Scalable architecture for spin-based quantum computers with a single type of gate

Dieter Suter* and Kyungwon Lim†
Fachbereich Physik, Universität Dortmund, 44221 Dortmund, Germany
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We propose a scalable design for a solid-state spin-based quantum computer. It uses endohedral fullerenes like $N@C_{60}$ or $P@C_{60}$, which can be positioned on Si surfaces with a scanning tunneling microscope. Each logical qubit is stored in two physical qubits, corresponding to the nuclear and electronic spins. We discuss the addressing of individual qubits by a magnetic field gradient, and the implementation of one- and two-qubit quantum gates by sequences of radio-frequency and microwave pulses.

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I. INTRODUCTION

Computers based on quantum mechanical systems [1] may be able to successfully tackle numerical problems that are exponentially difficult on classical computers [2]. While spin $\frac{1}{2}$ particles form an obvious choice for implementing a qubit, it was not until 1997 that it was shown that nuclear magnetic resonance (NMR) can actually implement a quantum computer in an ensemble of molecules [3,4]. These results and the subsequent work on NMR quantum computing in liquids opened the first possibility of studying quantum algorithms in an actual experiment. It appears unlikely, however, that such a scheme will be scalable to the number of qubits required for increasing the speed of a quantum computer over that of a classical computer [5]. It is therefore generally believed that scalable spin-based quantum computers will have to rely on solid-state systems [6–9]. In particular Kane's proposal [6], which uses single donor spins in Si, appears very attractive if the engineering problems can be overcome. For current technology, the placement of the impurity spins inside the silicon crystal is probably the most demanding part of the scheme.

This difficulty is avoided in the approach suggested by Twamley [10] and by Harneit *et al.* [11–13], where the qubits are placed on the surface rather than inside the crystal. These authors show that the long decoherence time of the electronic spin in $N@C_{60}$ makes it an ideal candidate for the implementation of a qubit. The C_{60} cage represents a nanometer sized trap for the nitrogen atom [14], which can be precisely positioned on a Si surface using state of the art scanning tunneling microscopy (STM) techniques [15,16]. The nitrogen and phosphorus atoms inside these cages are virtually free atoms, with very long relaxation times [17]. The electronic spin is $S=\frac{3}{2}$, and the nuclear spin either $I=\frac{1}{2}$ (^{31}P, ^{15}N), or $I=1$ (^{14}N).

While $N@C_{60}$ appears as a very promising candidate for storing quantum information, Ref. [11] contains only vague suggestions for addressing individual qubits by shifting electron density onto the cages. No experimental evidence exists to date that indicates whether interactions due to electrostatic gates can be used for addressing such qubits.

It is therefore the purpose of this paper to introduce an alternative architecture that uses only the Zeeman and dipole-dipole interactions, both of which are well characterized. Addressing of qubits can be performed with magnetic field gradients generated by micropatterned wires and selective microwave pulses. In this respect this concept resembles a proposal by Goldman *et al.* [18], who suggested using static field gradients for addressing qubits through their Larmor frequencies. Since we use electronic spins here, rather than nuclear spins, the frequency difference between adjacent qubits is some three orders of magnitude larger, with correspondingly faster switching times. Furthermore, generation of the magnetic field gradient with electrical currents rather than with permanent magnets allows one to change the addressing by changing the gradient field during the experiment.

II. QUBIT IMPLEMENTATION

The degrees of freedom relevant for us are the electronic spin, which is $S=\frac{3}{2}$ for the ground state nitrogen atom, and the nuclear spin $I=\frac{1}{2}$ for ^{15}N and ^{31}P or $I=1$ for ^{14}N. For the present purpose, the size of the spin is not relevant, so we simplify the discussion by considering a chain of $S=\frac{1}{2}$ electronic spins, each coupled to a single $I=\frac{1}{2}$ nuclear spin.

Each logical qubit in our system is represented by two physical qubits, an electron and a nuclear spin. The relevant spin Hamiltonian for a single logical qubit is then (setting $\hbar=1$)

$$\mathcal{H}_S = g_B\mu_B \mathbf{B}_0\cdot\mathbf{S} - \gamma_n \mathbf{B}_0\cdot\mathbf{I} + A\mathbf{S}\cdot\mathbf{I}, \tag{1}$$

where the first two terms are the electron and nuclear Zeeman Hamiltonians and the last term is the hyperfine interaction Hamiltonian. μ_B is the Bohr magneton, g_B the g factor, and γ_n the gyromagnetic ratio of the nucleus. **S** and **I** are the electron and nuclear spin operators.

