

# Preparation of effective pure states $|00 \cdots 0\rangle$ on an NMR quantum computer with any number of spins

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## Abstract

A method is proposed to prepare an effective pure state corresponding to the pure state  $|0\rangle|0\rangle \cdots |0\rangle$  for any number of spins on a nuclear magnetic resonance quantum computer, where  $|0\rangle$  stands for the spin-up state of a nuclear spin. The method is based on the spatial labeling proposed by Cory *et al.*

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## 1 Introduction

Quantum computers [1] have been shown to be able to solve some problems exponentially faster than classical computers [2], which seems to have sparked enormous interest in this field of research. A quantum computer uses a set of two-state systems as quantum bits (qubits) and executes a computation by a sequence of controlled unitary transformations on them. The desired useful information (output) is extracted by measuring the resulting final state of the qubits. Of course, the task of practically realizing even a prototype quantum computer poses a daunting challenge primarily because of the decoherence of the quantum system used. Despite the difficulty, simple quantum logic gates have been tested successfully for the first time using cold trapped ions [3].

Recently several groups proposed the use of nuclear magnetic resonance (NMR) for the implementation of a quantum computer and demonstrated their usefulness [4–24]. Nuclear spin systems are rather well isolated from the environment and have longer decoherence (relaxation) times. Several

simple quantum algorithms have been implemented [11–14] by using room-temperature NMR with only a small number of qubits. NMR uses of the order of Avogadro’s number of spin systems (molecules), where the energy difference between the spin-up ( $|0\rangle$ ) and the spin-down ( $|1\rangle$ ) states is very small compared to the thermal energy except at extremely low temperatures [25]. For this reason, the ensemble of the spin systems used for an NMR quantum computer is not in a pure state but in a mixed state. However, as with any computation on modern (classical) computers, quantum computation has to start from a pure input state of the form, e.g.,  $|00\dots 0\rangle = |0\rangle|0\rangle\dots|0\rangle$ . (Exceptions are for the cases of only one qubit [26] and of the Deutsch-Jozsa problem [15].) Several methods [4–9] have been proposed to prepare states that are transformed identically (at least on NMR) to the pure states. Such states are termed “effective pure states” or “pseudopure states,” and the methods include spatial labeling [4,5], temporal labeling [6], and logical labeling [7,8]. Although a general algorithm to prepare an effective pure state has been described for the latter two methods, this does not seem to be the case with spatial labeling.

We propose here a method to prepare, by spatial labeling, an effective pure state corresponding to the pure state  $|00\dots 0\rangle$  (which will henceforth be called simply “an effective pure state  $|00\dots 0\rangle$ ”) on an NMR quantum computer with any number of qubits. Once the effective pure state  $|00\dots 0\rangle$  is prepared, it is easy, at least in principle, to produce various input states including entangled states [4–24].

## 2 Basic operations

Let us consider an ensemble of linear  $n$ -spin molecules placed in a static magnetic field along the  $z$  axis, and assume that each spin is coupled only to its neighboring spins. (Details of the system will be described in the following section.) The  $i$ th spin will be denoted as  $I^i$ . The method presented here consists essentially of the following two operations. The first is the operation that transforms the term  $I_z^i$  in the density matrix into the form  $I_z^i[\frac{1}{2}(1 + 2I_z^{i+1})]$ . Assume that we are given the density operator described as

$$\rho = I_z^i. \quad (1)$$

Application of a  $\pi/4$  pulse along the  $x$  axis of the rotating frame of reference on the  $i$ th spin, denoted as  $(\pi/4)_x(i)$ , gives

$$\rho = \frac{1}{\sqrt{2}}(I_z^i + I_y^i). \quad (2)$$

By evolving the system solely under the influence of the spin-spin coupling  $J_{i,i+1}$  between spin  $I^i$  and its nearest-neighbor spin  $I^{i+1}$  for a time period of  $t = 1/(2J_{i,i+1})$  (this operation will henceforth be denoted as  $1/2J_{i,i+1}$ ), we have

$$\rho = \frac{1}{\sqrt{2}}(I_z^i - 2I_x^i I_z^{i+1}). \quad (3)$$

Then, we apply a  $(\pi/4)_{-y}(i)$  pulse to generate

$$\rho = \frac{1}{2}[I_z^i + I_x^i - 2(I_x^i - I_z^i)I_z^{i+1}]. \quad (4)$$

If we finally apply the pulsed field gradient along the  $z$  axis  $G_z$  to annihilate all transverse magnetizations, we get the state described as

$$\rho = I_z^i \left[ \frac{1}{2}(1 + 2I_z^{i+1}) \right]. \quad (5)$$

Thus, the sequence of operations

$$\left(\frac{\pi}{4}\right)_x(i) - 1/2J_{i,i+1} - \left(\frac{\pi}{4}\right)_{-y}(i) - G_z \quad (6)$$

is equivalent to multiplying  $I_z^i$  by the bracketed factor of Eq. (5) that involves the nearest-neighbor spin  $I^{i+1}$ . The procedure represented by Eq. (6) can be applied, of course, only between spin-spin coupled (nearest) neighbors.

