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NMR simulation of an eight-state quantum system

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The propagation of excitation along a one-dimensional chain of atoms is simulated by means of nuclear magnetic resonance (NMR). The physical system used as an analog quantum computer is a nucleus of ^{133}Cs (spin 7/2) in a liquid-crystalline matrix. First, a pseudopure state of the spin system is prepared. Then, the Hamiltonian of migration is simulated by using a special seven-frequency pulse. The dynamics is monitored by following the transfer of population from one of the eight spin energy levels to the others.

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I. INTRODUCTION

In 1981 Feynman conceived the concept of the quantum computer because classical computers were not efficient in simulating quantum physics [1]. The reason for the inefficiency is the large dimensionality of the Hilbert spaces in even simple quantum systems. For example, accurate simulation of the dynamics of only a dozen coupled spins with $I=\frac{1}{2}$ is beyond the reach of modern computers. Thus, simulation of quantum objects was the first and natural goal that inspired attempts by researchers to build quantum computers. After the discovery of quantum algorithms [2–4], which are more efficient than classical algorithms, an intense search began for systems that can perform as universal quantum computers. At present, systems of interacting nuclear spins are among the best candidates because (1) they can have long relaxation and decoherence times; (2) they can be manipulated in desired ways; and (3) the spin degrees of freedom are well isolated from other degrees of freedom (lattice). The idea of using pseudopure (effective pure) states instead of pure quantum states [5,6] opened the possibility of using liquid-state NMR for ensemble quantum computing. Since then, a large number of works has been published, where various aspects of quantum computing have been realized by means of NMR (see [7] for a recent review).

While the possibility of building universal quantum computers of practical importance is still in dispute, the task of creating specialized or analog quantum computers seems eminently more feasible. An obvious reason for such optimism is that any quantum system simulates itself. At the same time, we consider that the goal of quantum simulations is not to copy any existing physical system, but rather to reproduce the behavior of idealized model systems with well-defined Hamiltonians. The Hamiltonian of the physical system used for simulation should be as close as possible to that of the model, and flexibility in altering the parameters of the Hamiltonian is desirable. Again, nuclear spins are good candidates for the actual implementation of quantum computing capability, and modern NMR spectrometers give the possibility of necessary manipulations with a high degree of coherent control. The first results of quantum simulations using NMR have been presented recently [8,9]. The two simulated model systems were a four-level truncated oscillator [8] and a three-spin effective Hamiltonian [9]. Here we present the results of the simulation of quantum dynamics in a more realistic physical model that describes the migration of excitation along a linear chain of atoms. While previous NMR quantum simulations studied the dynamics of other spin systems [8,9], the work described here reproduces the motion of a quantum particle in real space by studying the evolution in the spin space of a single nucleus. For reference, an excellent analysis of the use of one-dimensional chains with excitations to model real physical systems was presented in a monograph [10].

II. SIMULATED MODEL SYSTEM

We will consider a model system with the Hamiltonian

$$\mathcal{H}=\lambda\sum_{n=0}^{6}(a_n^\dagger a_{n+1}+a_n a_{n+1}^\dagger), \tag{1}$$

where a_n and $a_n^\dagger$ are the annihilation and creation operators, respectively, for the nth site, and λ is the interaction constant. This Hamiltonian describes the migration of excitation or particle of any physical nature in an eight-site linear chain. The total number of particles is conserved. Since we will model the motion of a single particle, the necessary Hilbert space is reduced to eight dimensions and the Hamiltonian can be written as

$$\mathcal{H}=\lambda\begin{pmatrix}0&1&0&0&0&0&0&0\\1&0&1&0&0&0&0&0\\0&1&0&1&0&0&0&0\\0&0&1&0&1&0&0&0\\0&0&0&1&0&1&0&0\\0&0&0&0&1&0&1&0\\0&0&0&0&0&1&0&1\\0&0&0&0&0&0&1&0\end{pmatrix}. \tag{2}$$

In what follows, we will use a dimensionless time scale by setting $\lambda=1$. The quantum state $|n\rangle$, $0\leqslant n\leqslant 7$, corresponds to an excitation localized at the nth atom. The population of a particular state gives the probability of finding the excitation at this location. The initial condition $\rho(0)=|0\rangle\langle 0|$ corresponds to excitation initially localized at one end of the chain.

