Dynamics of entanglement between quantum dot spin-qubits

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Abstract

We briefly review the physics of gate operations between quantum dot spin-qubits and analyze the dynamics of quantum entanglement in such processes. The indistinguishable character of the electrons whose spins realize the qubits gives rise to further entanglement-like quantum correlations that go beyond simple antisymmetrization effects. We also summarize further recent results concerning this type of quantum correlations of indistinguishable particles. Finally we discuss decoherence properties of spin-qubits when coupled to surrounding nuclear spins in a semiconductor nanostructure.

1 Introduction

Quantum entanglement is one of the most intriguing features of quantum mechanics. It is one of the decisive properties of the quantum world which distinguishes it from classical physics. Moreover, in the last decade, entanglement has proved to be the key ingredient of the emerging field of quantum information theory.

In the beginning of modern quantum theory, the notion of entanglement was first noted by Einstein, Podolsky, and Rosen [11], and by Schrödinger [12]. While in those days quantum entanglement and its predicted physical consequences were (at least partially) considered as an unphysical property of the formalism (a “paradox”), the modern perspective on this issue is very different. Nowadays quantum entanglement is to be seen as an experimentally verified property of nature providing a resource for a vast variety of novel phenomena and concepts such as quantum computation, quantum cryptography, or quantum teleportation.

While the basic notion of entanglement in pure quantum states of bipartite systems (Alice and Bob) is theoretically well understood, fundamental questions are open concerning entanglement in mixed states (described by a proper density matrix), or entanglement of more than two parties [8, 9, 10]. The most elementary example for entanglement in a pure quantum state is given by a spin singlet composed from two spin-1/2-objects (qubits) owned by A(lice) and B(ob), respectively,

\[
\frac{1}{\sqrt{2}}((|\uparrow\rangle_A \otimes |\downarrow\rangle_B - |\downarrow\rangle_A \otimes |\uparrow\rangle_B).
\] (1)
For such a state, the state of the combined system cannot be described by specifying the state of Alice’s and Bob’s qubit separately. It is a standard result of quantum information theory [1, 4] that this property does not depend on the basis chosen in Alice’s or Bob’s Hilbert space. As we shall see below, the entanglement of such a quantum state (quantified by an appropriate measure) is invariant under (independent) changes of basis in both spaces.

Physically measurable consequences of quantum entanglement of the above kind arise typically (but not exclusively) in terms of two-body correlations between the subsystems. In this case the effects of entanglement can typically be cast in terms of so-called Bell inequalities [13] whose violation manifests the presence of entanglement in a given quantum state. Using this formal approach the physical existence of quantum entanglement (as opposed to classical correlations) has unambiguously been verified by Aspect and coworkers for the polarization state of photons [14]. Moreover, quantum entanglement is an essential ingredient of algorithms for quantum computation [2, 3, 4], in particular for Shor’s algorithm for decomposing large numbers into their prime factors [15]. This problem is intimately related to public key cryptography systems such as RSA encoding which is widely used in today’s electronic communication.

Among the many proposals for experimental realizations of quantum information processing solid state systems have the advantage of offering the perspective of scalability, i.e. the integration of a large number of quantum gates into a quantum computer once the single gates and qubits are established. In the recent years, several proposals for using spins of electrons and/or nuclei in solid state systems have been put forward, starting with the work of Ref. [16], see Refs. [17, 18, 19, 20, 21]. Specifically, in Ref. [16] it was proposed to use the spin of electrons residing in semiconductor quantum dots as qubits [22, 23, 24, 25, 26].

The central idea is to store the information in the spin-degree-of freedom of the electron, while the manipulation of the spin, like single spin rotations and spin-spin interactions, are achieved via electrical gates acting on the charge degree-of-freedom of the electron. In this contribution we briefly review essential aspects of this proposal and analyze the dynamics of quantum entanglement in gate operations between qubits of this type. During such processes, the indistinguishable character of the electrons leads to entanglement-like quantum correlations which require a description different from the usual entanglement between distinguishable parties (Alice, Bob, ...) in bipartite (or multipartite) systems. In such a case the proper statistics of the indistinguishable particles has to be taken into account [24].

This article is organized as follows. In section 2 we give a brief overview on elementary results on entanglement between distinguishable parties. In section 3 we briefly review essential aspects of the quantum dot spin qubit proposal of Ref. [16]. After some general remarks we summarize in subsection 3.2 recent results on decoherence properties of electron spins interacting with surrounding nuclear spins in semiconductor nanostructures [53, 54]. In subsection 3.3 we give a brief description of the low-energy physics of lateral quantum dot molecules consisting of two spin-qubits. This discussion will lead us to the question of “entanglement” (or entanglement-analogous quantum correlations) between indistinguishable particles, which are in our case here electrons in the joint system of two (or more) quantum dots [24]. The research and literature on quantum entanglement has so far fairly concentrated on distinguishable parties; the issue of indistinguishable (or, in other words, identical) objects has been addressed only very recently [24, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38]. We therefore give also a short overview on this new direction of work in quantum information theory. In section 5 we discuss results on gate operations between quantum dot spin qubits with the emphasis on the dynamics of quantum entanglement. Specifically we present results on swap processes (interchanging the state of two qubits) and the “square root of a swap” generating a maximally entangled state from a tensor product. We close with a summary in section 6.
2 Quantum Entanglement between distinguishable parties

We now give an introduction to basic concepts of characterizing and quantifying entanglement between distinguishable parties. We concentrate on pure states (i.e. elements of the joint Hilbert space) of bipartite systems. We then comment only briefly on the case of mixed states (described by a proper density operator), and entanglement in multipartite systems.

One of the most prominent examples of an entangled state was already given in the previous section, namely a spin singlet built up from two qubits. More generally, if Alice and Bob own Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with dimensions $m$ and $n$, respectively, a state $|\psi\rangle$ is called nonentangled if it can be written as a product state,

$$|\psi\rangle = |\alpha\rangle_A \otimes |\beta\rangle_B$$

(2)

with $|\alpha\rangle_A \in \mathcal{H}_A$, $|\beta\rangle_B \in \mathcal{H}_B$. Otherwise $|\psi\rangle$ is entangled. The question arises whether a given state $|\psi\rangle$, expressed in some arbitrary basis of the joint Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, is entangled or not, i.e. whether there are states $|\alpha\rangle_A$ and $|\beta\rangle_B$ fulfilling (2). Moreover, one would like to quantify the entanglement contained in a state vector.

An important tool to investigate such questions for bipartite systems is the biorthogonal Schmidt decomposition [1]. It states that for any state vector $|\psi\rangle \in \mathcal{H}$ there exist bases of $\mathcal{H}_A$ and $\mathcal{H}_B$ such that

$$|\psi\rangle = \sum_{i=1}^r z_i (|a_i\rangle \otimes |b_i\rangle)$$

(3)

with coefficients $z_i \neq 0$ and the basis states fulfilling $\langle a_i|a_j \rangle = \langle b_i|b_j \rangle = \delta_{ij}$. Thus, each vector in both bases for $\mathcal{H}_A$ and $\mathcal{H}_B$ enters at most only one product vector in the above expansion. As a usual convention, the phases of the basis vectors involved in (3) can be chosen such that all $z_i$ are positive. The expression (3) is an expansion of the state $|\psi\rangle$ into a basis of product vectors $|a\rangle \otimes |b\rangle$ with a minimum number $r$ of nonzero terms. This number ranges from 1 to $\min\{m,n\}$ and is called the Schmidt rank of $|\psi\rangle$.

