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Control of Non-Resonant Effects in a Nuclear Spin Quantum Computer with a Large Number of Qubits

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We discuss how to simulate simple quantum logic operations with a large number of qubits. These simulations are needed for experimental testing of scalable solid-state quantum computers. Quantum logic for remote qubits is simulated in a spin chain. Analytical estimates are presented for possible correlated errors caused by non-resonant transitions. A range of parameters is given in which non-resonant effects can be minimized.

INTRODUCTION

Several proposals for scalable solid-state quantum computers have been recently published[1–3]. The simulation of quantum information processing with a large number of qubits will be necessary to test these computers. We show in this paper how to implement the Control Not (CN) gate between remote qubits in a spin chain using a sequence of electromagnetic pulses. The errors generated by non-resonant effects are estimated analytically and computed numerically. We give the probability of error as a function of the Rabi frequency and the number of qubits.

The two-level approximation for an individual transition used in this paper for analysis of the system (see also Ref. [4]) allows one to simulate the quantum dynamics in a system with an enormous number (2^L, where L is the number of qubits) of quantum states. This technique is based on selection of states generated as a result of the resonant or near-resonant transitions, while other transitions are neglected.

In Sec. I we give the Hamiltonian of the nuclear spin quantum computer. In Sec. II we use the resonance approximation to show that each quantum state interacts resonantly only with a single state. This allows us to decrease from exponential in L to polynomial in L the number of differential equations in the system. In Sec. III we use the solution of the problem in the resonance approximation to estimate error probabilities in the implementation of a CN gate caused by finite detuning from exact resonance.

I. DYNAMICS OF THE SPIN CHAIN

We consider a chain of identical nuclear spins placed in a nonuniform high external magnetic field B, with a uniform gradient. The nuclear magnetic resonance (NMR) frequency for the kth spin is $\omega_k = \gamma_n B_k$, where γ_n is the nuclear gyromagnetic ratio and B_k is the z-component of the magnetic field at the location of the kth spin. The gradient of the magnetic field (in the direction of the chain) provides a shift of ω_k by the value $\delta\omega$ between the neighboring spins. (For the physical parameters see Ref. [4].)

The Hamiltonian of the spin chain in an external radio-frequency (rf) field is,

$$H_n = -\sum_{k=0}^{L-1} \omega_k I_k^z - 2J \sum_{k=0}^{L-1} I_k^z I_{k+1}^z + V_n = H_0 + V_n, \quad (1)$$

where J is the Ising interaction constant and I_k^z is the operator of the z-component of spin 1/2. The operator, V_n, describing the interaction of spins with the rf pulses, can be written in the form,[5] $V_n = -(\Omega_n/2)\sum_{k=0}^{L-1}[I_k^- \exp(-i(\nu_n t + \varphi_n) + I_k^+ \exp(i\nu_n t + \varphi_n)]$, where Ω_n, ν_n and φ_n are the Rabi frequency, the frequency and the phase of the nth pulse; $I_k^{\pm} = I_k^x \pm I_k^y$. Each quantum state of the spin chain can be described as a superposition of eigenstates of H_0, for example, $|00\ldots00\rangle$, $|00\ldots01\rangle$, and so on, where the state $|\ldots 0_k \ldots\rangle$ corresponds to the direction of the kth nuclear spin along the direction of the magnetic field (spin up), and the state $|\ldots 1_k \ldots\rangle$ corresponds to the spin being in the opposite direction (spin down). The wave function, Ψ, of the spin chain can be written in the interaction representation as a linear combination of the individual states, $\Psi(t) = \sum_p C_p(t)|p\rangle \exp(-iE_p t)$, where E_p is the energy of the state $|p\rangle$. The contribution of each quantum state to the wave function, $\Psi(t)$, is given by the coefficient $C_p(t)$. The quantity $|C_p(t)|^2$ is the probability of finding the spin chain in the state $|p\rangle$ at time t.

