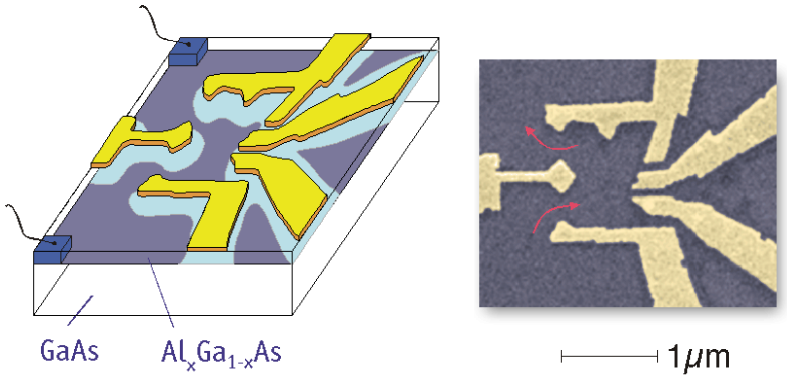

Figure 8: Example for a real implementation of an 2-qubit-system (from http://marcuslab.harvard.edu/images/dots.gif)

Another very interesting technique, is to place quantum dots in microcavities, whereby the exchange is done by virtual photons. This proceeds as follows: make holes in the GaAs photonic cristal by EBL (electron beam lithography) and chemical etching, then produce a line defect by removing some holes (see fig. 9). The optical confinement is inplane given by the 2-dim. photonic crystal and offplane by the GaAs-air-interface. This forms a so called microcavity in which the virtual photons can be exchanged.

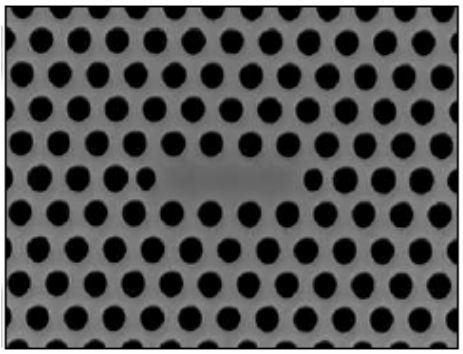

Figure 9: Example of a real implementation of a microcavity-quantum-dot-system. The quality Q of the microcavity is optimized by the hole radius, lattice spacing and membrane thickness. (done by M. T. Rakher, L. A. Coldren, Cavity QED with quantum dots in semiconductor microcavities, preprint version, University of California Santa Barbara)

The theoretical description differs from those shown above, because of the different exchange interaction (here described by the transverse-coupling), but the scheme remains the same:

1. find the Hamiltonian of the system
2. calculate the terms for the interaction
3. find a suitable description of the exchange energy
4. find a variation of exchange to produce non-classical operations

5 Summary

In this work, the idea of a qubit-implementation done by electron spins was presented by the example of a GaAs/AlGaAs heterostructure. To understand the physics behind these devices, we had a closer look at the exchange interaction and how the coupling is controlled by external gates. A simple description of the exchange interaction was presented and some approximate results for the exchange energy were given. As shown in former publications ([1] and references therein), operations on 2-qubit-systems can be realized by a time depending exchange between the dots. One sequence to achieve an essential quantum-operation, from which all computations can be gained, has been shown. In the last part we have seen one example for the heterostructure-realization and discussed the expectations of these devices and the problems which have to be solved by further research. In a second example, it was shown that the scheme, applied in this work, remains valid in a more general sense and leads to quantum operations which are necessary for the realization of a quantum computer

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6 References

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