With respect to arbitrary bases in $\mathcal{H}_A$ and $\mathcal{H}_B$ a given state vector reads

$$|\psi\rangle = \sum_{a,b} M_{ab} |a\rangle \otimes |b\rangle$$

(4)

with an $m \times n$ coefficient matrix $M$. Under unitary transformations $U_A$ and $U_B$ in $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, $M$ transforms as

$$M \mapsto M' = U_A M U_B^{T}$$

(5)

with $U_B^{T}$ being the transpose of $U_B$. The fact that there are always bases in $\mathcal{H}_A$ and $\mathcal{H}_B$ providing a biorthogonal Schmidt decomposition of $|\psi\rangle$ is equivalent to stating that there are matrices $U_A$ and $U_B$ such that the resulting matrix $M'$ consists of a diagonal block with only nonnegative entries while the rest of the matrix contains only zeros. For the case of equal dimensions of Alice’s and Bob’s space, $m = n$, this is also a well-known theorem of matrix algebra [39].

Obviously, $|\psi\rangle$ is nonentangled, i.e. a simple product state, if and only if its Schmidt rank is one. More generally, the Schmidt rank of a pure state can be viewed as a rough characterization for its entanglement. However, since the Schmidt rank is by construction a discrete quantity it does not provide a proper quantification of entanglement. Therefore finer entanglement measures are desirable. For the case of two distinguishable parties, a
useful measure of entanglement is the von Neumann-entropy of partial density matrices constructed from the pure-state density matrix \( \rho = |\psi\rangle\langle\psi| \) [40]:

\[
E(|\psi\rangle) = -\text{tr}_A (\rho_A \log_2 \rho_A) = -\text{tr}_B (\rho_B \log_2 \rho_B),
\]

where the partial density matrices are obtained by tracing out one of the subsystems, \( \rho_{A/B} = \text{tr}_{B/A} \rho \). With the help of the biorthogonal Schmidt decomposition of \( |\psi\rangle \) one shows that both partial density matrices have the same spectrum and therefore the same entropy, as stated in Eq. (6). In particular, the Schmidt rank of \( |\psi\rangle \) equals the algebraic rank of the partial density matrices. \( |\psi\rangle \) is nonentangled if and only if the partial density matrices of the pure state \( \rho = |\psi\rangle\langle\psi| \) are also pure states, and \( |\psi\rangle \) is maximally entangled if its partial density matrices are “maximally mixed”, i.e. if they have only one non-zero eigenvalue with a multiplicity of \( \min\{m, n\} \).

It is important to observe that the entanglement measure (6) of a given state \( |\psi\rangle \) does not depend on the bases used in Alice’s and Bob’s Hilbert space to express this state. This is because the trace operations in the definition of \( E(|\psi\rangle) \) are invariant under a change of bases (performed, in general, independently in both spaces). Therefore, entanglement in bipartite systems is a basis-independent quantity.

Thus, the problem of characterizing and quantifying quantum entanglement for pure states in bipartite systems can been seen as completely solved. Unfortunately, the situation is much less clear for mixed states [8, 9, 10], and for multipartite entanglement. The main obstacle in the latter issue is the fact that the biorthogonal Schmidt decomposition in bipartite systems does not have a true analogue in the multipartite case.

3 Quantum entanglement with electron spins in quantum dots

We will now illustrate the phenomenon of quantum entanglement on the example of a specific (possible) realization of a quantum information processing system [16]. The proposal to be discussed below deals with qubits realized by the spins of electrons residing on semiconductor quantum dots. As we shall see in this and the following section, the indistinguishable character of the electrons gives rise to quantum correlations which are beyond entanglement between distinguishable parties.

An study analogous to the one to be described below [24] has been carried out recently for the case of indistinguishable bosons (instead of electrons, i.e. indistinguishable fermions) in Refs. [41]. There the quantum dynamics (and generation of entanglement) between bosonic atoms trapped in neighboring potential minima of an optical lattice was studied and numerically simulated.

3.1 General remarks

An array of coupled quantum dots, see figure 1, each dot containing a top most spin 1/2, was found to be a promising candidate for a scalable quantum computer [16] where the qubit is defined by the spin 1/2 on the dot. Quantum algorithms can then be implemented using local single-spin rotations and the exchange coupling between nearby spins, see figure 1. This proposal is supported by experiments where, e.g., Coulomb blockade effects, [42] tunneling between neighboring dots, [43, 42] and magnetization [44] have been observed as well as the formation of a delocalized single-particle state in coupled dots [45].

The basic mechanism for two-qubit gate operations within quantum-dot spin-qubit proposal are gated (i.e. time-dependent) tunneling amplitudes between the dots. Then the two-qubit dynamics is driven by the effective exchange coupling between the electron spins on different dots arising from a finite tunneling amplitude.
In the following subsection we shall briefly address the issue of decoherence of spin-qubits. In subsection 3.3 we will summarize properties of a specific physical description of quantum dot spin-qubits which are necessary for our discussion here. For more comprehensive reviews of quantum computing with electron spins in quantum dots see Refs. [46, 47, 48].

3.2 Decoherence properties

The electron spin is a natural candidate for a qubit since its spin state in a given direction, |↑⟩ or |↓⟩, can be identified with the classical bits |0⟩ and |1⟩, while an arbitrary superposition α|↑⟩ + β|↓⟩ defines a qubit. In principle, any quantum two-level system can be used to define a qubit. However, one must be able to control coherent superpositions of the basis states of the quantum computer, i.e. no transition from quantum to classical behavior should occur. Thus, the coupling of the environment to the qubit should be small, resulting in a sufficiently large decoherence time $T_2$ (the time over which the phase of a superposition of |0⟩ and |1⟩ is well-defined). Assuming weak spin-orbit effects, the spin decoherence time $T_2$ can be completely different from the charge decoherence time (a few nanoseconds), and in fact it is known [50] that $T_2$ can be orders of magnitude longer than nanoseconds. Time-resolved optical measurements were used to determine $T_2^\ast$, the decoherence time of an ensemble of spins, with $T_2^\ast$ exceeding 100 ns in bulk GaAs [50]. More recently, the single spin relaxation time $T_1$ (usually $T_1 \geq T_2$) of a single quantum dot attached to leads was measured via transport to be longer than a few $\mu$s [51], consistent with calculations [52].