Equation (1) can be simplified if the electron Zeeman interaction is significantly stronger than the other interactions. In an external field of $B_0=1$ T, the resonance frequency of the electronic spin is $\nu_e=28$ GHz and the nuclear Larmor frequency is $\nu_n=4.3$ MHz for ^{15}N, while the isotropic hyperfine interaction is 22.35 MHz for ^{15}N [19]. We may then disregard those terms in the Hamiltonian that do not com-

*Electronic address: Dieter.Suter@physik.uni-dortmund.de
†Electronic address: lim@e3.physik.uni-dortmund.de

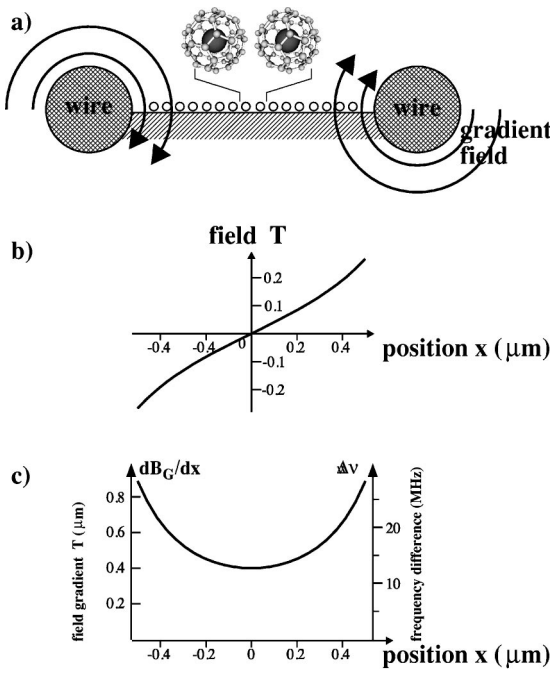

FIG. 1. (a) Arrangement of wires that generate the magnetic field gradient. The currents I in the two wires are equal and parallel. (b) Field distribution along the chain of the qubits for a separation of $\Delta=1$ μm and $I=1$ A. (c) Corresponding field gradient. The vertical axis also indicates the frequency separation between neighboring electron spins, for a separation of 1.14 nm.

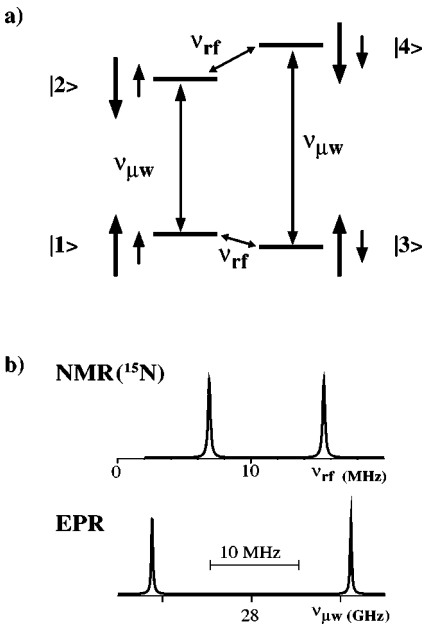

FIG. 2. (a) Relevant energy level scheme for electron and nuclear spin. (b) NMR and EPR transition frequencies in a 1 T field.

mute with the electron Zeeman interaction. With the conventional choice of the axis system, the Hamiltonian simplifies to

$$\mathcal{H}_S = g\mu_B B_0 S_z - \gamma_n B_0 I_z + A I_z S_z . \tag{2}$$

Logical gates can be applied to these qubits by microwave pulses that rotate the spin through a specific angle around an axis determined by the frequency and phase of the microwave. To address a specific qubit, we need a way to distinguish between them. Rather than relying on electrodes that access individual molecules, we propose to use magnetic field gradients, which can shift the resonance frequency of neighboring electron spins by several megahertz. Using integrated circuits, it is possible to apply currents of 1 A through a 1μm diameter wire [20]. Two parallel wires with radius r separated by a distance Δ generate an additional magnetic field in the space between the wires of

$$B_G = -\frac{\mu_0}{4\pi} 2I \left(\frac{1}{x+\Delta/2+r} + \frac{1}{x-\Delta/2-r} \right), \tag{3}$$

where I is the current in the wires and x the position, measured from the center between the wires. Figure 1(a) shows a schematic representation of the arrangement and Fig. 1(b) the resulting magnetic field for a current of $I=1$ A flowing parallel through the two wires.