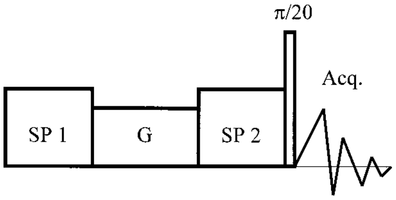

FIG. 1. The scheme of the NMR experiment. SP 1 is a shaped pulse for preparing the pseudopure ground state, G is a field gradient pulse, SP 2 is a shaped pulse for the evolution period, and $\pi/20$ is the reading pulse.

III. PHYSICAL SYSTEM

A multiqubit NMR system can consist of either several coupled spin $\frac{1}{2}$ nuclei or a single quadrupole nucleus. The latter is a multilevel spin system and can be described by the "virtual spin" formalism [11]. Experimentally, we have shown that ^{23}Na ($I=\frac{3}{2}$) in a lyotropic liquid crystal forms a two-qubit system [12]; more recently, the implementation of a complete set of two-qubit logic gates has been demonstrated for a similar system (^{7}Li in a liquid-crystalline medium [13]). Similarly, the ^{133}Cs nucleus ($I=\frac{7}{2}$, 100% natural abundance) in an anisotropic environment is a very convenient eight-level (three-qubit) system [14]. In this work, we used a 54% solution of cesium pentadecafluorooctanoate in D_2O at 48 °C. The presence of considerable residual quadrupole splitting (with a separation of 6.0 kHz between neighboring peaks in the equilibrium NMR spectrum) makes this system suitable for manipulations with selective pulses.

Instead of creating the pure initial state $\rho(0)=|0\rangle\langle 0|$, it is sufficient to prepare a pseudopure state [5,6] with only the deviation part of the density matrix having the desired form. A very efficient way to prepare such a pseudopure state for the ^{133}Cs nucleus is to simultaneously irradiate six upper single-quantum transitions so that the corresponding transition matrix elements (including the spin matrix elements) are about 0.7, 0.9, 1, 1, 0.9, and 0.7, respectively [14]. Under such irradiation, the populations of the seven upper levels begin to change from their equilibrium distributions and simultaneously cross at some point, while the population of the ground state remains unchanged. This point of crossing determines the duration of the radio-frequency (rf) pulse. The off-diagonal matrix elements can then be averaged, using either pulsed magnetic field gradients [6,12] or temporal averaging [15]. It was convenient to use both methods in our experiments.

In the interaction representation, the Hamiltonian of interaction with the rf magnetic field will have the form (2) if the system is simultaneously irradiated at all seven single-quantum transition frequencies, and if the amplitudes of the rf harmonics are inversely proportional to the corresponding spin matrix elements $\langle I,m-1|I_-|I,m\rangle = \sqrt{(I+m)(I-m+1)}$.

The scheme of the experiment is shown in Fig. 1. The first shaped pulse is the sum of six rf harmonics whose amplitudes are adjusted in the manner described above and has a duration of 600 μs. This pulse, followed by a 1-ms pulsed field gradient (5 G/cm) to average out the off-diagonal elements of the density matrix, creates the pseudopure ground state. The second shaped pulse, which is the sum of seven rf harmonics, creates the necessary Hamiltonian for the evolution period. Its length was varied from 0 to 600 μs. In each successive experiment the phase of the second shaped pulse was incremented by $\pi/2$ with respect to the phase of the final pulse (the $\pi/20$ reading pulse). The total number of transients was set to a multiple of 4. This averaged out the contributions to the observed signal of the off-diagonal elements of the density matrix generated during the evolution period. The small-angle reading pulse is chosen to satisfy the linear-response condition and to give accurate differences of populations for neighboring pairs of states.