A particularly relevant and, from a fundamental point of view, also interesting mechanism for electron spin decoherence in quantum dots (or other semiconductor nanostructures) is the hyperfine interaction with surrounding nuclear spins, which are ubiquitous in many materials such as GaAs. Thus, the Hamiltonian reads

$$\mathcal{H} = \vec{S} \cdot \sum_i A_i \vec{I}_i$$  \hspace{1cm} (7)

where $\vec{S}$ is the electron spin and $\vec{I}_i$ are the surrounding nuclear spins (both taken here to be dimensionless) The coupling constants $A_i$ have dimension of energy and are proportional to the square modulus of the electron wave function at the location of the $i$-th nucleus. Since the electron wave function is spatially varying across the dot (a typical typical form for such envelope wave functions is given by a Gaussian), the coupling is inhomogeneous, i.e. different nuclei couple with different strength to the electron spin. This system was investigated in detail very recently in Refs. [53, 54]. Generally, the quantum dynamics according to (7) lead to a decay of the electron spin as measured in terms of its expectation values $\langle \vec{S} \rangle$ (assuming an initially fully polarized spin, $|\langle \vec{S} \rangle| = 1/2$). This spin decay is generally a source of decoherence, i.e. loss of quantum information encoded in the qubit. However, a main finding in Ref. [53] is an exact analytical solution for the quantum dynamics for the situation of an initially fully polarized nuclear spin system with the electron spin pointing opposite to it. This exact solution can be evaluated explicitly in the limit of a large number $N$ of nuclear spins being involved. As a result, the decay of the electron spin is in this case only of order $1/N$ and occurs after a time interval of order $\hbar N/\sum_i A_i$, where $A = \sum_i A_i \propto 10^{-5} \text{eV}$ for GaAs. In a typical GaAs quantum dot $N$ is of order $10^3$. Therefore, for a sufficiently large number of nuclear spins being involved, the magnitude of the electron spin decay is small, and large decoherence times can be obtained.

The findings of Ref. [53] have been corroborated and extended by numerical work in Ref. [54]. These investigations revealed a striking dependence of the electron spin dynamics
on the character of the initial state of the nuclear spin system (having a general degree of polarization): If the initial state of the total system is a simple tensor or product of the states each spin (both electron and nuclei), the time evolution depends strongly on the initial nuclear spin state. However, this behavior is very different from the situation where the electron is initially still uncorrelated with the nuclei, but the nuclei are among themselves randomly correlated, i.e. in a random superposition of all tensor product basis states of the nuclear system. Then the time evolution is very reproducible, i.e. it does (almost) not depend on the specific randomly generated initial state of the nuclear system; examples of such observations are shown in figure 2. Moreover, the time evolution of such a randomly correlated initial state mimics closely the average over the dynamics of all possible tensor product initial states. This observation can be understood as a self-averaging property [54]. The above results are illustrated in figures 2 and 3.

Another observation from the numerical studies in Ref. [54] is that the spin decay occurs more slowly if the nuclear spins are initially in a tensor product (i.e. non-entangled) state. This result can be expected to be of quite general nature and independent of the specific model (7): Disentangling the environment suppresses decoherence.

The decay of the central electron spin $\vec{S}(t)$ in (7) is generally accompanied with the generation of entanglement between the electron and the nuclei [54]. This entanglement can be measured conveniently by the von-Neumann entropy of the partial density matrix where either the electron or the environment has been traced out from the pure-state density matrix of the total state [40], cf. Eq. (6). Tracing out the nuclear system we have

$$\rho_{el}(t) = \left( \begin{array}{cc} \frac{1}{2} + \langle S^z(t) \rangle & \langle S^+(t) \rangle \\ \langle S^-(t) \rangle & \frac{1}{2} - \langle S^z(t) \rangle \end{array} \right).$$

(8)

This matrix has eigenvalues $\lambda_{\pm} = 1/2 \pm |\langle \vec{S}(t) \rangle|$, and the measure of entanglement reads $E = -\lambda_+ \log \lambda_+ - \lambda_- \log \lambda_-$. Thus, the formation of expectation values $|\langle \vec{S}(t) \rangle| < 1/2$ is a manifestation of the entanglement between the electron spin and the nuclear spin system. The maximum entanglement, $E = \log 2$, is achieved if the electron spin has decayed completely as measured by the expectation values of its components, $\langle \vec{S}(t) \rangle = 0$. The generation of quantum entanglement between the electron spin and the nuclear spin system signaled by a reduced value of $\langle \vec{S}(t) \rangle$ is a main and crucial difference between the quantum system studied here and its classical ‘counterpart’ described by a system of Landau-Lifshitz equations.

### 3.3 Modeling of the double quantum dot system

Let us now consider a system of two laterally tunnel-coupled dots having one electron each. Using an appropriate model [22, 23, 24] theoretical calculations have demonstrated the possibility of performing two-qubit quantum gate operations in such a system by varying the tunnel barrier between the dots. An important point to observe here is the fact that the electrons whose spins realize the qubits are indistinguishable particles [24]. Differently from the usual scenario of distinguishable parties (Alice, Bob, ...) the proper quantum statistics has to be taken into account when a finite tunneling between the dots is present [24, 27, 28].

The Hamiltonian of the double dot system is given by $H = T + C$, where $C$ denotes the Coulomb repulsion between the electrons, and $T = \sum_{i=1,2} \hbar_i$ is the single-particle part with

$$h_i = \frac{1}{2m} \left( \vec{p}_i + \frac{e}{c} \vec{A}(\vec{r}_i) \right)^2 + V(\vec{r}_i).$$

(9)

The single-particle Hamiltonian $h_i$ describes electron dynamics confined to the $xy$-plane in a perpendicular magnetic field $B$. The effective mass $m$ is a material-dependent parameter.
The coupling of the dots (which includes tunneling) is modeled by a quartic potential

$$V(x, y) = \frac{m\omega_0^2}{2} \left( \frac{1}{4a^2} (x^2 - a^2)^2 + y^2 \right),$$

(10)

which separates into two harmonic wells of frequency $\omega_0$ (one for each dot) in the limit $2a \gg 2a_0$, where $a$ is half the distance between the dots and $a_0 = \sqrt{\hbar/m\omega_0}$ is the effective Bohr radius of a dot.

Following Burkard et al. [22] we employ the Hund-Mulliken method of molecular orbits to describe the low-lying spectrum of our system. This approach concentrates on the lowest orbital states in each dot and is an extension of the Heitler-London method also discussed in [22]. The Hund-Mulliken approach accounts for the fact that both electrons can, in the presence of a finite tunneling amplitude, explore the entire system of the two dots. Therefore this approach is suited to investigate the issue of entanglement-analogous quantum correlations between indistinguishable particles. In particular, the Hund-Mulliken approach includes two-particle states with both electrons being on the same dot. This issue of double occupancies will be discussed in more detail below.

In the usual symmetric gauge $\vec{A} = B(-y, x, 0)/2$ the Fock-Darwin ground state of a single dot with harmonic confinement centered around $\vec{r} = (\pm a, 0, 0)$ reads

$$\varphi_{\pm a}(x, y) = \sqrt{m\omega \pi \hbar} \exp \left( \frac{m\omega}{2\hbar} \left( (x \mp a)^2 + y^2 \right) \right) \cdot \exp \left( \frac{i}{2} y a l_B \right) ,$$

(11)

where $l_B = \sqrt{\hbar c/eB}$ is the magnetic length, and the frequency $\omega$ is given by $\omega^2 = \omega_0^2 + \omega_L^2$ where $\omega_L = eB/2mc$ is the usual Larmor frequency. From these non-orthogonal single-particle states we construct the orthonormalized states $|A\rangle$ and $|B\rangle$ with wave functions

$$\langle \vec{r}|A\rangle = \frac{1}{\sqrt{1 - 2Sy - g^2}} (\varphi_+ - g\varphi_-) ,$$

(12)

$$\langle \vec{r}|B\rangle = \frac{1}{\sqrt{1 - 2Sy - g^2}} (\varphi_- - g\varphi_+) ,$$

(13)

with $S$ being the overlap between the states (11) and $g = (1 - \sqrt{1 - S^2})/S$. For appropriate values of system parameters such as the interdot distance and the external magnetic field, the overlap $S$ becomes exponentially small [22]. In this limit an electron in one of the states $|A\rangle$, $|B\rangle$ is predominantly localized around $\vec{r} = (\pm a, 0, 0)$. In the following we consider this case and use these states as basis states to define qubits, i.e. qubits are realized by the spin state of an electron in either orbital $|A\rangle$, or orbital $|B\rangle$.