The Schrödinger equation for the coefficients $C_p(t)$ has the form (we put $\varphi_n = 0$), $i\dot{C}_p(t) = \sum_{m=0}^{2^L-1} V_{pm}^n \exp[i(E_p - E_m)t + ir_{pm}\nu_n t]C_m(t)$, where $r_{pm} = \mp 1$ for $E_p > E_m$ and $E_p < E_m$, respectively. $V_{pm}^n = -\Omega_n/2$ for the states $|p\rangle$ and $|m\rangle$ connected by a single-spin transition. $V_{pm}^n = 0$ for all other states.

II. THE APPROXIMATE SOLUTION

The Schrödinger equation can be numerically integrated only for a spin chain with small enough number of spins since the number of states increases exponentially with L. The problem can be simplified when the Rabi frequency, Ω_n, is much less than the difference, $\delta\omega$, between the NMR frequencies of the neighboring spins, $\Omega_n \ll \delta\omega$. Suppose that a pulse is resonant with the kth spin in the chain, $\nu_n \approx \omega_k$. Then one can admit that this pulse affects in some approximation only the kth spin in the chain and does not interact with other spins. In this case, only

the term with the energy $E_{m'} \approx E_p + \nu_n$ effectively contributes to the right-hand side of the Schrödinger equation, so that the states $|m'\rangle$ and $|p\rangle$ are connected by a single-spin flip of the kth spin. In this case, we reduce the Schrödinger equation to the set of two differential equations,

$$i\dot{C}_m(t) = -\frac{\Omega_n}{2}\exp[i(E_p - E_m - \nu_n t]C_m(t),$$

$$i\dot{C}_p(t) = -\frac{\Omega_n}{2}\exp[-i(E_p - E_m - \nu_n t]C_p(t), \qquad (2)$$

where $E_p > E_m$, and $|p\rangle$ and $|m\rangle$ are two stationary states which are connected by a single-spin transition of the kth spin, $\nu_n \approx \omega_k$.

The solution of Eq. (2), for initial conditions, $C_m(t_{n-1}) = 1$, $C_p(t_{n-1}) = 0$, after the action of the nth pulse has the form,

$$C_m(t_n) = \left[\cos(\lambda_n\tau_n/2) + i\frac{\Delta_n}{\lambda_n}\sin(\lambda_n\tau_n/2)\right] e^{\left(\frac{-i\tau_n\Delta_n}{2}\right)},$$

$$C_p(t_n) = i\frac{\Omega_n}{\lambda_n}\sin(\lambda_n\tau_n/2)\, e^{\left(it_{n-1}\Delta_n + i\frac{\tau_n\Delta_n}{2}\right)}, \qquad (3)$$

where t_{n-1} and t_n are the beginning and the and of the nth pulse, τ_n is the duration of the nth pulse, $\Delta_n = E_p - E_m - \nu_n$ (we do not indicate the dependence of Δ_n on the indices p and m), $\lambda_n = \sqrt{\Omega_n^2 + \Delta_n^2}$ is the precession frequency in the frame rotating with the frequency ν_n. Suppose that at t_{n-1} the system was in the state $|m\rangle$. In the case of the exact resonance ($\Delta_n = 0$) and for $\Omega_n\tau_n = \pi$ (a π pulse) Eqs. (3) describe the resonant transition from the state $|m\rangle$ to the state $|p\rangle$. If the frequency of the next pulse also satisfies the resonance condition, $\Delta_{n+1} = E_l - E_p - \nu_{n+1} = 0$, then the system with probability equal to unity will transform to the state $|l\rangle$, and so on.

III. ERRORS IN CREATION OF ENTANGLED STATE FOR REMOTE QUBITS

The advantages given by the two-level approximation described above are obvious: (a) we solve the problem by using the discrete map (3) instead of integrating differential equations; (b) we can consider only the states with large enough probabilities and neglect all other states in a controlled way; (c) we can estimate errors caused by non-resonant effects and minimize them by choosing optimal parameters.