The second operation essential to the present method is the SWAP (or EXCHANGE) operation [27,28] which exchanges the states of the two qubits in question. The necessary condition for the SWAP operation to work is that the two spins to be swapped are spin-spin coupled, which is clear from the fact that the SWAP operation is equivalent to three consecutive controlled-NOT operations. For example, if we denote the controlled-NOT operation with spin  $I$  as the control and spin  $S$  as the target by  $\text{CNOT}(I, S)$ , then

$$\text{SWAP}(I, S) = \text{CNOT}(I, S)\text{CNOT}(S, I)\text{CNOT}(I, S). \quad (7)$$

The essential ingredient of  $\text{CNOT}(I, S)$  and  $\text{CNOT}(S, I)$  is, in turn, to evolve the spin system solely under the influence of the spin-spin coupling  $J_{IS}$ , an operation  $1/2J_{IS}$  that is similar to that denoted as  $1/2J_{i,i+1}$  in Eq. (6). An exact operator form of the SWAP operation is [29,30], apart from an irrelevant overall phase factor,

$$\text{SWAP}(I, S) = e^{i\pi I_z S_z} e^{i\pi I_y S_y} e^{i\pi I_x S_x}, \quad (8)$$

where the order of the three factors of the right-hand side is immaterial as is evident from the commutation relation

$$[I_k S_k, I_l S_l] = 0 \quad (k, l = x, y, \text{ or } z). \quad (9)$$

We note that by combining the two operations described above we can create and multiply by factors that are similar to those in Eq. (5) but contain remote spins  $I^j$ , where  $i + 1 < j \leq n$ . For example, if we wish to create the factor  $[\frac{1}{2}(1 + 2I_z^{i+2})]$  from the magnetization  $I_z^i$ , we first bring  $I_z^i$  to the position of  $I^{i+1}$  which neighbors  $I^{i+2}$  by a SWAP operation, then create the desired factor by a process similar to that of Eq. (6), and then bring back to their original positions by a second SWAP. Thus, if we have the state given by Eq. (5), we get the following:

$$\begin{aligned} \rho &= I_z^i \left[ \frac{1}{2}(1 + 2I_z^{i+1}) \right], \\ \text{SWAP}_{\rightarrow} (I^i, I^{i+1}) \rho &= I_z^{i+1} \left[ \frac{1}{2}(1 + 2I_z^i) \right], \\ \text{the sequence of Eq. (6)}_{\rightarrow} \text{ with } i \text{ increased by } 1 \\ \rho &= I_z^{i+1} \left[ \frac{1}{2}(1 + 2I_z^{i+2}) \right] \left[ \frac{1}{2}(1 + 2I_z^i) \right], \\ \text{SWAP}_{\rightarrow} (I^i, I^{i+1}) \rho &= I_z^i \left[ \frac{1}{2}(1 + 2I_z^{i+2}) \right] \left[ \frac{1}{2}(1 + 2I_z^{i+1}) \right]. \end{aligned} \quad (10)$$

Therefore, it will be convenient to incorporate the two operations into one procedure  $F(i, j)$ , which is defined as the operation to create the term  $I_z^i [\frac{1}{2}(1 + 2I_z^j)]$  from  $I_z^i$  for any spin pair of  $I^i$  and  $I^j$ . In this notation, the procedure of Eq. (6) is simply  $F(i, i + 1)$ , and the whole process in Eq. (10) is  $F(i, i + 2)$ . To execute  $F(i, j)$ , one applies the SWAP operation  $(j - i - 1)$  times, then applies the operation of Eq. (6) with  $i$  replaced by  $(j - 1)$ , and finally applies the SWAP operation  $(j - i - 1)$  times again:

$$(\text{SWAP})^{j-i-1} - [\text{Eq. (6) with } i \text{ replaced by } (j - 1)] - (\text{SWAP})^{j-i-1}. \quad (11)$$

### 3 Preparation of effective pure states

The system we have in mind is an ensemble of the order of Avogadro's number of identical  $n$ -spin molecules in a liquid state, placed in an external static

magnetic field along the  $z$  axis and at room temperature. To simplify the discussion, we assume, for now, a linear chain of spins as the spin system that comprises a quantum computer and nonzero spin-spin couplings only between nearest neighbors (no long-range spin-spin couplings). All the spins are assumed to have different chemical shifts (Larmor precession frequencies in a static magnetic field), enabling us to address each spin individually. Each spin (except the terminal ones) has to be coupled at least to two neighboring spins in the chain. Otherwise the molecule cannot function as a universal quantum computer, being unable to perform the controlled-NOT operation that is requisite to a universal quantum computer [28]. For the moment, we also assume that the system is homonuclear in order to avoid cluttering the notation. It would be understood that these assumptions are not unrealistic if the number of qubits is moderate.