An appropriate basis set for the six-dimensional two-particle Hilbert space is given (using standard notation) by the three spin singlets

$$|S_1\rangle = \frac{1}{\sqrt{2}} \left( c_{A_1}^+ c_{B_1}^+ - c_{A_1}^+ c_{B_1}^+ \right) |0\rangle ,$$

(14)

$$|S_2\rangle = \frac{1}{\sqrt{2}} \left( c_{A_1}^+ c_{B_1}^+ + c_{A_1}^+ c_{B_1}^+ \right) |0\rangle ,$$

(15)

$$|S_3\rangle = \frac{1}{\sqrt{2}} \left( c_{A_1}^+ c_{A_1}^+ - c_{B_1}^+ c_{B_1}^+ \right) |0\rangle ,$$

(16)

and the triplet multiplet,

$$|T^{-1}\rangle = c_{A_1}^+ c_{B_1}^+ |0\rangle ,$$

(17)
\[ |T^0\rangle = \frac{1}{\sqrt{2}} \left( c_{A^\uparrow} c_{B^\downarrow} + c_{A^\downarrow} c_{B^\uparrow} \right) |0\rangle, \]  
(18)  
\[ |T^1\rangle = c_{A^\uparrow} c_{B^\downarrow} |0\rangle. \]  
(19)

The three triplet states are degenerate (typically we can ignore possible Zeeman splittings [22]) and have the common eigenvalue,

\[ \varepsilon_T = 2 \varepsilon + V_-, \]  
(20)

where we have defined

\[ \varepsilon = \langle A | h | A \rangle = \langle B | h | B \rangle \]  
(21)

and

\[ V_- = \langle T^a | C | T^a \rangle, \quad V_+ = \langle S_1 | C | S_1 \rangle. \]  
(22)

An important further observation is that, as a consequence of inversion symmetry along the axis connecting the dots, the Hamiltonian does not have any non-zero matrix elements between the singlet state \(|S_3\rangle\) and other states. Hence, \(|S_3\rangle\) is, independently of the system parameters, an eigenstate. The eigenvalues of the triplet and \(|S_3\rangle\), however, do depend on system parameters. The Hamiltonian acting on the remaining space spanned by \(|S_1\rangle\) and \(|S_2\rangle\) can be written as

\[ H = 2 \varepsilon + \frac{1}{2} U_H + V_+ - \begin{pmatrix} U_H/2 & 2t_H \\ 2t_H & -U_H/2 \end{pmatrix}, \]  
(23)

where

\[ t_H = -\langle A | h | B \rangle - \frac{1}{2} \langle S_2 | C | S_1 \rangle \]  
(24)

and

\[ U_H = \langle S_2 | C | S_2 \rangle - V_+. \]  
(25)

The nontrivial part of (23) is a simple Hubbard Hamiltonian and can be identified as the Hamiltonian of a pseudospin-1/2-object in a pseudomagnetic field having a component \(U_H\) in the \(\hat{z}\)-direction and \(4t_H\) in the \(\hat{x}\)-direction of pseudospin space. [Note that this pseudospin is not related to the spin degree of freedom which provides the qubit!] The space spanned by \(|S_1\rangle\) and \(|S_2\rangle\) contains the ground state of the system. The basis states themselves are eigenstates only in the case of vanishing tunneling amplitude \(t_H\) where \(|S_1\rangle\) is the ground state. In all other cases, the ground state has an admixture of doubly occupied states contained in \(|S_2\rangle\). The energy gap between the triplet and the singlet ground state is

\[ \varepsilon_T - \varepsilon_{S_0} = V_+ - V_- - \frac{U_H}{2} + \frac{1}{2} \sqrt{U_H^2 + 16t_H^2}. \]  
(26)

A key challenge is the construction of systems composed of two coupled quantum dots which can be coupled to perform swap operations \(U_{SW}\), i.e. unitary two-qubit operations which interchange the spin states (qubits) of the electrons on the two dots. By combining the “square root” \(U_{SW}^{1/2}\) of such a swap with other isolated-qubit manipulations one can construct a quantum XOR gate. A quantum XOR gate, along with isolated-qubit operations, has been shown to be sufficient for the implementation of any quantum algorithm [55]. Hence a practical and reliable realization of a swap gate would be an important step toward the fabrication of a solid state quantum computer. A swap operation in the present system is a unitary transformation which turns a state having the qubits in different states, say,

\[ c_{A^\uparrow} c_{B^\downarrow} |0\rangle = \frac{1}{\sqrt{2}} \left( |T^0\rangle + |S_1\rangle \right), \]  
(27)
into a state where the contents of the qubits is interchanged,

$$c_{A_1}^+ c_{B_1}^+ |0\rangle = \frac{1}{\sqrt{2}} (|T^0\rangle - |S_1\rangle) .$$

(28)

These two states are eigenstates in the case $V_+ = V_-$ and $t_H = 0$ for which the singlet-triplet splitting vanishes.

As discussed in references [16, 22, 24], swapping may be achieved by the action of a gate that lowers the potential barrier between the quantum dots. This leads to exponentially larger values for both $V_+ - V_-$ and $t_H$. It is adequate for our purposes to consider a model where $V_+ = V_-$ (consistent with the above limit of small overlap $S$), and the singlet-triplet splitting results entirely from $t_H$. If the duration and amplitude of a tunneling pulse is adjusted appropriately, the relative phase between the singlet and the triplet state involved picks up a shift of $\pi$, and a swapping operation is performed.

A finite tunneling amplitude necessarily leads to a finite probability for double occupancies of qubit states where both electrons are on the same dot. If double occupancy errors occur to any sizable extent as a result of the swapping process, any quantum computation based on this hardware is likely to fail. However, if the double occupancies are sufficiently rare after the swapping process, errors in the quantum computation can likely be corrected dynamically. An important observation is that the double-occupancy probability after the swap vanishes in the adiabatic limit, i.e. if the ramp time $\tau$ of the quantum gate is such that $\hbar/\tau$ is much larger than the pseudospin splitting $\sqrt{U_H^2 + 16t_H^2}$. This follows since the non-adiabatic effects can arise only from the states $|S_1\rangle$ and $|S_2\rangle$, which have a non-trivial time evolution when the tunneling amplitude $t_H$ is time-dependent. Thus, the question of whether double occupancies are problematic for swap operations in the present system is reduced to the question of how close the motion of a spin-$\frac{1}{2}$ object in a time-dependent magnetic field is to its adiabatic limit. This will be investigated further in Sec. 5.