In this paper we will estimate the error in implementation of a unitary operation for remote qubits (which is a particular case of the well-known Control-Not (CN) gate) using a sequence of π-pulses. This CN gate is defined as the unitary operator, U, with the following properties:

$$U|0_{L-1}0_{L-2}\ldots 0_1 0_0\rangle = e^{i\varphi_1}|0_{L-1}0_{L-2}\ldots 0_1 0_0\rangle, \quad (4a)$$

$$U|1_{L-1}0_{L-2}\ldots 0_1 0_0\rangle = e^{i\varphi_2}|1_{L-1}0_{L-2}\ldots 0_1 1_0\rangle, \quad (4b)$$

where φ_1 and φ_2 are known phases. The target qubit (0) should change its state only when the control qubit $(L-1)$ is in the state $|1\rangle$. The operator, U, can be used to create an entangled state for remote qubits: $U(\alpha|0_{L-1}...0_0\rangle + \beta|1_{L-1}...0_0\rangle) = \alpha e^{\varphi_1}|0_{L-1}...0_0\rangle + \beta e^{\varphi_2}|1_{L-1}...1_0\rangle$. To accomplish the (4b) operation in the system described by the Hamiltonian (1), we choose a sequence of π-pulses with resonant frequencies (for which all $\Delta_n = 0$). In this case, the state $|10\ldots00\rangle$ transforms to the state $|10\ldots01\rangle$, with probability equal to unity, by the following scheme: $|1000\ldots0\rangle \to |1100\ldots0\rangle \to |1110\ldots0\rangle \to |1010\ldots0\rangle \to |1011\ldots0\rangle \to |1001\ldots0\rangle \to \ldots \to |100\ldots11\rangle \to |100\ldots01\rangle$. The sequence of pulses which realizes this protocol has the following form: $\nu_1 = \omega_{2L-2}$, $\nu_2 = \omega_{2L-3}$, $\nu_3 = \omega_{2L-2} - 2J$, $\nu_{2L-4} = \omega_6$, $\ldots$, $\nu_{2L-4} = \omega_0 - J$, $\nu_{2L-3} = \omega_1$. If we apply the same protocol to the state $|00\ldots00\rangle$, then with some probability the system will remain in this state because all transitions are non-resonant with the detuning $\Delta_n = \pm J, \pm 2J$. Since $\Delta_n \neq 0$ these non-resonant transitions have the probabilities (see Eq. (3)),

$$\varepsilon_n = (\Omega_n/\lambda_n)^2 \sin^2(\lambda_n\tau_n/2). \qquad (5)$$

In this paper we study the errors generated during the operation (4a) under the condition that the transitions in Eq. (4b) are resonant. The operator U in Eqs. (4a) and (4b) can be written as a product, $U = U_{2L-3}U_{2L-4}\ldots U_2U_1$, of operators of individual pulses U_n, where $n = 1, , 2, \ldots, 2L-3$. We take the Rabi frequency to be the same, $\Omega_n = \Omega$, for all pulses. Then the error, ε_n, generated by the nth pulse is defined only by the detuning, Δ_n. The values of detuning, $|\Delta_n|$, are the same for all pulses, $|\Delta_n| = J$, except for the third pulse, where $|\Delta_3| = 2J$. We denote $\varepsilon_n \equiv \varepsilon$ for $n \neq 3$ and $\varepsilon_{n=3} \equiv \varepsilon'$.

Each unwanted state generated by the nth pulse can produce other unwanted states under the action of the other $(n+m)$ pulses. This causes the generation of a hierarchy of different states. Instead of one ground state, which should be the result of (4a), we generate a series of different unwanted states.