As shown in Fig. 1(c), the resulting field gradient between the wires would be more than 4×10^5 T/m. Since N@C_{60} molecules must be separated by at least 1.14 nm, this implies a frequency difference of more than 12.7 MHz between nearest-neighbor electronic spins. Increasing the separation between molecules, which is possible in increments of 0.38 nm for C_{60} on Si(100), increases the frequency separation roughly linearly with the distance.

The logical qubits that we consider here allow us to store the information in the nuclear or in the electronic spin. Figure 2 summarizes the relevant energy level scheme and shows the allowed magnetic dipole transitions, which can be assigned to NMR and electron paramagnetic resonance (EPR) transitions. Generally the nuclear spins have longer decoherence times, while the electronic spins interact more strongly with the applied magnetic fields, thus providing shorter gate times. As we show below, using both degrees of freedom allows one to optimize the number of gate operations before decoherence becomes relevant. Furthermore, it provides a possible way to effectively switch the interaction between neighboring qubits on and off, as is required for the implementation of two-qubit gates.

To optimize the number of logical operations during the decoherence time of the system, we distinguish a passive state of the logical qubit, during which the information is stored in the nuclear spin, and an active state, where the information is stored in the electron spin. The passive state serves to preserve the information while it is not accessed. To perform logical operations, the qubit is activated by switching it from the passive to the active state.

This conversion between the two states, corresponding to an exchange of quantum information between two physical qubits, can be achieved by SWAP operations. This operation has already been implemented in liquid-state NMR [21,22], using pulse sequences of the type

$$U_{\mathrm{SWAP}}=[I_z+S_z][2I_zS_z][-I_y-S_y][2I_zS_z][I_x+S_x][2I_zS_z]\times[I_y+S_y]. \quad (4)$$

Here we use the notation $e^{i(\pi/2)I_r}=[I_r]$. The operators appear in time-reversed order, i.e., the sequence starts with the nonselective $(\pi/2)_y$ pulse represented by $[I_y+S_y]$. I and S represent the two spins that contribute to the logical qubit. Here, we write I for the nuclear spin and S for the electronic spin.

This implementation requires ideal (="hard") radio-frequency and microwave pulses. In the system we are considering here, it would be experimentally very difficult to implement such hard radio-frequency pulses on the nuclear spins, whose transition frequencies are split by 8 MHz. A better approach is to use two-frequency pulses at the two satellite transitions, which can be implemented in any double resonance NMR spectrometer. The electron spin system can also be manipulated with selective pulses, which act on only one of the two hyperfine-split transitions. Using such selective pulses, the SWAP operation can be implemented (up to an overall phase) by sequences of three π pulses applied to adjacent transitions, e.g.,

$$U_{\mathrm{SWAP}_1}=[2S_y^{(12)}][2I_x^{(13)}][-2S_y^{(12)}][-0.5F_z],$$

$$U_{\mathrm{SWAP}_2}=[2I_y^{(13)}][2S_x^{(12)}][-2I_y^{(13)}][-0.5F_z],$$

$$U_{\mathrm{SWAP}_3}=[-2I_y^{(13)}][2S_x^{(12)}][2I_y^{(13)}][0.5F_z]. \quad (5)$$

The upper index refers to a single transition of the corresponding spin [23]. A term $[2S_x^{(12)}]$ thus represents a rotation by π around the x axis of transition $|1\rangle\leftrightarrow|2\rangle$. The operator $F_z=I_z+S_z$ corresponds to a rotation of both spins around the z axis, which can be implemented either by composite z pulses or as a phase shift during the overall pulse sequence.

III. ONE-QUBIT GATES

Universal quantum computation requires arbitrary rotations of single qubits. As is well known, these rotations can be implemented for spins with radio-frequency or microwave pulses. Addressing individual qubits can in our case be implemented by the magnetic field gradient and frequency-selective pulses. For the geometry described above, the electronic and the nuclear spins are both shifted by the magnetic field gradient. For the numbers considered above, the separation between the nuclear Larmor frequencies of adjacent molecules is a few kilohertz. The duration of selective radio-frequency pulses would therefore be of the order of 1 ms. Considerably faster gate operations are possible if the frequency separation between neighboring electron spins is used. Since the frequency separation is more than 10 MHz, selective gate operations can be shorter than 1 μs.

