

Solid-State Quantum Computer Based on Scanning Tunneling Microscopy

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We propose a solid-state nuclear-spin quantum computer based on application of scanning tunneling microscopy (STM) and well-developed silicon technology. It requires the measurement of tunneling-current modulation caused by the Larmor precession of a single electron spin. Our envisioned STM quantum computer would operate at the high magnetic field (~ 10 T) and at low temperature ~ 1 K.

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I. Introduction.—Recently, we suggested a solid-state nuclear-spin quantum computer based on magnetic resonance force microscopy (MRFM) [1,2]. In this proposal, a ferromagnetic particle, which is attached to the tip of the cantilever, moves along a chain of paramagnetic ions (atoms) located below the surface of silicon. The ferromagnetic particle targets a particular ion, providing selective excitation of its electron or nuclear spin, a measurement of the state of the nuclear spin, and initial polarization and one-qubit rotations of nuclear spins. A two-qubit control-NOT (CN) gate for two neighboring nuclear spins utilizes the dipole-dipole interaction between the nuclear spin of one ion and the electron of the neighboring ion.

There are three basic disadvantages in the suggested MRFM proposal: (1) The motion of the ferromagnetic particle along the chain of paramagnetic ions can induce additional dephasing in the spin system. This dephasing must be taken into account. (2) Fluctuations of the position of a ferromagnetic particle cause additional decoherence in a spin system. (3) The accurate positioning of the ferromagnetic particle relative to an ion is a complicated experimental problem.

In this paper, we suggest a quantum computer architecture which seems to be free of all these disadvantages. At the same time, it retains the main advantage of the MRFM proposal—it does not require an array of single-atom gates, which is an essential part of well-known solid-state proposals based on silicon technology [3,4]. We give estimates for characteristic parameters required for realization of a quantum computer based on the scanning tunneling microscopy (STM) technique.

II. STM detection of an electron spin resonance and a nuclear spin state.—Our proposal utilizes recent results in STM experiments which seem to allow detection of the precessing electron spin from a single ion (atom). In these experiments [5], the STM technique was used to measure the frequency of the Larmor precession of an electron spin of an individual iron atom in silicon in the presence of a small, static applied magnetic field. This measurement utilizes the interaction between a localized electron spin

in a surface of a sample and the current produced by tunneling electrons. Because of this interaction the tunneling probability is affected by the Larmor precession of a localized spin, and the tunneling current is modulated at the Larmor frequency.

The mechanism causing the tunnel current modulation is, however, not well understood. While this requires additional consideration, in this paper we assume that the STM technique is able to detect the frequency of electron spin precession for an individual ion (atom) in a silicon surface. This results in the possibility for the STM technique to detect the state of a nuclear spin in the same ion. Indeed, suppose that the hyperfine interaction between electron and nuclear spins of the ion is greater than the Zeeman interaction between a high external magnetic field, \vec{B}_0 , and the nuclear spin. Then, the frequency of an electron spin precession depends on the state of the nuclear spin. As an example, following [2], we consider a $^{125}\text{Te}^+$ ion (A center) in the surface of silicon. The Hamiltonian of the electron-nuclear spin system of the ion has the form

$$\mathcal{H} = g_e \mu_B B_0 S_z + g_n \mu_n B_0 I_z - A \vec{S} \vec{I}, \quad (1)$$

where \vec{S} and \vec{I} are electron and nuclear spin operators ($S = I = 1/2$); B_0 is a high magnetic field pointed in the positive z direction; $g_e \approx 2$, $g_n \approx 0.882$; and $A/2\pi\hbar \approx 3.5$ GHz is the constant of the hyperfine interaction. The magnetic moments of the ^{125}Te nucleus and the electron are both negative. Figure 1 demonstrates the energy levels of the electron and nuclear spins of the $^{125}\text{Te}^+$ ion in a high magnetic field.

If the nuclear magnetic moment points “up,” the modulation frequency is

$$f = f_{e0} = g_e \mu_B B_0 / 2\pi\hbar + A/4\pi\hbar. \quad (2)$$

In the opposite case,

$$f = f_{e1} = g_e \mu_B B_0 / 2\pi\hbar - A/4\pi\hbar. \quad (3)$$

The hyperfine splitting is $A/2\pi\hbar$. If the tunneling current is observed to oscillate with the frequency f_{e0} , the nuclear spin of the ion is in its ground state. Otherwise the nuclear spin is in the excited state.