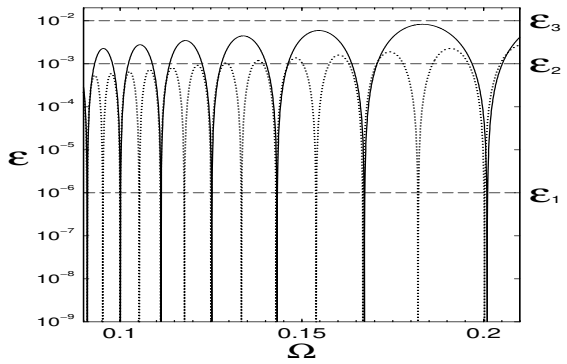

FIG. 1. Dependence of ε (solid line) and ε' (dotted line) on Ω. $J = 1$.

Since the dynamics is generated by the discrete map (3), probability of error can be estimated analytically. Suppose that we can measure only the states with prob-

ability $P \geq P_0$, where P_0 can be defined by the experimental conditions. Then, if $\varepsilon, \varepsilon' < \varepsilon_1 = P_0$, we shall not find in the system any unwanted states and the CN gate is realized with probability equal to unity. In Fig. 1, we plot ε (solid line) and ε' (dotted line) as functions of Ω. We suppose that $\varepsilon_1 = P_0 = 10^{-6}$. One can see from Fig. 1 that $\varepsilon(\Omega)$ and $\varepsilon'(\Omega)$ are less than ε_1 only in very narrow regions of the values of Ω (in the vicinity of $\Omega_k = |\Delta_n|/\sqrt{4k^2-1}$, $k = 1, 2, ...$[4,5]). Hence, high precision is required to implement the CN gate, (4a), (4b), without error.

Let us consider now in detail the case of arbitrary ε: $0 \leq \varepsilon \leq 1$, and explain how the errors can be estimated analytically in the operation (4a). The first pulse U_1 generates one unwanted state $U_1|0000\ldots0\rangle \to |0100\ldots0\rangle$ with the probability ε. The probability to remain in the ground state is $1-\varepsilon$. The second pulse, U_2, generates an additional unwanted state from the ground state, $U_2|0000\ldots0\rangle \to |0010\ldots0\rangle$, with probability $\varepsilon(1-\varepsilon)$, and transforms the state $|0100\ldots0\rangle$ to the state $|0110\ldots0\rangle$ without generating additional states, since the second pulse is resonant to this transition. The probability of remaining in the ground state is now $(1-\varepsilon)^2$. The total number of states after the action of two pulses is three. The probabilities of all generated states after the action of the U_3 pulse are:

$$\begin{aligned} &|0000\ldots0\rangle: && (1-\varepsilon)^2(1-\varepsilon'),\\ &|0100\ldots0\rangle: && \varepsilon'(1-\varepsilon)^2,\\ &|0010\ldots0\rangle: && \varepsilon(1-\varepsilon+\varepsilon^2),\\ &|0110\ldots0\rangle: && \varepsilon(1-\varepsilon^2). \end{aligned}$$

(Note, that above expressions can be considered only as estimates because we estimated probabilities instead of complex amplitudes.) One can continue to calculate the states generated by subsequent pulses and estimate their probabilities in a similar way. However, for $\varepsilon, \varepsilon' \ll 1$, one can omit the contribution from the higher order terms in ε, and neglect the states with the probabilities less than P_0.

Suppose, that $\varepsilon' \approx \varepsilon$ and $\varepsilon_1 < \varepsilon < \varepsilon_2 \equiv \sqrt{P_0}$. In this case, each pulse generates only one unwanted state from the ground state. Then, only

$$N_1(L) = 2L - 3 \tag{6}$$

unwanted states will be generated with probabilities (with the accuracy up to ε^2) ε, $\varepsilon(1-\varepsilon)$, $\varepsilon(1-2\varepsilon)$, ..., $\varepsilon(1-(2L-4)\varepsilon)$. After the action of $2L-3$ pulses there are $L-1$ unwanted states of the form,