The reduction of the dynamics to the time evolution of a two-level-system relies on the fact that the system has inversion symmetry along the $\hat{x}$-axis in real space connecting the dots. This symmetry can be broken if odd powers of the particle coordinates $x_i$ are added to the Hamiltonian (9) like for example the potential of a homogeneous electric field. However, the only additional matrix element due to such terms in the Hamiltonian occurs in the subspace of double occupied states between the singlets $|S_1\rangle$ and $|S_2\rangle$. Thus, in the presence of an electric field $E = -eE \sum_i x_i$ the Hamiltonian acting on the singlet subspace spanned by $|S_1\rangle$, $|S_2\rangle$, $|S_3\rangle$ reads

$$\mathcal{H} = 2\varepsilon + \frac{1}{2} U_H + V_+$$

$$-\begin{pmatrix} U_H/2 & 2t_H & 0 \\ 2t_H & -U_H/2 & F \\ 0 & F & -U_H/2 + 2X \end{pmatrix}$$

with the real matrix element $F = \langle S_2|E|S_3\rangle$ and

$$2X = \langle S_2|C|S_2\rangle - \langle S_3|C|S_3\rangle = 2\langle A|\langle A|C|B\rangle|B\rangle .$$

(30)

With a finite matrix element $F$ the dynamics of the system is slightly more complicated, but also in this case the only coupling of the two-qubit states (27) and (28) to the subspace of double occupied states is provided by the tunneling amplitude $t_H$. Therefore, with respect to the adiabaticity of the swapping process, the situation can be expected to be not very different from the one with inversion symmetry between the dots. This will be verified in Sec. 5.

So far we have not considered a possible Zeeman coupling to the electron spin. This would not change the situation essentially since all states involved in the swapping process ($|T^0\rangle$, $|S_1\rangle$, $|S_2\rangle$, and possibly $|S_3\rangle$) have the total spin quantum number $S^z = 0$. 

9
In the following section we give an elementary introduction to the theory of “entanglement-like” quantum correlations in systems of indistinguishable particles. We concentrate on the fermionic case and illustrate our findings on the above example of coupled quantum dots.

4 Quantum Correlations between indistinguishable particles

For indistinguishable particles a pure quantum state must be formulated in terms of Slater determinants or Slater permanents for fermions and bosons, respectively. Generically, a Slater determinant contains correlations due to the exchange statistics of the indistinguishable fermions. As the simplest possible example consider a wave function of two (spinless) fermions,

\[ \Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} [\phi(\vec{r}_1)\chi(\vec{r}_2) - \phi(\vec{r}_2)\chi(\vec{r}_1)] \] (31)

with two orthonormalized single-particle wave functions \(\phi(\vec{r})\), \(\chi(\vec{r})\). Operator matrix elements between such single Slater determinants contain terms due to the antisymmetrization of coordinates (“exchange contributions” in the language of Hartree-Fock theory). However, if the moduli of \(\phi(\vec{r})\), \(\chi(\vec{r})\) have only vanishingly small overlap, these exchange correlations will also tend to zero for any physically meaningful operator. This situation is generically realized if the supports of the single-particle wave functions are essentially centered around locations being sufficiently apart from each other, or the particles are separated by a sufficiently large energy barrier. In this case the antisymmetrization present in Eq. (31) has no physical effect.

Such observations clearly justify the treatment of indistinguishable particles separated by macroscopic distances as effectively distinguishable objects. So far, research in Quantum Information Theory has concentrated on this case, where the exchange statistics of particles forming quantum registers could be neglected, or was not specified at all.

The situation is different if the particles constituting, say, qubits are close together and possibly coupled in some computational process. This the case for all proposals of quantum information processing based on quantum dots technology [16, 22, 23, 24, 25, 26]. Here qubits are realized by the spins of electrons living in a system of quantum dots. The electrons have the possibility of tunneling eventually from one dot to the other with a probability which can be modified by varying external parameters such as gate voltages and magnetic field. In such a situation the fermionic statistics of electrons is clearly essential.

Additional correlations in many-fermion-systems arise if more than one Slater determinant is involved, i.e. if there is no single-particle basis such that a given state of \(N\) indistinguishable fermions can be represented as an elementary Slater determinant (i.e. fully antisymmetric combination of \(N\) orthogonal single-particle states). These correlations are the analog of quantum entanglement in separated systems and are essential for quantum information processing in non-separated systems.

As an example consider a “swap” process, as discussed in the previous subsection, exchanging the spin states of electrons on coupled quantum dots by gating the tunneling amplitude between them [22, 24]. Before the gate is turned on, the two electrons in the neighboring quantum dots are in a state represented by a simple Slater determinant, and can be regarded as distinguishable since they are separated by a large energy barrier. When the barrier is lowered, more complex correlations between the electrons due to the dynamics arise. Interestingly, as shown in Refs. [22, 24], during such a process the system must necessarily enter a highly correlated state that cannot be represented by a single Slater determinant. The final state of the gate operation, however, is, similarly as the initial one,
essentially given by a single Slater determinant. Moreover, by adjusting the gating time appropriately one can also perform a “square root of a swap” which turns a single Slater determinant into a “maximally” correlated state in much the same way [24]. Illustrative details of these processes will be given in section 5. In the end of such a process the electrons can again be viewed as effectively distinguishable, but are in a maximally entangled state in the usual sense of distinguishable separated particles. In this sense the highly correlated intermediate state can be viewed as a resource for the production of entangled states.

In the following we give an elementary introduction to recent results in the theory of quantum correlations in systems of indistinguishable particles [24, 27, 28]. This issue has attracted recently considerable interest and intense discussions [29, 30, 31, 32, 33, 34, 35, 36, 37, 38]. The correlations to be discussed below are analogues of entanglement between distinguishable parties. However, to avoid confusion with the existing literature and in accordance with Refs. [27, 28, 29], we shall reserve in the following the term “entanglement” for separated systems and characterize the analogous quantum correlation phenomenon in nonseparated systems in terms of the Slater rank and the correlation measure to be defined below. The results and concepts presented below and in the references given are in various respect complementary to a recent approach by Zanardi [31, 32] stressing the dependence of the notion of entanglement of the way a certain system is split into subsystems.