In the high temperature limit, the density operator for our ensemble of the linear  $n$ -spin systems at thermal equilibrium in an external static magnetic field may be written concisely by [25]

$$\rho = \sum_{i=1}^n I_z^i, \quad (12)$$

where we omitted the proportionality constants and NMR-irrelevant, unitarily invariant constants. The density matrix in Eq. (12) corresponds to the traceless part of the density matrix of our ensemble and is sometimes termed as the deviation density matrix [7]. (All the density matrices used in this work refer to deviation density matrices.) The preparation starts by transforming the thermal equilibrium state in Eq. (12) into

$$\rho = \sum_{i=1}^n \left(\frac{1}{2}\right)^{i-1} I_z^i. \quad (13)$$

This is easily accomplished by tipping each magnetization  $I_z^i$  by an angle  $\theta_i$ , where  $\cos \theta_i = (\frac{1}{2})^{i-1}$ , and then applying a field-gradient  $G_z$ . Incidentally, in a heteronuclear case, a similar procedure will be used in realizing this type of density operator from the density operator at thermal equilibrium, which is proportional to

$$\rho = \sum_{i=1}^n \omega_0^i I_z^i, \quad (14)$$

where  $\omega_0^i$  is the resonance frequency of the  $i$ th spin [25].

Now, apply first the procedure  $F(n-1, n)$  to spin  $I^{n-1}$  of Eq. (13) to get

$$\rho = \sum_{i=1}^{n-2} \left(\frac{1}{2}\right)^{i-1} I_z^i + \left(\frac{1}{2}\right)^n [(1 + 2I_z^{n-1})(1 + 2I_z^n) - 1]. \quad (15)$$

Next apply  $F(n-2, n-1)$  to spin  $I_z^{n-2}$  to obtain

$$\begin{aligned} \rho &= \sum_{i=1}^{n-3} \left(\frac{1}{2}\right)^{i-1} I_z^i + \left(\frac{1}{2}\right)^{n-3} I_z^{n-2} \left[\frac{1}{2}(1 + 2I_z^{n-1})\right] \\ &\quad + \left(\frac{1}{2}\right)^n [(1 + 2I_z^{n-1})(1 + 2I_z^n) - 1], \end{aligned} \quad (16)$$

and then  $F(n-2, n)$  to obtain

$$\begin{aligned} \rho &= \sum_{i=1}^{n-3} \left(\frac{1}{2}\right)^{i-1} I_z^i + \left(\frac{1}{2}\right)^{n-3} I_z^{n-2} \left[\frac{1}{2}(1 + 2I_z^{n-1})\right] \left[\frac{1}{2}(1 + 2I_z^n)\right] \\ &\quad + \left(\frac{1}{2}\right)^n [(1 + 2I_z^{n-1})(1 + 2I_z^n) - 1] \\ &= \sum_{i=1}^{n-3} \left(\frac{1}{2}\right)^{i-1} I_z^i + \left(\frac{1}{2}\right)^n [(1 + 2I_z^{n-2})(1 + 2I_z^{n-1})(1 + 2I_z^n) - 1]. \end{aligned} \quad (17)$$

For the  $k$ th spin  $I_z^k$ , we apply a sequence of  $(n-k)$  procedures,  $F(k, k+1)$ ,  $F(k, k+2)$ , ...,  $F(k, n-1)$ , and  $F(k, n)$ , as follows:

$$\begin{aligned} \rho &= \sum_{i=1}^{k-1} \left(\frac{1}{2}\right)^{i-1} I_z^i + \left(\frac{1}{2}\right)^{k-1} I_z^k \\ &\quad + \left(\frac{1}{2}\right)^n [(1 + 2I_z^{k+1})(1 + 2I_z^{k+2}) \cdots (1 + 2I_z^n) - 1], \\ &\quad \xrightarrow{F(k, k+1)} \quad \xrightarrow{F(k, k+2)} \quad \cdots \quad \xrightarrow{F(k, n)} \\ \rho &= \sum_{i=1}^{k-1} \left(\frac{1}{2}\right)^{i-1} I_z^i \\ &\quad + \left(\frac{1}{2}\right)^{k-1} I_z^k \left[\frac{1}{2}(1 + 2I_z^{k+1})\right] \left[\frac{1}{2}(1 + 2I_z^{k+2})\right] \cdots \left[\frac{1}{2}(1 + 2I_z^n)\right] \\ &\quad + \left(\frac{1}{2}\right)^n [(1 + 2I_z^{k+1})(1 + 2I_z^{k+2}) \cdots (1 + 2I_z^n) - 1] \\ &= \sum_{i=1}^{k-1} \left(\frac{1}{2}\right)^{i-1} I_z^i \\ &\quad + \left(\frac{1}{2}\right)^n [(1 + 2I_z^k)(1 + 2I_z^{k+1}) \cdots (1 + 2I_z^n) - 1]. \end{aligned} \quad (18)$$