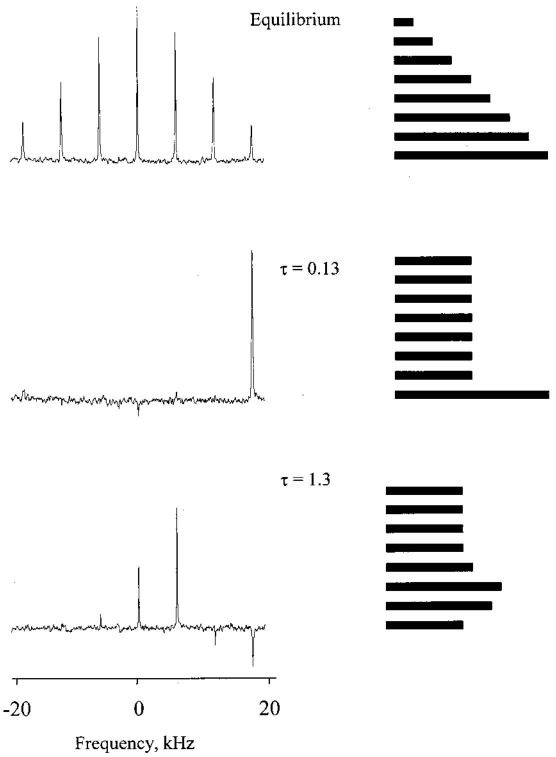

FIG. 2. ^{133}Cs NMR equilibrium spectrum (top) and the spectra corresponding to two different evolution times. The bars on the right show excessive populations of the levels.

IV. RESULTS AND DISCUSSION

The equilibrium ^{133}Cs NMR spectrum is shown in the top of Fig. 2. Bars on the right schematically represent the excess populations of the levels. At equilibrium, all the differences of populations are equal and the intensities of the peaks are proportional to squares of the spin matrix elements, which are 7:12:15:16:15:12:7. Because of relaxation and exchange effects, the linewidths of the seven peaks are different, ranging from 10 Hz for the central peak to 130 Hz for the outermost peaks. These differences are reduced in the displayed spectra by using a 100-Hz broadening factor for the Fourier transform. The spectrum in the middle of Fig. 2 shows the spectrum of the initial pseudopure ground state after an evolution time $\tau=0.13$, and it is still very close to the initial state. At longer evolution times the excessive population propagates, in the form of a wave packet, to other