As we discussed above, the quantum information is usually stored in the nuclear spin. Applying a one-qubit gate to a specific qubit therefore involves three steps: first, the information is activated by SWAP-ing it from the nuclear to the electronic spin. There, the selective rotation is applied and a second SWAP operation brings the information back into the nuclear spin. We will denote by U_{SWAP_i} a SWAP operation that acts selectively on the logical qubit i. Its effect can be summarized as

$$U_{\mathrm{SWAP}_i}I_\alpha^k U_{\mathrm{SWAP}_i}=S_\alpha^k\delta_{ik}+I_\alpha^k(1-\delta_{ik}),$$

$$U_{\mathrm{SWAP}_i}S_\alpha^k U_{\mathrm{SWAP}_i}=I_\alpha^k\delta_{ik}+S_\alpha^k(1-\delta_{ik}),$$

$$U_{\mathrm{SWAP}_i}U_{\mathrm{SWAP}_i}=1. \quad (6)$$

As a specific example, we consider the pseudo-Hadamard operation h_i [24] (a $[\pi/2]_y$ rotation) applied to logical qubit i. It can be implemented as

$$h_i=[I_y^{(i)}]=U_{\mathrm{SWAP}_i}[S_y^{(i)}]U_{\mathrm{SWAP}_i}. \quad (7)$$

To keep pulse sequences short, the radio-frequency pulses should not be selective with respect to the nuclear spins. Accordingly, all nuclear spins will be affected by this pulse sequence, not only the nuclei of the target qubit. However, for the passive qubits, the electronic spin is not affected. This can be used to construct sequences $U_{\mathrm{SWAP}}[S_a]U_{\mathrm{SWAP}}$ that do not affect the passive qubits. As an example, the combination $U_{\mathrm{SWAP}_2}U_{\mathrm{SWAP}_3}$, defined in Eq. (5), evaluates to a unity operator for the passive qubits.

IV. TWO-QUBIT GATES

Universal quantum computation requires, in addition to the single qubit gates, a two-qubit gate, such as an XOR or controlled-NOT (c-NOT) gate, that can be applied to any two nearest neighbors. In magnetic resonance, a c-NOT gate to spins A,B can be implemented by the pulse sequence [25]

$$U_{c\text{-}\mathrm{NOT}_{AB}}=[-B_y][-A_z-B_z][2A_zB_z][+B_y]. \quad (8)$$

The notation for the evolution is the same as above. The terms $[2A_zB_z]$ represent free precession under the coupling Hamiltonian, while the term $[B_y]$ represents a $\pi/2$ rotation of spin B around the y axis.

As in this example, two-qubit gates always use a precession under a coupling Hamiltonian for a duration τ. To implement such an operation, the coupling has to be turned on for the appropriate duration. While dipolar couplings between nearest-neighbor $N@C_{60}$ molecules are of a suitable size, they can only be turned off by moving the molecules apart, which is difficult to achieve within the time windows available.

Kane's proposal [6] for a scalable spin-based quantum computer uses "J gates," which shift electrons that mediate an exchange interaction between the nuclear spin qubits. In the case of endohedral fullerenes, this scheme appears not to be feasible, since the exchange of electrons between the cen-

tral N atom and the cage is very weak. We therefore suggest an alternative possibility, again SWAP-ing the quantum information between the nuclear and the electronic spin. When the information is stored in the electron spin, the interaction between neighboring molecules becomes effective, correlating neighboring qubits. When the information is SWAP-ed into the nuclear spins, the interaction is effectively switched off, since the nuclear dipole-dipole interaction is more than six orders of magnitude smaller than that between two electron spins (of the order of a few hertz at a separation of 1 nm). On the time scales relevant to us, it can be safely neglected.

For a formal analysis of this scheme, we start with the spin Hamiltonian for two logical qubits

$$\mathcal{H}_{ik}=\omega_i S_z^i+\omega_k S_z^k+\omega_n(I_z^i+I_z^k) +A(S_z^i I_z^i+S_z^k I_z^k)+dS_z^i S_z^k, \quad (9)$$

where $\omega_i=g_B\mu_B[B_0+B_G(\vec{r}_i)]$ represents the Larmor frequency of the electron spin at position $\vec{r}_i$ and ω_n is the nuclear Larmor frequency. For the nuclear spins, we neglect the difference in the Larmor frequency, and we assume that the difference between the Zeeman frequencies of neighboring electron spins is large compared to their dipole-dipole coupling, thus allowing us to truncate the dipolar interaction. This condition can always be fulfilled by increasing the distance between the molecules, which is possible in increments of 0.38 nm for C_{60} on Si(100). At the smallest possible distance of 1.14 nm, the dipolar interaction would be as large as 50 MHz [26], thus exceeding the difference of the Larmor frequencies. Increasing the separation Δ decreases the dipolar interaction ($\propto\Delta^{-3}$) while increasing the difference of the Larmor frequencies ($\propto\Delta$).