For the purposes of this article we shall concentrate on elementary results for the case of pure states of two identical fermions. Results for mixed states and more than two fermions can be found in [24, 28]. Results for the case of identical bosons can be found in [30, 29, 28]

We consider the case of two identical fermions sharing an $n$-dimensional single-particle space $\mathcal{H}_n$ resulting in a total Hilbert space $\mathcal{A}(\mathcal{H}_n \otimes \mathcal{H}_n)$ with $\mathcal{A}$ denoting the antisymmetrization operator. A general state vector can be written as

$$\left| w \right\rangle = \sum_{a,b=1}^{n} w_{ab} f^+_a f^+_b \left| 0 \right\rangle$$  \hspace{1cm} (32)$$

with fermionic creation operators $f^+_a$ acting on the vacuum $\left| 0 \right\rangle$. The antisymmetric coefficient matrix $w_{ab}$ fulfills the normalization condition

$$\text{tr}(\bar{w}w) = -\frac{1}{2},$$  \hspace{1cm} (33)$$

where the bar stands for complex conjugation. Under a unitary transformation of the single-particle space,

$$f^+_a \mapsto U f^+_a U^+ = U_{ba} f^+_b,$$

$$w \text{ transforms as } w \mapsto U w U^T,$$  \hspace{1cm} (35)$$

where $U^T$ is the transpose (not the adjoint) of $U$. For any complex antisymmetric matrix $n \times n$ matrix $w$ there is a unitary transformation $U$ such that $w' = U w U^T$ has nonzero entries only in $2 \times 2$ blocks along the diagonal [27, 39]. That is,

$$w' = \text{diag}[Z_1, \ldots, Z_r, Z_0]\text{ with } Z_i = \begin{bmatrix} 0 & z_i \\ -z_i & 0 \end{bmatrix},$$  \hspace{1cm} (36)$$

$z_i \neq 0$ for $i \in \{1, \ldots, r\}$, and $Z_0$ being the $(n-2r) \times (n-2r)$ null matrix. Each $2 \times 2$ block $Z_i$ corresponds to an elementary Slater determinant in the state $\left| w' \right\rangle$. Such elementary Slater determinants are the analogues of product states in systems consisting of distinguishable parties. Thus, when expressed in such a basis, the state $\left| w \right\rangle$ is a sum of elementary
Slater determinants where each single-particle basis state enters not more than one term. This property is analogous to the biorthogonality of the Schmidt decomposition discussed above. The matrix (36) represents an expansion of $|w\rangle$ into a basis of elementary Slater determinants with a minimum number $r$ of non-vanishing terms. This number is analogous to the Schmidt rank for the distinguishable case. Therefore we shall call it the (fermionic) Slater rank of $|w\rangle$ [27], and an expansion of the above form a Slater decomposition of $|w\rangle$.

We now turn to the case of two fermions in a four-dimensional single-particle space. This case is realized in a system of two coupled quantum dots hosting in total two electrons which are restricted to the lowest orbital state on each dot. In such a system, a simple correlation measure can be defined as follows [24, 27, 28]: For a given state (32) with a coefficient matrix $\omega_{ab}$ one defines a dual state $|\tilde{\omega}\rangle$ characterized by the dual matrix

$$\tilde{w}_{ab} = \frac{1}{2} \sum_{c,d=1}^{4} \varepsilon^{abcd} \tilde{w}_{cd},$$

with $\varepsilon^{abcd}$ being the usual totally antisymmetric unit tensor. Then the correlation measure $\eta(|w\rangle)$ can be defined as $^2$

$$\eta(|w\rangle) = |\langle \tilde{w} | w \rangle| = \left| \sum_{a,b,c,d=1}^{4} \varepsilon^{abcd} w_{ab} w_{cd} \right| = |8 (w_{12} w_{34} + w_{13} w_{42} + w_{14} w_{23})|.$$  

(38)

Obviously, $\eta(|w\rangle)$ ranges from zero to one. Importantly it vanishes if and only if the state $|w\rangle$ has the fermionic Slater rank one, i.e. $\eta(|w\rangle)$ is an elementary Slater determinant. This statement was proved first in Ref. [24]; an alternative proof can be given using the Slater decomposition of $|w\rangle$ and observing that

$$\det w = \left( \frac{1}{8} \langle \tilde{w} | w \rangle \right)^2.$$  

(39)

This is just a special case of a general relation expressing the determinant of an antisymmetric $(2K) \times (2K)$ matrix $w$ by the square of its Pfaffian,

$$\det w = \left( \frac{1}{(2K)!} \sum_{i_1,\ldots,i_{2K}=1}^{2K} \varepsilon^{i_1\ldots i_{2K}} w_{i_1 i_2} \cdots w_{i_{2K-1} i_{2K}} \right)^2.$$  

(40)

The quantity $\eta(|w\rangle)$ measures quantum correlation contained in the two-fermion state $|w\rangle$ which are beyond simple antisymmetrization effects. This correlation measure in under many aspects analogous to the entanglement measure “concurrence” used in systems of two distinguishable qubits [56]. These analogies are discussed in detail in [28] including also the case of indistinguishable bosons. An important difference between just two qubits, i.e. two distinguishable two-level systems, and the present case of two electrons in a two-dot system is that in latter system both electrons can possibly occupy the same dot while the other is empty. Therefore the total Hilbert space is larger than in the two-qubit system, and a generalized correlation measure becomes necessary. Furthermore, similar as in the two-qubit case, the correlation measure $\eta$ defined here for pure states of two fermions has a natural extension to mixed fermionic and bosonic states [27, 28].

A convenient choice to make contact between the general state labels $a, b, \ldots \in \{1, 2, 3, 4\}$ used here and the basis states of the preceding section is given by $(1,2,3,4) = (A \uparrow, A \downarrow)$

---

$^2$The notation $\eta$ for the correlation measure was first used in Refs. [24, 27]. In Ref. [28] the notation $\mathcal{C}$ was used in order to stress the analogy to the “concurrence “ introduced by Wootters [56].
With this convention, a state vector spanned by \(|S_2\rangle\) and \(|S_3\rangle\) only has \(w_{12}\) and \(w_{34}\) as its only independent non-zero coefficients in \(w\). Such a state lies fully in the subspace of double occupancies, and its entanglement is purely due to the orbital degrees of freedom:

\[
\eta_{\text{orb}} = 8|w_{12}w_{34}|. \tag{41}
\]

On the other hand, a state spanned by \(|S_1\rangle\) and \(|T_0\rangle\) has no double occupancies and is entangled purely with respect to the spin degrees of freedom,

\[
\eta_{\text{spin}} = 8|w_{14}w_{23}|. \tag{42}
\]

For a general state vector, both kinds of correlations (orbital and spin) contribute to \(\eta(w)\).

A direct connection of the degree of quantum correlation \(\eta\) in the singlet ground state of the double dot system and its tunneling amplitude was found recently in [46]. The ground state reads

\[
|w_0\rangle = \frac{1}{\sqrt{2(1 + \phi^2)}} (((1 + \phi)|S_1\rangle + (1 - \phi)|S_2\rangle) \tag{43}
\]

with an energy given in (26). Here the “interaction parameter”

\[
\phi = \sqrt{1 + \left(\frac{4t_H}{U_H}\right)^2 - \frac{4t_H}{U_H}}. \tag{44}
\]

has been introduced, and the correlation measure of the ground state is given by

\[
\eta = \frac{2\phi}{1 + \phi^2}. \tag{45}
\]

At zero tunneling \(t_H = 0\) the ground state singlet does not contain any double occupancies and is degenerate with the triplet. At large tunneling \(t_H \gg U_H\) both electrons are in symmetric orbital states differing in spin. This state is a single Slater determinant, and the correlation measure is zero.

### 5 Dynamics of entanglement in quantum gate operations

We now continue with our investigation of the dynamics of the double quantum dot qubit swapping process generated by a time-dependent tunneling amplitude.

