Magnetic Resonance Force Microscopy Quantum Computer with Tellurium Donors in Silicon

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We propose a magnetic resonance force microscopy (MRFM)-based nuclear spin quantum computer using tellurium impurities in silicon. This approach to quantum computing combines well-developed silicon technology and expected advances in MRFM. Our proposal does not use electrostatic gates to realize quantum logic operations.

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Introduction.—Recently, Kane [1] proposed a silicon-based nuclear spin quantum computer. This proposal linked the theoretical field of quantum computation with the well-developed silicon industry technology. It was proposed in [1] to use the nuclear spins, $I = 1/2$, of impurity phosphorus atoms (^{31}P) in silicon (^{28}Si) as qubits for quantum computation. Selective one-qubit rotations of nuclear spins can be implemented by combining the action of electrostatic gates and resonant radio frequency (rf) pulses. The electrostatic gate increases the size of the electron cloud of the selected phosphorus atom, changing the hyperfine interaction between the electron spin ($S = 1/2$) and the nuclear spin of the phosphorus atom. A two-qubit quantum CONTROL-NOT (CN) gate can be implemented by applying resonant rf pulses and electrostatic gates acting on the neighboring phosphorus atoms. Under the action of electrostatic gates, the electron clouds of the neighboring atoms increase their size and overlap. This causes an exchange interaction between electron spins which, in turn, generates an indirect coupling between the associated nuclear spins.

To measure the state of a nuclear spin, it was proposed in [1] to transfer the state of the nuclear spin to the electron spin. Then, using an electrostatic gate, one induces a transfer of the electron from the measured phosphorus atom to the auxiliary phosphorus atom. Because of the Pauli principle, this transfer is possible only if the electron spins of the measured atom and the auxiliary atom have opposite directions. The change of the charge of the auxiliary atom can be measured by a single-electron transistor. This attractive proposal may, however, face difficulties associated with the following: (a) the precise manipulation of the electron clouds using electrostatic gates, (b) the complicated procedure for transferring the nuclear spin state to the electron spin state, and (c) the application of the single-electron transistor. Vrijen *et al.* [2] proposed a way to overcome these problems. But their proposal implements qubits in the electron spins of the phosphorus atoms. It is clear that unlike nuclear spins, electron spins cannot be isolated from their surroundings. So, the price of simplification of the original proposal [1] seems to be a significantly shorter decoherence time.

In our previous paper [3] we proposed the solid-state magnetic resonance force microscopy (MRFM) quantum computer. This proposal relies on rapidly developing MRFM methods which promise single spin detection combining magnetic resonance techniques, atomic force microscopy, and novel optical methods for detection of mechanical vibrations [4–6]. Our proposal relies also on the hyperfine interaction in the impurity paramagnetic atoms but it does not use electrostatic gates. The selective change of the spin resonant frequency is caused by the magnetic field produced by a ferromagnetic particle. The two-qubit CN gate is implemented using the hyperfine interaction and the dipole-dipole interaction between the electron and the nuclear spins of the neighboring atoms. So, the exchange interaction between the neighboring electron spins is not important. It would be very attractive to apply the idea of the MRFM quantum computer to paramagnetic impurities in silicon. However, the phosphorus atom does not fit our proposal because of the large size of its electron cloud and relatively weak hyperfine interaction. In this paper, we propose a MRFM quantum computer based on a silicon substrate with tellurium impurities. Unlike phosphorus, a tellurium atom in silicon is a "deep donor" with a small electron cloud and with an extremely large hyperfine interaction. Application of tellurium impurities in silicon could combine the advantages of MRFM with the well-developed techniques of silicon technology. In section II, we discuss the design of this quantum computer. In section III, we describe quantum computation using this nuclear spin quantum computer. We discuss a one-qubit rotation, a two-qubit quantum CN gate, the measurement of the state of a nuclear spin, and the initialization of the nuclear spins in their ground states.

MRFM Si:Te nuclear spin quantum computer.—A diagram of the proposed quantum computer is shown in Fig. 1. Tellurium-125 donors are placed near the surface of the silicon-28 substrate. We use pure ^{125}Te nuclei, whose natural abundance is only 7%. We also use silicon containing only ^{28}Si nonmagnetic nuclei. ^{29}Si magnetic nuclei whose natural abundance is 4.7% must be removed. When the host atom in silicon is replaced by a tellurium donor, two extra electrons become available. The properties
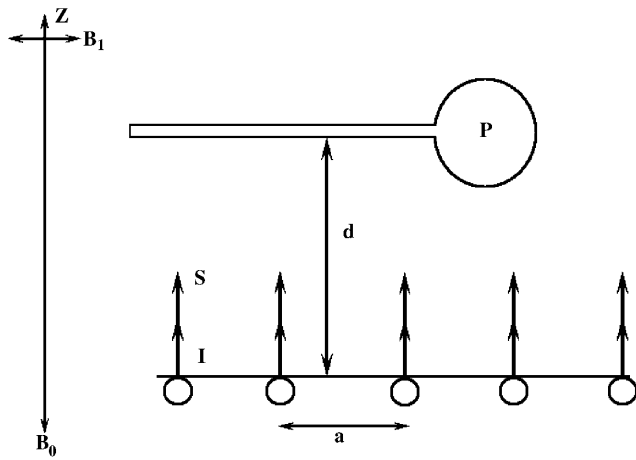
FIG. 1. A diagram of the proposed quantum computer. The circles indicate $^{125}\text{Te}^+$ ions implanted near the surface of the silicon substrate; I is the nuclear spin; S is the electron spin (spins are shown in their ground states); P is the ferromagnetic particle (vibrating or nonvibrating); $d = 15$ nm; $a = 5$ nm.