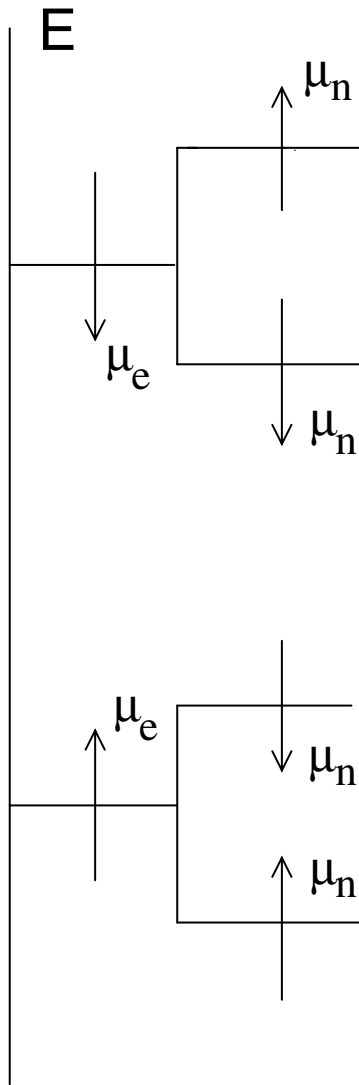


FIG. 1. Energy levels for electron (μ_e) and nuclear (μ_n) magnetic moments in a high magnetic field.

III. Selective excitation of a nuclear spin.—To provide a selective excitation of the nuclear spin (qubit), we assume that a permanent magnetic field is slightly nonuniform in the x direction (see Fig. 2). Assuming that the distance between the neighboring ions is a , we have, for the difference in the precession frequencies for these ions,

$$\Delta f_e = (g_e \mu_B / 2\pi \hbar) a \frac{\partial B_0}{\partial x}. \quad (4)$$

The corresponding difference for nuclear magnetic resonance (NMR) frequencies is

$$\Delta f_n = (g_n \mu_n / 2\pi \hbar) a \frac{\partial B_0}{\partial x}. \quad (5)$$

[In Eq. (4) we assume that nuclear spins of the neighboring ions are in the same state. In Eq. (5) we assume that the electron spins of the neighboring ions are in the same state.] As an example, taking $a = 5$ nm and $\partial B_0 / \partial x = 10^5$ T/m, we obtain for ^{125}Te $\Delta f_n \approx 6.75$ kHz.

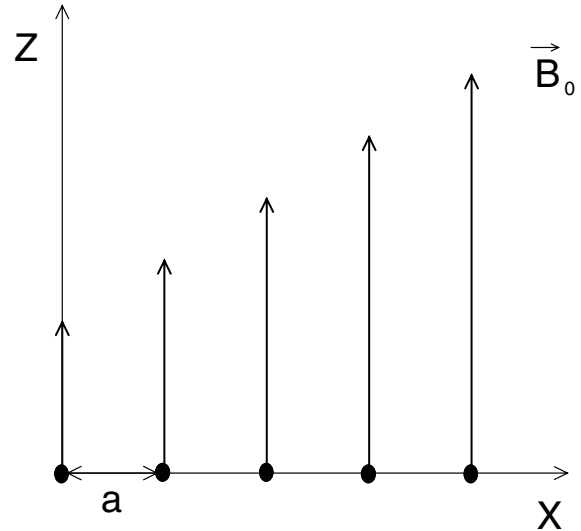


FIG. 2. The magnitude of the permanent magnetic field slightly increases in the x direction. a is the distance between the neighboring ions.

For selective excitation of a nuclear spin, one can apply a π - or $\pi/2$ -pulse of a rotating magnetic field, \vec{B}_\perp . The nuclear Rabi frequency, f_{nR} , is given by

$$f_{nR} = (g_n \mu_n / 2\pi \hbar) B_\perp. \quad (6)$$

For selective excitation, this quantity must be less than Δf_n . It imposes a restriction on the duration, τ , of a π -pulse,

$$\tau = \pi / 2\pi f_{nR} > 1 / 2\Delta f_n \approx 74 \mu\text{s}. \quad (7)$$

Using selective nuclear π -pulses one can drive a nuclear spin chain into the ground state. For this purpose one prepares the system in a high magnetic field at a low temperature, so that all electron spins are in their ground state. (As an example, $B_0 \sim 10$ T, $T \sim 1$ K.) Then, one measures the modulation frequency of the tunneling current at any position, x_k . If the modulation frequency fits the value, $f_{e1}(x_k)$, one applies a selective nuclear π -pulse with the frequency, $f_n(x_k)$, which drives the nuclear spin into the ground state.

IV. A control-NOT gate.—The ability to implement a CN gate is important for quantum computation as any quantum algorithm can be decomposed into a sequence of one-qubit rotations and CN gates [6]. We propose to use a scheme close to that outlined in our MRFM proposal [1,2]. It consists of three steps.

(1) One applies an electronic π -pulse with the frequency $f = f_{e1}(x_k)$. This pulse drives the electron spin of the ion “ k ” into the excited state only if the nuclear spin of the ion k (a control qubit) is in the excited state. The difference, Δf_e , of electron spin resonance (ESR) frequencies of neighboring ions for $\partial B_0 / \partial x = 10^5$ T/m is $\Delta f_e = 14$ MHz. This is much smaller than the hyperfine splitting, $A / 2\pi \hbar \approx 3.5$ GHz. Thus, for a chain containing up to 250 spins the frequency, $f_{e1}(x_k)$, is unique in

the chain. For a longer chain, additional conditions are required to prevent a coincidence of the ESR frequencies for remote ions. (The dipole-dipole contribution to the ESR frequency is small in comparison to the hyperfine splitting.)