Let us first consider the case of inversion symmetry along the axis connecting the dots. As explained in Sec. 3.3 this problem can be reduced essentially to the time evolution of a pseudospin-\(\frac{1}{2}\)-object in a magnetic field having a time-dependent component in the \(x\)-direction of the pseudospin space. In the course of swapping, the triplet contribution to the incoming state (27) will just pick up a phase factor according to its constant eigenvalue, while the singlet contribution will mix with the other singlet \(|S_2\rangle\). Therefore, a finite probability for double occupancies will necessarily arise during the swapping process. However, if these amplitudes can be suppressed sufficiently when the swapping is complete (as in the adiabatic limit), errors in the quantum computation can be avoided. Thus we are left with the question of how close the dynamics of our formal spin-\(\frac{1}{2}\) object is to its adiabatic limit. We note that, in the adiabatic limit, no Berry phase occurs in the time evolution of the singlet states, since the motion of the formal spin is restricted to a plane. Hence the solid angle encircled in a round trip is strictly zero.
The integration of the Schrödinger equation for our time-dependent two-level problem is in general non-elementary. However, there is a considerable body of literature, starting with early work by Landau [57], Zener [58], and Rosen and Zener [59], where particular cases of this problem were reduced to well-known differential equations of mathematical physics such as the hypergeometric equation. This work was reviewed and generalized very recently in [60]. However, such an approach still works only for special time-dependent Hamiltonians, i.e., in the present context, only for special shapes of the tunneling pulse $t_H(t)$, and many quantities of interest are given by complicated non-elementary expressions which require numerical evaluation. For this reasons, and for the sake of brevity of our presentation, we shall resort to numerical integrations of the Schrödinger equation. From such studies we will see that the range of adiabaticity is remarkably large. Our numerical findings will be corroborated and made physically plausible by well-known analytical results for Landau-Zener-type transitions in simplified cases.

To be specific, we consider a time-dependent tunneling of the form

$$t_H(t) = \frac{\Delta}{1 + \frac{\cosh(t/\tau)}{\cosh(T/(2\tau))}}.$$  \hspace{1cm} (46)

This is a tunneling pulse which is switched on and off exponentially with a characteristic time $\tau$. It has a duration of $T$ and an amplitude given by $\Delta$ (for $T \gg \tau$). Therefore this form is flexible enough to describe the essential features of a pulse. The exponential switching is motivated by the exponential-like dependence of the tunneling matrix element on external parameters [22].

A typical situation is shown in figure 4 for a switching time of $\tau = 4\hbar/U_H$, an amplitude of $\Delta = U_H/8$ and the duration $T$ adjusted to enable single swap operation. The figure shows the results of a numerical integration of the time-dependent Schrödinger equation using the fourth order Runge-Kutta scheme. The time-dependent tunneling amplitude $t_H(t)$ is plotted (in units $U_H$) as a dotted line. The square amplitude of the incoming state (27) and the outgoing state (28) are shown as thick lines. The square amplitudes of the singlets $|S_1\rangle$ and $|S_2\rangle$ are denoted by $|\varphi_1|^2$ and $|\varphi_2|^2$, respectively, and plotted as long-dashed lines. The probability of double occupancies is given by $|\varphi_2|^2$. As one can see from the figure, this quantity is finite during the swapping process but strongly suppressed afterwards. The measure of entanglement $\eta(t)$ is also shown in the figure. It is zero for the non-entangled incoming and outgoing state, and achieves its maximum value of almost unity in the middle of the process. This quantifies and shows explicitly the entanglement of the quantum state during the swapping process.

The probability $|\varphi_2|^2$ for double occupancy after switching off the tunneling depends on the switching time $\tau$, the amplitude $\Delta$ and also on the duration $T$ of the tunneling pulse, i.e. on the exact time when the switching off sets in. However, our numerics suggest that there is an upper bound for $|\varphi_2|^2$ at given $\tau$ and $\Delta$. In the above example the double occupancy probability after the swapping process is smaller than $10^{-10}$, which is a very tiny value. A typical order of magnitude for the double occupancy probability is $10^{-8}$ for amplitudes $\Delta < U_H$ and switching times $\tau > 4\hbar/U_H$. In fact, also larger values of $\Delta$ (being still comparable with $U_H$) can be possible, leading to double occupancy probabilities of the same order, while this probability significantly increases if $\tau$ becomes smaller than $4\hbar/U_H$. Thus, this value characterizes the region where the motion of the system is close to its adiabatic limit and is remarkably small on the natural time scale of the system given by $\hbar/U_H$, while adiabatic behavior is in general expected for a particularly slow time evolution.

This large range of quasi-adiabatic behavior can be understood qualitatively by considering a simplified situation where the tunneling is switched on and off linearly in time and is constant otherwise. Then, non-adiabatic effects can occur only during the sharply
defined switching processes. For simplicity, we consider the first switching process only where the tunneling has the time dependence $t_H = (\Delta/\tau)t$, $t \in [0, \tau]$. To enable analytical progress let us further assume $t \in [-\infty, \infty]$, which should lead to an upper bound for the probability of non-adiabatic transitions due to the switching. This problem was considered a long time ago by Landau [57] and by Zener [58]. The result of reference [58] for the probability of non-adiabatic transitions reads

$$P_{\text{nad}} = e^{-\alpha}$$

with an adiabaticity parameter

$$\alpha = \frac{\pi U_H^2}{8 \hbar (\Delta/\tau)}.$$  \hspace{1cm} (48)

We see that the probability for non-adiabatic transitions is exponentially suppressed with increasing switching time $\tau$. This exponential dependence explains qualitatively the above observation of a large range of quasi-adiabatic behavior. To obtain an estimate for a nonlinear switching one may replace the ratio $(\Delta/\tau)$ in the denominator of (48) by the maximum time derivative of the tunneling $t_H(t)$ (giving $\alpha = \pi U_H^2/3\hbar (\Delta/\tau)$ for the pulse (46)).

A similar exponential dependence of the probability for non-adiabatic transitions on the switching time $\tau$ was also found analytically by Rosen and Zener [59] for a particular two-parametric pulse of the form

$$t_H(t) = \Delta/\cosh(t/\tau).$$

In this case non-adiabatic transitions occur with a probability

$$P_{\text{nad}} = \sin^2 \left(\frac{\Delta \tau}{2\hbar}\right) / \cosh^2 \left(\frac{U_H \tau}{2\hbar}\right).$$

To illustrate the behavior in the strongly non-adiabatic case we have plotted in figure 5 $|\phi_1|^2$ and $|\phi_2|^2$ for the same situation as in figure 4 but with a four times smaller ramp time of only $\tau = \hbar/U_H$. In this case small oscillations occur in the time-evolution of these two quantities during the tunneling pulse, which can be understood in terms of the eigenspectrum at a given tunneling $t_H = \Delta$. Additionally, a sizable double occupancy probability of about 0.005 remains after the pulse, as shown in the inset.