Application of similar procedures will finally yield

$$\rho = \left(\frac{1}{2}\right)^n \left[ \prod_{i=1}^n (1 + 2I_z^i) - 1 \right], \quad (19)$$

which is exactly the target state we want to prepare, i.e., the effective pure state  $|00 \cdots 0\rangle$  expressed in the deviation density matrix.

#### 4 Discussion

Although we do not claim the present method to be optimal for preparing an effective pure state  $|00 \cdots 0\rangle$ , it should be worthwhile to estimate how difficult it is to carry it out. A difficulty is concerned with the preparation of the state given by Eq. (13) from the state in Eq. (12). We have to apply radiofrequency pulses for all spins, the pulse angle for the  $i$ th spin being  $\theta_i$ . As the number of qubits  $n$  increases, the value of the factor  $\cos \theta_i = \left(\frac{1}{2}\right)^{i-1}$  approaches zero and  $\theta_i$  approaches  $90^\circ$ . For example, even for  $i = 6, 7,$  and  $8$ , the necessary pulse angles are  $\theta_6 = 88.21^\circ$ ,  $\theta_7 = 89.10^\circ$ , and  $\theta_8 = 89.55^\circ$ . Thus, it gets more and more difficult to prepare these factors exactly by radiofrequency pulses.

Another difficulty concerns the problem of decoherence. The time needed to obtain the effective pure state  $|00 \cdots 0\rangle$  by the present method may be estimated roughly in terms of the number of necessary operations. The preparative procedure leading to Eq. (13) from Eq. (12) needs  $n$  pulses. The operation of Eq. (6) works between nearest neighbors and requires about nine pulses. (This operation also works for spin pairs with  $J$  couplings.) For distant spin pairs with no direct  $J$  coupling, we have to operate  $F(i, j)$  repeatedly. As noted above, for the  $k$ th spin we have to apply the  $F(k, j)$  procedure  $(n - k)$  times ( $j = k + 1, k + 2, \dots, n$ ). The number of necessary SWAP operations increases quadratically as the number of intervening chemical bonds between the spins in question and the terminal  $n$ th spin. A (simplified) SWAP operation as proposed by Mádi *et al.* [24], which exchanges only the  $z$  component of the two magnetizations in question, needs 12 pulses. In this way, one may estimate that the total number of operations needed to prepare the state of Eq. (19) grows roughly as  $O(n^3)$ . Fortunately an improvement is possible if we note that it is not necessary to swap back [as in Eq. (10)] at all. Elimination of all swap-back operations reduces the total number to the order  $O(n^2)$ .

More importantly, we have to consider the fact that the operation  $1/2J_{ij}$  requires a time period of free precession of length  $t = 1/(2J_{ij})$ , and each (simplified) SWAP operation involves two  $1/2J_{ij}$  operations [24], where  $J_{ij}$  is the coupling constant between the spin pairs  $I^i$  and  $I^j$  in question. The necessary number of SWAP operations increases (approximately) as  $\frac{1}{2}n^2$  with the number of qubits  $n$ , and that of  $1/2J_{ij}$  operations also increases as  $\frac{1}{2}n^2$ . Thus a total time needed is  $\frac{3}{2}n^2$  times  $t = 1/(2J_{ij})$ . Assuming that all the

$J$  values are 20 Hz, we estimate the contribution from the SWAP and  $1/2J_{ij}$  operations to be around 0.6 s and 0.9 s even for  $n = 5$  and 6, respectively. Note that we did not take into account the time necessary for applying selective (soft) pulses. The pulse duration time for a selective pulse, rather than a nonselective (hard) pulse, is typically of the order of 1 ms for, e.g.,  $^1\text{H}$  and  $^{13}\text{C}$ , which is far from negligible when accumulated. Note also that these estimates refer only to the preparation of input state and do not include an actual quantum computation at all.

According to some (optimistic) estimation [31], an NMR quantum computer with about 30 qubits might exceed the power of modern supercomputers. In this context, we recall that Warren [32] pointed out previously that if we resort to effective pure states for quantum computation, the output (strength of NMR signals) scales as  $(\frac{1}{2})^n$ . The present estimate reiterates another challenge, the notorious problem of decoherence, unless we have a purpose-built spin system (computer molecule) for which the decoherence time is long.

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