of tellurium donors in silicon have been investigated elsewhere. (See, for example, Ref. [7] and references therein.) It was found that most of the implanted tellurium atoms occupy substitutional sites.

The ground states of the tellurium donors, as well as those of other atoms with two extra electrons, are referred to as "deep impurity levels," in contrast to "shallow" impurities like phosphorus with one extra electron whose ground state energies are of the order 50 meV. Because of the two extra electrons, tellurium donors form singly ionized A centers, Te^+, and neutral B centers, Te^0. The temperature-independent ground state energies were found in [7] to be 410.8 meV for A centers, and 198.8 meV for B centers.

Electron spin resonance (ESR) for A centers [7] can be described by the simple spin Hamiltonian,

$$\mathcal{H} = g_e \mu_B \vec{B}\vec{S} + g_n \mu_n \vec{B}\vec{I} - A\vec{S}\vec{I}, \qquad (1)$$

where $\vec{S}$ is the electron spin ($S = 1/2$) of Te^+, $\vec{I}$ is the nuclear spin ($I = 1/2$) of ^{125}Te nuclei, μ_B and μ_n are the Bohr and nuclear magnetons, g_e and g_n are the electron and nuclear g factors: $g_e \approx 2$ and $g_n \approx 0.882$, A is the isotropic hyperfine (hf) interaction constant, and $A/2\pi\hbar \approx 3.5$ GHz. The first two terms in (1) have the same signs because the nuclear magnetic moment of ^{125}Te is negative, as is the electron magnetic moment. For the same reason, we put in (1) a negative sign for the hyperfine interaction.

We propose to use as qubits the nuclear spins of the ^{125}Te donors (A centers). We assume that future advances in silicon technology will allow one to place a regular chain of ^{125}Te donors near the surface of silicon with the distance between donors being approximately 5 nm. (See Fig. 1.) To initialize the ground states of the nuclear spins and to measure their final states, we propose using MRFM. For this purpose, the ferromagnetic particle, P, in Fig. 1, attached to the end of the cantilever, can move along the impurity chain selecting an appropriate tellurium ion. To

implement quantum computation, we propose using the same (but nonvibrating) ferromagnetic particle which can move along the impurity chain. Next, we shall describe the operations of the proposed quantum computer.

Quantum computer operations.—Following our proposal [3], we assume that electron spins are polarized in the positive z direction. (As an example, for $B_0 = 10$ T and at a temperature of 1 K, the probability for an electron to change its direction is approximately 1.4×10^{-6}.) In contrast to the electrons, approximately 44% of nuclear spins are in their excited states. To detect these nuclear spins one moves the ferromagnetic particle placed on the cantilever to a selected tellurium ion. Assuming that the distance between the ferromagnetic particle and the selected ion is 10 nm, the radius of the ferromagnetic particle is 5 nm, and the magnetic induction of the ferromagnetic particle is $\mu_0 M \approx 2.2$ T, one finds that the shift of the ESR frequency for the selected ion is $\Delta f_e \approx 1.5$ GHz. (The corresponding magnetic field produced by the ferromagnetic particle is approximately 5.4×10^{-2} T [3].) The "natural" ESR frequency for $B_0 = 10$ T is $f_e \approx 280$ GHz. The hyperfine shift of the ESR frequency is $f_{\text{hf}} = A/4\pi\hbar \approx 1.75$ GHz [7]. For a tellurium ion, the magnetic dipole field produced by its two neighbor electron spins is approximately 1.5×10^{-5} T. The magnetic dipole field produced by all other electron spins does not exceed 3×10^{-6} T [3]. The corresponding shifts of the ESR frequency are $f_{ed} \approx 0.42$ MHz and $f'_{ed} < 0.08$ MHz. We assume that the amplitude of the rf pulse, B_1, in frequency units (the Rabi frequency) is greater than f_{ed}. So, the dipole contribution to the ESR frequency can be ignored. Thus, applying the rf pulses with the frequency,

$$f \approx f_e + f_{\text{hf}} + \Delta f_e, \qquad (2)$$

one induces oscillations of the electron spin of a selective tellurium ion only if the nuclear spin of the ion is in its ground state. The oscillating electron spin, in turn, induces resonant vibrations of the cantilever which can be detected by MRFM methods. A discussion of modified MRFM techniques for detection of a single-electron spin and related estimates for the MRFM quantum computer can be found in our previous papers [3,8].

