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Title:

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Submitted to:

New Phenomena in Mesoscopic Structures
Kauai, HI
12/7-11/98

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Form 836 (10/96)

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Electron-Nuclear Spin Dynamics in a Mesoscopic Solid-State Quantum Computer

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We numerically simulate the process of nuclear spin measurement in Kane's quantum computer. For this purpose, we model the quantum dynamics of two coupled nuclear spins located on ^{31}P donors implanted in Si. We estimate the minimum time of measurement necessary for the reliable transfer of quantum information from the nuclear spin subsystem to the electronic one and the probability of error for typical values of external noise.

Recently ^{31}P donors in silicon were proposed as candidates for quantum logic gates based on nuclear spin dynamics¹. It was shown that a quantum Control-Not operation may be performed using a pair of donor nuclear spins indirectly coupled via hyperfine interactions with electrons. Because of a very weak interaction of nuclear spins with the environment, they exhibit huge decoherence times², which is advantageous for quantum computations. However the almost perfect isolation of the spins from the environment also makes difficult reading out the computation result. The traditional NMR methods do not allow sufficient accuracy to measure the signal from a single spin. Therefore, Kane proposed a special procedure for measuring the quantum states of nuclear spins¹. In the course of this procedure, the information about the spin state of nuclear subsystem is transferred to the electron subsystem, so that the latter finally finds itself either in singlet or triplet state depending on the initial state of nuclear spins. The latter states may be distinguished through their different charge properties, e.g., by means of single-electron capacitance techniques. We present simulations of dynamics of two coupled electron and nuclear spins in the course of the read-out procedure and estimations of minimum time necessary for a reliable measurement of the computation result. We also study the effects of external noise on the measuring results.

Figure 1. Two ^{31}P donors in silicon. The nuclear spins are coupled to the outer electrons by the hyperfine interactions controlled by A gates, and the electrons are mutually coupled via exchange interaction controlled by the J gate.

The Hamiltonian of the system is of the form

$$\mathcal{H} = 2\mu_B B(\hat{S}_{1z} + \hat{S}_{2z}) - 2g_n\mu_n B(\hat{I}_{1z} + \hat{I}_{2z}) + 4A_1\hat{S}_1\hat{I}_1 + 4A_2\hat{S}_2\hat{I}_2 + 4J\hat{S}_1\hat{S}_2,$$

where $\hat{S}_i$ and $\hat{I}_i$ are electron and nuclear spin operators corresponding to donors 1 and 2, μ_B and μ_n are the Bohr and nuclear magnetons, $g_n = 1.13$ is the nuclear g -factor, B is the external magnetic field, A_i are the hyperfine interaction constants for nuclei 1 and 2, and J is the constant of exchange interaction between the electrons.

Generally, $\mathcal{H}$ possesses 16 energy levels, which correspond to different projections of the four spins on the direction of magnetic field. Of these 16, four states with total projection $S_z + I_z = -1$ form a closed group that is of interest to us. The dependences of these levels on the exchange coupling are shown in Fig. 2. After the quantum computation is performed at $J \rightarrow 0$, the system may find itself either in the state $|E_2\rangle = |\downarrow\downarrow\rangle_e |\uparrow\downarrow + \downarrow\uparrow\rangle_n$ or in the state $|E_4\rangle = |\downarrow\downarrow\rangle_e |\uparrow\downarrow - \downarrow\uparrow\rangle_n$. As the exchange coupling between the hydrogen-like electron levels of the donors is adiabatically increased by means of an external gate, state $|E_2\rangle$ retains its structure, whereas state $|E_4\rangle$ evolves into $|\uparrow\downarrow - \downarrow\uparrow\rangle_e |\downarrow\downarrow\rangle_n$, i.e., the electron and nuclear subsystems exchange their spins. As a result, the electron subsystem finally finds itself in a singlet or triplet state depending on the initial state of the nuclear subsystem. However, if J is increased too rapidly, the system may be excited from state $|E_4\rangle$ into state $|E_3\rangle$, which has the same symmetry yet evolves in the opposite sense from $|\uparrow\downarrow - \downarrow\uparrow\rangle_e |\downarrow\downarrow\rangle_n$ to $|\downarrow\downarrow\rangle_e |\uparrow\downarrow - \downarrow\uparrow\rangle_n$. This would result into an erroneous measurement. By numerically simulating the quantum dynamics of the system in the course of measurement, we calculated the dependence of P_4 , the probability for the system to finally find itself in state $|E_4\rangle$, on the duration of measurement T for the case of $A_1 = A_2 = A$ (see Fig. 3).

Figure 2. Energy levels of the system of two coupled nuclear and electron spins vs. exchange coupling J . Inset shows the bottleneck between states $|E_3\rangle$ and $|E_4\rangle$ at larger scale.

For small T , $P_4 \rightarrow 0$ because the short-term dynamics of electrons is only weakly affected by hyperfine interaction and the electron subsystem retains its spin. For sufficiently large T , P_4 tends to 1 according to the law $1 - P_4 \propto \exp(-T/\tau)$. For the typical values of $B = 2$ Tesla and $A/\hbar = 1.8 \times 10^8 \text{ sec}^{-1}$ one obtains $\tau^{-1} = 5.7 \times 10^5 \text{ sec}^{-1}$.

By scaling A , we found that $\tau^{-1} \propto A^2/2\mu_B B\hbar$. This result can be explained as follows. The width of the bottleneck between the states $|E_4\rangle$ and $|E_3\rangle$ is $\Delta E = 4A$ (see Fig. , inset) and the corresponding interval of J is also on the order of A . Hence $T/\tau \sim \Delta E \Delta t/\hbar$, where Δt is the time of passage of the system through this bottleneck.

Amplitude of state $|E_4\rangle$ vs. duration of measurement for $B = 2$ Tesla and $A/\hbar = 1.8 \times 10^8 \text{ sec}^{-1}$ (solid curve). The dash-dot and dashed curves show the same dependences for $A/\hbar = 1.8 \times 10^9 \text{ sec}^{-1}$ and $A/\hbar = 1.8 \times 10^{10} \text{ sec}^{-1}$.

It is a pleasure to thank C. Hammel, B. Kane, and D. Pelekhov for valuable discussions. K.E.N. is grateful to the Theoretical Division and the CNLS of the Los Alamos National Laboratory for their hospitality. This work was supported by the Department of Energy under contract W-7405-ENG-36, and by the Linkage Grant 93-1602 from the NATO Special Programme Panel on Nanotechnology.

¹ B.E. Kane, *Nature* **393**, 133 (1998).

² J.S. Waugh and C.P. Slichter, *Phys. Rev. B* **37**, 4337 (1988).