To implement a two-qubit operation, such as a c-NOT between the neighboring logical qubits *i* and *k*, the two target logical qubits are first activated using the single qubit addressing scheme discussed above. Then the c-NOT operation (8) is applied to the electron spins and the resulting information SWAP-ed back into the nuclear spins. The sequence of operations is then

$$U_{c\text{-NOT}_{ik}}=U_{c\text{-NOT}_{I_iI_k}} =U_{\text{SWAP}_i}U_{\text{SWAP}_k}U_{c\text{-NOT}_{S_iS_k}}U_{\text{SWAP}_k}U_{\text{SWAP}_i}. \quad (10)$$

After the operation, the information is again in the nuclear spin and remains unaffected by the coupling between the electron spins. The double SWAP operation has therefore the effect of switching the dipole interaction on for a limited time. As in the single qubit gates discussed above, the pulses should be nonselective with respect to the nuclear spins. Again, an overall effect on the nuclear spins can be avoided by proper combinations of SWAP sequences.

In the Hamiltonian of Eq. (9), we did not take into account the couplings to the passive qubits, which are also present, but should not affect the evolution of the qubits *i* and *k*. Since we assume only nearest-neighbor interactions in this context, this can be achieved by selective irradiation of the neighboring electron spins. Alternatively, it would be possible to simultaneously invert both *S* spins in the middle of the c-NOT sequence. The critical part is the free precession period $[2A_zB_z]=[2S_z^iS_z^k]$, which then becomes $[S_z^iS_z^k][2S_y^i+2S_y^k][S_z^iS_z^k]$. The decoupled c-NOT sequence becomes, e.g.,

$$U_{c\text{-NOT}_{AB}}^{dec}=[-B_y][-A_z-B_z][A_zB_z][-2A_y-2B_y] \times[A_zB_z][-2A_y-B_y]. \quad (11)$$

This sequence refocuses not only the couplings to the passive *S* spins, but also the hyperfine interaction, thus avoiding the necessity of nuclear spin decoupling during the $U_{c\text{-NOT}_{S_iS_k}}$ operation.

V. DISCUSSION AND CONCLUSION

We have presented an architecture for a scalable spin-based quantum computer. Addressing of the qubits is achieved with a magnetic field gradient and selective microwave pulses. A central aspect of our architecture is that each logical qubit uses electronic as well as nuclear spin degrees of freedom. SWAP-ing the information between the nucleus and the electron allows one to optimize the number of gate operations that can be completed before decoherence becomes relevant. Furthermore, it allows one to effectively switch the dipole-dipole interaction on for a well defined period. As a consequence, only one type of addressing capability for the individual spins is required, which corresponds to the *A* gates in Kane's design.

While it is motivated by a specific type of molecule (endohedral fullerenes), it uses only the fact that nuclear and electronic spins have vastly different gyromagnetic ratios. Applications to similar systems should therefore be straightforward.

A major difficulty in any spin-based quantum computer is the readout problem. While single spin magnetic resonance by optical detection has been demonstrated in several systems [27,28], these experiments are possible only in a relatively narrow parameter range, which may not include $N@C_{60}$. Another technique that may allow single spin detection is magnetic force detection [7,29,30]. This approach has the advantage that it requires less specific parameters, but present implementations are still far from single spin sensitivity. Single spin detection has also been reported with a STM [31], but the experiment is not well understood so far and no other group has reproduced the results. Another possible approach could combine spin-dependent tunneling with single electron detection [32].

The SWAP operation, which was used in this architecture, may also be useful for the readout problem. It may be possible, e.g., to swap the information from the qubits where they are processed to a readout qubit, such as a single electron device. Such elements tend to have shorter decoherence times, making them less suitable for the processor part of the quantum computer, but the stronger coupling to the environment facilitates the readout, where the decoherence will be less critical.

Another problem, which is shared by most spin-based ar-

chitectures, is the initialization: quantum error correction requires a supply of qubits in a well defined state, such as the ground state. While thermal relaxation may bring most spins into their ground state if the field is sufficiently high and the temperature low, this process cannot be faster than the decoherence for the same spin, and is therefore not useful for quantum error correction. Again, the SWAP operation may be used for this purpose: Spins in an environment of lower symmetry than $N@C_{60}$ tend to have significantly shorter relaxation times. They could therefore provide qubits in the $|0\rangle$ state at a high rate, and a SWAP operation could transfer this state to the qubits of the quantum register.

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