Thus, tellurium ions detected by MRFM have their nuclear spins in their ground state. To drive other nuclear spins to their ground states, one moves the nonvibrating ferromagnetic particle to a selected tellurium ion whose nuclear spin is in the excited state. The natural NMR frequency for ^{125}Te nuclear spin in an external magnetic field of 10 T is 134.5 MHz. The hyperfine "shift," $f_{\text{hf}} \approx 1.75$ GHz is larger than the natural frequency. The additional shift caused by the magnetic field of the ferromagnetic particle is $\Delta f_n \approx 0.73$ MHz. Applying an rf π pulse with frequency,

$$f = f_n + f_{\text{hf}} + \Delta f_n - f_{nd} - f'_{nd}, \qquad (3)$$

one drives the nuclear spin into its ground state.

In Eq. (3), the frequency, f_{nd}, is the NMR shift caused by the dipole field of the electron spins of the neighbor ions, and f'_{nd} is due to electron spins of all other ions. For ^{125}Te, the frequency $f_{nd} \approx 200$ Hz, and $f'_{nd} < 40$ Hz. Applying an rf pulse with a nuclear Rabi frequency larger than f_{nd}, one can neglect the dipole contribution in (3). The same method can be used to implement a one-qubit rotation. To implement a two-qubit gate, we propose using the magnetic dipole interaction between electron and nuclear spins of neighboring tellurium ions. For this purpose, one moves the nonvibrating ferromagnetic particle to a tellurium ion containing a control nuclear spin (a control qubit). Then, one applies an rf pulse with frequency (2). This pulse drives the electron spin into its excited state if the control nuclear spin is in the ground state. Next, one moves the nonvibrating ferromagnetic particle to the neighboring tellurium ion containing the target nuclear spin (a target qubit). Now, it is important to use a selective rf pulse whose frequency is

$$f = f_n + f_{\text{hf}} + \Delta f_n - f_{nd} - f'_{nd}, \qquad (4)$$

and whose Rabi frequency is less than 200 Hz. This pulse changes the state of the target nuclear spin if the dipole contribution from neighbor electron spins does not cancel out. This happens only if the control nuclear spin was in the excited state. Finally, one moves the nonvibrating ferromagnetic particle back to the ion containing the control nuclear spin and applies a π pulse with the frequency (2), to return the electron spin to its ground state (if it had been in the excited state). Thus, three rf pulses together implement a quantum CN gate: the target qubit changes its state if the control qubit is in the excited state. The final measurement of the nuclear states can be implemented using MRFM in the same way as the measurement of the initial nuclear states.

Certainly, a very important problem is connected to the relaxation time for electron spins, as the electron spins are supposed to be used in quantum operations. The longest characteristic time which limits the speed of quantum transformations in our proposal is the duration of the "nuclear" rf pulse in the CN gate. The Rabi frequency for this pulse must be less than $f_{nd} \approx 200$ Hz. It means that the duration of the pulse must be greater than 2.5 ms. During this time interval, the electron spin of the control qubit must be in the excited state. It is known that the electron spin relaxation time for paramagnetic impurities in a diamagnetic host can be of the order of an hour, which is much greater than the time needed for a CN gate [9].

The second important problem is to position a ferromagnetic particle near the targeted tellurium ion. In our proposal the distance between the neighboring tellurium ions is 5 nm, the same as the radius of the ferromagnetic particle. Thus, the uncertainty in positioning the center of the particle must be much less than its radius. This requires further development of MRFM techniques.

Finally, we compare our MRFM proposal with the well-known Kane proposal [1]. We consider our MRFM proposal as an alternative approach to implement the same idea as in [1]—to create a scalable nuclear spin quantum computer based on silicon technology. This MRFM quantum computer does not require any electrostatic gates which manipulate individual qubits. It also does not require a complicated scheme to transfer the nuclear spin state to the electron spin state and then to the charge state which must be measured by a single-electron transistor. In the MRFM quantum computer, all operations are performed using a "magnetic head" which moves along the array of qubits like a read/write head in a conventional computer. The requirements for the magnetic head are very high. In particular, they include a single electron spin measurement and high precision positioning near the targeted tellurium ions.

Conclusion.—We describe a MRFM nuclear spin quantum computer using tellurium-125 singly ionized donors placed near the surface of silicon-28. It is shown that a MRFM single-electron spin measurement can provide three essential requirements for quantum computation: (a) preparation of the ground state of nuclear spins, (b) one- and two-qubit quantum logic gates, and (c) a measurement of the final state. Our design requires further developments in silicon technology and advances in MRFM including the detection of a single spin. The proposed quantum computer can operate at temperatures up to 1 K.

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