$$|011\ldots11\rangle,\ |0011\ldots11\rangle, ..., |00\ldots011\rangle,\ |00\ldots01\rangle, \tag{7}$$

with the target spin in the state $|1\rangle$, and $L-2$ unwanted states of the form,

$$|011\ldots110\rangle,\ |0011\ldots110\rangle,\ \ldots,\ |00\ldots010\rangle, \tag{8}$$

with the target spin in the state $|0\rangle$. As one can see from Eqs. (7) and (8), already in the first order of ε many states have correlated error with many qubits in excited states. The estimate of the total probability of unwanted states is

$$P_1(\mathcal{E}) = \varepsilon \sum_{n=0}^{2L-4} (1-n\varepsilon) \approx \mathcal{E}\left(1 - \frac{1}{2}\mathcal{E}\right), \tag{9}$$

where $\mathcal{E} = (2L-3)\varepsilon$.

The probability of unwanted effect of finding a target qubit in the state $|1\rangle$ while the control qubit is in the state $|0\rangle$ (i.e. the probability of the process $U|0\ldots0\rangle \to |0\ldots1\rangle$) is,

$$\mathcal{P}_1(\varepsilon) = \varepsilon + \varepsilon \sum_{n=0}^{L-3} (1-(2n+1)\varepsilon) \approx \Gamma(1-\Gamma), \tag{10}$$

where $\Gamma = (L-2)\varepsilon$.

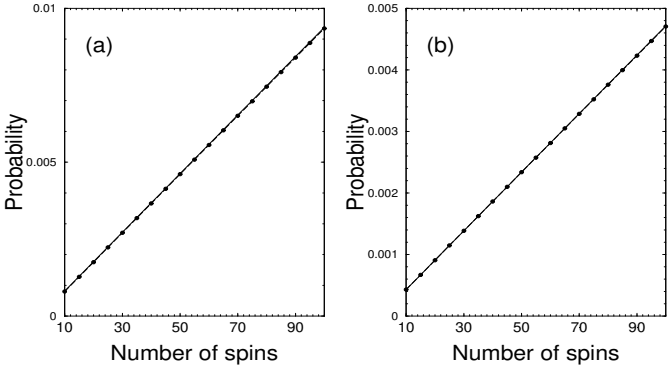

FIG. 2. (a): The total probability, P_1, of unwanted states in the execution of the CN logic gate as a function of the number of qubits, L, in the spin chain. Solid line: analytical estimate (9), filled circles connected by dashed line: numerical results. (b) Probability, $\mathcal{P}_1$, of observing the target spin in the state $|1\rangle$, while the control qubit is in the state $|0\rangle$, after the CN operation; solid line: analytical estimate (10), filled circles connected by dashed line: numerical results. $J = 1$, $\Omega = 0.0906$.

In Figs. 2 (a), (b) we plot the probabilities, P_1 and $\mathcal{P}_1$, as functions of the number of spins, L, in the chain, for $\Omega = 0.0906$, so that $\varepsilon_1 < \varepsilon(\Omega) = 4.78 \times 10^{-5} < \varepsilon_2 = 10^{-3}$ ($\varepsilon'(\Omega) = 3.23 \times 10^{-5}$). The number of unwanted states in our calculations was exactly equal to N_1 in Eq. (6). From Figs. 2 (a) and (b) one can see that the analytical estimates agree with the results of numerical calculations.

In a similar way one can calculate the probabilities of unwanted states for the case $\varepsilon_2 < \varepsilon < \varepsilon_3 \equiv (P_0)^{1/3}$. In this situation one should take into account states with the probabilities up to ε^2. Each of these states is generated as a result of two successive non-resonant processes. However, since the ground state generates only unwanted states with the probabilities of order ε, the total probability of unwanted states will be given again by Eq. (9). But the number of generated states increases and at the condition, $\varepsilon_2 < \varepsilon < \varepsilon_3$, it is proportional to L^2.