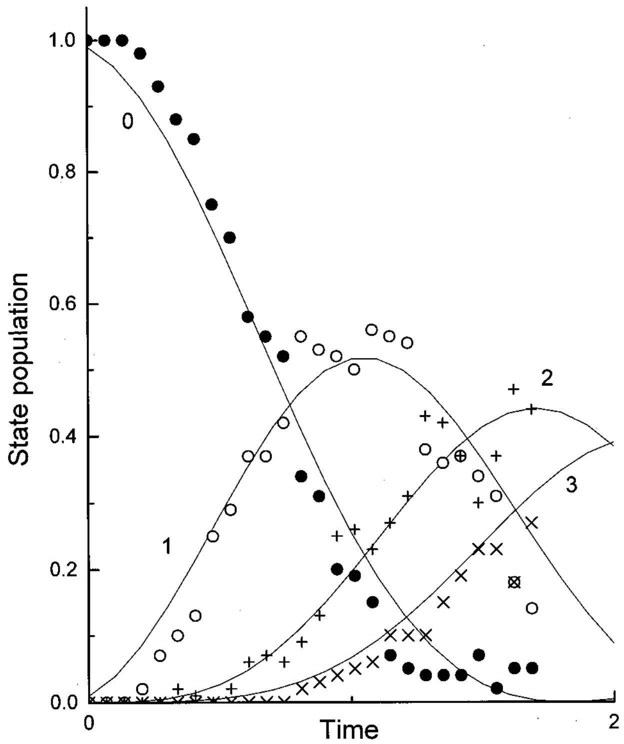

FIG. 3. Simulated populations of the four states (sites); the curves are theoretical results. "0" is the ground state, "1" is the first excited state, and so on. The axes are dimensionless, and the time scale is equal to the product of the actual evolution time and the amplitude ($\gamma B_1/2\pi$) of the rf harmonics in the shaped pulse.

states (sites). At $\tau = 1.3$, as seen in the bottom spectrum, deviations of populations for the three neighbor sites have developed.

After each evolution period the populations can be obtained by integrating the spectra (an integral for each peak is proportional to the difference in the populations of the corresponding pair of states). The results are presented in Fig. 3. The populations of only four of the states are shown. The excess populations of the other four states remain small at the time scale displayed. The dimensionless time in Fig. 3 is equal to the product of the actual evolution time and the amplitude ($\gamma B_1/2\pi$) of the rf harmonics in the shaped pulse. The duration of the evolution period is limited by the relaxation processes (T_2 for the outer peaks is less than 10 ms). In principle it is possible to increase the maximum dimensionless time by increasing the amplitudes of the rf harmonics, but this will lead to the loss of selectivity because a larger amplitude rf pulse would start to excite transitions at neighboring frequencies. The parameters used in our experiment were a compromise between the effect of relaxation and sufficient selectivity of the pulses.

To assess the validity of the results of the experiment, a theoretical calculation of the migration produced by the Hamiltonian (2) was made. Although this dynamic problem can be solved exactly even for a finite number of sites [16], it was more convenient to perform a numerical simulation for our small system. The solid curves in Fig. 3 were numerically simulated, and the data points are the experimental quantum simulation results. The comparison shows that, although the accuracy is quite moderate, our NMR system simulates the propagation of excitation in the idealized model system, up to the third neighbor along the chain, without substantial loss of quantum coherence. If rapid dephasing of the off-diagonal elements of the density matrix were to occur (large quantum decoherence), the evolution would have been reduced to jumps to neighboring sites with equal probabilities. In that case, the results would be qualitatively different from those observed in Fig. 3; for example, in such a case, the population of the initially populated site would always remain the highest. Therefore, the results presented in Fig. 3 clearly indicate that a high degree of quantum coherence is maintained during the experimental evolution time. Nevertheless, due to noticeable spin-lattice relaxation, the lifetime of quantum coherence is insufficient to simulate the longer evolution times required for the wave of excitation to reach the opposite end of the chain, reflect, and move back.

The use of a multifrequency excitation provides flexibility for changing the parameters of the Hamiltonian. For example, it is possible to create a diagonal disorder by changing the frequencies of the harmonics, or an off-diagonal disorder by changing their amplitudes. These irregular models are no longer analytically solvable. Furthermore, when a different pseudopure state (except the highest state) [12] is used as the starting point, the situation would correspond to excitation in the middle of the linear chain. Although these experiments have not yet been carried out, they are completely feasible and will be considered in further studies.

An amazing feature of the "quantum processor" used in this work is that it is not even an atomic size object, but a single nucleus, which is eight orders of magnitude smaller. Of course, there were about 3×10^{20} nuclei in the sample, but this number was used only to produce a detectable signal and avoid statistical averaging. The nontrivial dynamical problem was solved by the quantum motion of a single nucleus in external electric and magnetic fields.

The goal of quantum simulation is to build systems that will account for the quantum dynamics of theoretical models, for which the problem is too complicated for numerical simulation using classical computers. Although the model system studied here is still very simple and can be simulated by classical computers, our work is a step in the right direction and demonstrates the potential of NMR simulation in the development of quantum information processors.

ACKNOWLEDGMENT

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