(2) One tunes the frequency of the nuclear π -pulse for the ion “ $k + 1$ ” (or “ $k - 1$ ”) taking into consideration the dipole field produced by an electron spin on the nuclear spin of the ion $k + 1$ (a target qubit). If the electron spin of the ion k did not change its direction, the NMR frequency for the ion $k + 1$ (taking into account a dipole field of electron spins) is

$$f = f_n(x_{k+1}) - f_{nd} - f'_{nd}, \quad (8)$$

where f_{nd} is the dipole shift due to two neighboring electron spins, and f'_{nd} is the dipole shift due to all other electron spins. (For $a = 5$ nm, $f_{nd} \approx 200$ Hz, $f'_{nd} < 40$ Hz, the nuclear-nuclear dipole interaction is negligible.) If the electron spin of the ion k has changed its direction, then the NMR frequency for the ion $k + 1$ is

$$f = f_n(x_{k+1}) - f'_{nd}. \quad (9)$$

The difference, f_{nd} , between the frequencies (8) and (9) must be smaller than Δf_n . In our case this condition is satisfied, so both frequencies (8) and (9) are unique in a spin chain. If the frequency of a nuclear π -pulse is tuned to (9), and the Rabi frequency, f_{nR} , of the nuclear π -pulse is less than f_{nd} , then the nuclear spin of the ion $k + 1$ changes its direction only when the control qubit is in the excited state. This provides an implementation of a CN gate. This step imposes a most severe restriction on the duration of a quantum gate: $\tau = \pi/2\pi f_{nR} > 2.5$ ms. The same step imposes a restriction on the electron relaxation time which must be greater than τ . (Available data [7] show that the electron relaxation time for paramagnetic impurities can be of the order of hours.)

(3) Finally, one repeats the first step to drive an electron spin of the ion k back to the ground state, if the control qubit is in the excited state.

V. Conclusion.— We proposed a nuclear spin solid-state quantum computer based on STM. Our proposal does not require sophisticated single-atom electrostatic gates. A single-spin measurement is provided by measuring the modulation of the tunneling current. Selective excitation of a nuclear spin can be achieved using an inhomogeneous permanent magnetic field. A control-NOT gate is provided by utilizing the dipole-dipole interaction between the electron and nuclear spins. Our envisioned STM quantum computer would operate at high magnetic field (~ 10 T) and at low temperature ~ 1 K.

To complete our discussion on the STM quantum computer, we should mention some experimental difficulties which must be overcome. First, the NMR frequency, f_n , is very sensitive to an exact location of a paramagnetic ion. Taking the distance between paramagnetic ions (5 nm) to be equal to 30 interatomic distances, one obtains the NMR frequency shift about 200 Hz between two neighboring atoms. This problem could be solved by accurate initial measurement of the NMR frequency for each paramagnetic ion. A resonant nuclear π -pulse of duration greater than 2.5 ms will drive a nuclear spin from one state into the other state changing the ESR frequency and the modulation frequency of the tunneling current. Thus, the exact placement of a paramagnetic atom is not required in our proposal. Because of the same reason, the precise value of the external magnetic field on a paramagnetic ion with the accuracy to 1.5×10^{-5} T (which corresponds to the NMR frequency shift 200 Hz) is also not required. On the other hand, the stability of the external magnetic field must be greater than 1.5×10^{-5} T. Also, the frequency resolution of the tunneling current modulation must be greater than the ESR hyperfine splitting, 3.5 GHz. Certainly, the whole idea of our proposal assumes the opportunity for an adequate measurement of a nuclear spin state via the ESR frequency using the STM technique. This opportunity is yet to be proved in experiments.

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- [1] G. P. Berman, G. D. Doolen, P. C. Hammel, and V. I. Tsifrinovich, *Phys. Rev. B* **61**, 14 694 (2000).
 - [2] G. P. Berman, G. D. Doolen, P. C. Hammel, and V. I. Tsifrinovich, *Phys. Rev. Lett.* **86**, 2894 (2001).
 - [3] B. E. Kane, *Nature (London)* **393**, 133 (1998).
 - [4] R. Vrijen, E. Yablonovitch, K. Wang, H. W. Jiang, A. Balandin, V. Roychowdhury, T. Mor, and D. DiVincenzo, *Phys. Rev. A* **62**, 012306 (2000).
 - [5] Y. Manassen, I. Mukhopadhyay, and N. R. Rao, *Phys. Rev. B* **61**, 16 223 (2000).
 - [6] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. Smolin, and H. Weinfurter, *Phys. Rev. A* **52**, 3457 (1995).
 - [7] G. Feher and E. A. Gere, *Phys. Rev.* **114**, 1245 (1959).