In Fig. 3 we compare the numerical results with the analytical estimates for the total probability of unwanted

states given by Eq. (9) when the value ε is relatively large. From Fig. 3 one can see that formula (9) correctly describes the behavior of the system for large value of ε. When L becomes large enough, one should also include into consideration in Eq. (9) the terms of order $(L\varepsilon)^3$.

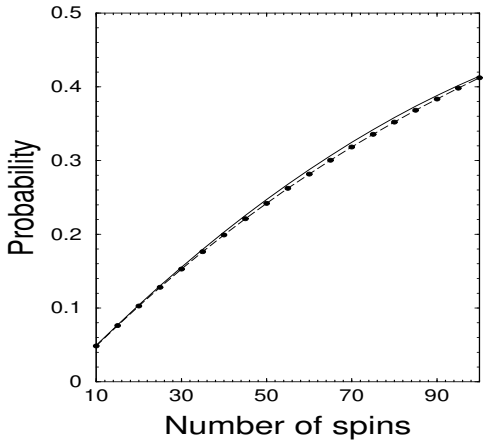

FIG. 3. The total probability of unwanted states for the case of relatively large ε, when $\varepsilon_1 < \varepsilon < \varepsilon_2$. Solid line: analytical estimate (9), filled circles connected by dashed line: numerical results. $J = 1$, $\Omega = 0.20844$, $\varepsilon(\Omega) = 2.98 \times 10^{-3}$, $\varepsilon'(\Omega) = 2.41 \times 10^{-3}$.

The probabilities of unwanted states are shown in Figs. 4 (a) and (b) in two different scales. Two types of states are clearly seen. The states in Fig. 4 (a) are generated as a result of one non-resonant transition, so the probabilities of these states are proportional to ε. On the other hand, the states in Fig. 4 (b) are generated by two successive non-resonant transitions, and they have the probabilities of the order ε^2.

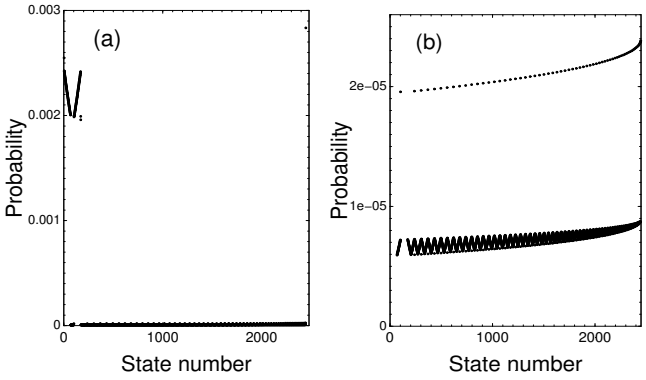

FIG. 4. The probabilities of generated states in two different scales. $L = 70$. All other parameters are the same as in Fig. 3.

IV. CONCLUSION

We have demonstrated how one can simulate a simple logic operation for a large number of qubits. We analyzed the probability of correlated errors in the implementation of a CN gate between remote qubits in a spin chain with a large number of qubits. In the limit when the Rabi frequency Ω is much less than the difference between the NMR frequencies of neighboring spins, it is shown that the probability of error, P, is mainly defined by the small parameter ε defined by (5) and by the number of qubits in the spin chain. It is demonstrated that at definite values of Ω the value of ε is small and there is no correlated error in the implementation of the CN gate. The total probability of unwanted states at other values of ε is estimated analytically and computed numerically.

Since the Hamiltonian of the system only allows transitions between the states connected by a single spin transformation, and because the electromagnetic field interacts resonantly only with one spin in the spin chain, the probability of error cannot accumulate in a definite single unwanted state. The probability of each unwanted state is always less than the value of the small parameter of the problem $\varepsilon(\Omega)$. The considered approach can be useful for experimental testing of scalable solid-state quantum computers.

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