Figure 6 shows a square root of a swap, which is obtained from the situation of figure 4 by halving the duration $T$ of the tunneling pulse. The resulting state is a fully entangled complex linear combination of the states $|S_1\rangle$ and $|T_0\rangle$, or, equivalently, of the incoming state (27) and the outgoing state (28) of the full swap. Again, the weight of the doubly occupied state $|S_2\rangle$ is strongly suppressed after the tunneling pulse. As a consequence, Eq. (41) implies that $\eta_{\text{orb}} = 0$ after completion of switching, while $\eta = \eta_{\text{spin}} = 8|w_{14}w_{23}| = 1$. This shows that the entanglement of the two electrons is entirely in the spin (and not in the orbital) degrees of freedom after switching.

Let us finally consider swapping processes when the inversion symmetry along the axis connecting the dots is broken. Such processes are governed by the Hamiltonian (29) in the presence of a finite matrix element $F$. Our numerical results are in this case qualitatively the same as before with the admissible switching times $\tau$ slightly growing with increasing $F$. In figure 7 we illustrate our findings for a comparatively large off-diagonal element $F = 0.4U_H$. The additional Coulomb matrix element is $X = 0.2U_H$, and the parameters of the tunneling pulse are $\tau = 8\hbar/U_H$ and $\Delta = U_H/8$ with a duration $T$ appropriate for a single swapping. As a result, a clean swapping operation can be performed also in the absence of inversion symmetry.

We note that the Hund-Mulliken scheme used here is restricted to the low-energy sector where only the lowest single-particle energy levels (with typical spacings $\delta\epsilon$) are kept.
this scheme to be valid also in a switching process, we need to require that time-dependent changes must be performed adiabatically also with respect to the time scale set by $\hbar/\delta \epsilon$, i.e. we need $\tau > \hbar/\delta \epsilon$[22]. On the other hand, to suppress double occupancy errors we have seen that the adiabaticity parameter $\alpha$ of Eq. (48) must exceed unity, implying that $\tau > 8\hbar \Delta / (\pi U_H^2)$. Thus, the adiabaticity condition for switching becomes more generally,

$$\tau > \tau_{\min} := \max \left\{ \frac{\hbar}{\delta \epsilon}, \frac{8\hbar \Delta}{\pi U_H^2} \right\} .$$  \hspace{1cm} (51)

There are now two particular cases we can distinguish. First, if the effective Coulomb charging energy exceeds the level spacing, i.e. $U_H > \delta \epsilon$, we obtain $\tau_{\min} = h/\delta \epsilon$, since for consistency we have $\Delta < \delta \epsilon$. Thus, when the switching is adiabatic with respect to the scale set by $\delta \epsilon$, errors due to double occupancy are automatically excluded. In the second case with $U_H < \sqrt{\Delta \delta \epsilon} < \delta \epsilon$ ("ultrasmall quantum dots"), we obtain $\tau_{\min} = 8\hbar \Delta / (\pi U_H^2)$, which means that the overall condition for adiabaticity is determined by the no-double occupancy criterion. Using typical material parameters for GaAs quantum dots[43], we can estimate[22] that $\tau_{\min}$ is of the order of 50 ps.

6 Summary

We have given an overlook on the physics of gate operations between quantum dot spin-qubits emphasizing the dynamics of quantum entanglement between such objects. For these purposes, the low-energy physics of a lateral pair of identical quantum dots can be effectively reduced to a (time-dependent) two-state problem. In particular we have analyzed the swap and "square root of a swap" operations by means of numerical simulations of the time-dependent Schrödinger equation. One of the main conclusions is that double occupancy error will not be a fatal problem for the operation of such quantum gates. This is due to a surprisingly large range of the quasiadiabatic regime in the quantum dynamics of the aforementioned two-state system Our numerical results are corroborated and physically made plausible by analytical results on related Landau-Zener-type transitions. We have also reported on recent results on electron spin decoherence in semiconductor nanostructures due to hyperfine interaction with surrounding nuclear spins.

Finally, the indistinguishable character of the electrons involved in the realization of quantum dot spin-qubits leads to the interesting question of entanglement-analogous quantum correlations between indistinguishable particles. Here we have provided an introduction to this issue, which has been addressed in the literature since only very recently and constitutes a new direction of work in quantum information theory.

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Figure 1: Quantum dot array, controlled by electrical gating. The electrodes (dark gray) define quantum dots (circles) by confining electrons. Additional gates and (dc and ac) external magnetic fields enable single-qubit rotations. Two-qubit operations are achieved by gating the effective tunneling amplitude between neighboring quantum dots. This introduces an effective time-dependent exchange coupling between the electron spins.

Figure 2: Upper panels: $\langle S^z(t) \rangle$ for a system of size $N = 19$ being initially in a randomly correlated nuclear spin state in the subspace with $J^z = 7$ where $\vec{J} = \vec{S} + \sum_i \vec{I}_i$ denotes the total spin of the system. The two panels represent two different randomly chosen initial conditions. Lower panels: Analogous data for $N = 14$ and a completely unpolarized nuclear spin system ($J^z = -1/2$). In both cases the simulation data does practically not depend on the initial condition.
Figure 3: Upper panels: time evolution of the electron spin \( \langle S^z(t) \rangle \) for a system with 14 nuclear spins being initially in an uncorrelated tensor product state in the subspace \( J^z = 9/2 \). The time evolution of the electron spin depends strongly on the initial state of the nuclear spins. Lower left panel: data of the same type as above but averaged over all possible uncorrelated initial states with \( J^z = 9/2 \). Lower right panel: \( \langle S^z(t) \rangle \) for the same system being initially in a randomly chosen correlated state. This time evolution closely mimics the averaged data of the lower left panel.

Figure 4: A swap process as a function of time. The tunneling amplitude \( t_H(t) \) is plotted (in units of \( U_H \)) as a dotted line. The square amplitude of the incoming state (27) and the outgoing state (28) are shown as thick lines. The square amplitudes of the singlets \( |S_1\rangle \) and \( |S_2\rangle \) are denoted by \( |\varphi_1|^2 \) and \( |\varphi_2|^2 \), respectively, and plotted as long-dashed lines. The measure of entanglement \( \eta(t) \) is also shown.
Figure 5: The square amplitudes of the singlet states $|S_1\rangle$ and $|S_2\rangle$ for the same situation as in figure 4, but with a four times smaller ramp time of only $\tau = \hbar/U_H$. The inset shows $|\varphi_2(t)|^2$ on a magnified scale. The dynamics of the system is clearly in the non-adiabatic regime.

Figure 6: A square root of a swap, which is obtained from the situation of figure 4 by halving the pulse duration $T$. The probability of double occupancies is again strongly suppressed after the tunneling pulse. The resulting state is a fully entangled complex linear combination of $|S_1\rangle$ and $|T^0\rangle$, or, equivalently, of the incoming state (27) and the outgoing state (28) of the full swap. The quantum mechanical weights of the latter states are plotted as thick solid lines.
Figure 7: A swapping processes in the absence of inversion symmetry along the axis connecting the dots. The square amplitudes of the singlet states $|S_i\rangle$, $i \in \{1, 2, 3\}$, are denoted by $|\varphi_i|^2$. The additional matrix elements entering the Hamiltonian (29) are $X = 0.2U_H$ and $F = 0.4U_H$. The parameters of the tunneling pulse are $\tau = 8\hbar/U_H$ and $\Delta = U_H/8$ with a duration $T$ appropriate for a single swapping. As a result, a clean swapping operation can be performed also in the absence of inversion symmetry.