Initialization Algorithm of NMR Quantum Computers

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In NMR quantum computers, nuclear spins in a molecule are used as qubit. Since the sensitivity of NMR is so low that we cannot observe a single nuclear spin but we need 10^{14} or more molecules. Spins are initially in the thermal equilibrium state. Unless the temperature is 0 K, each spin is in mixed state . At room temperature, the population difference is merely about 10^{-5} and the state is almost maximally mixed. Even at low temperature the state is still highly mixed. Anyway, we must extract the signal from qubits initially in $|0\rangle^{\otimes n}$.

Exhaustive averaging [1] is known to work for this purpose, but it requires 2^n experiments and the advantage of quantum computation is lost.

Recently new initialization based on typical states is proposed [2]. Although this method is demonstrated by making pseudo typical states [3], the efficient algorithm for initialization has not been shown. In this paper, we discuss efficient initialization algorithm of NMR quantum computers.

We consider n-qubit system in which each qubit is in $|0\rangle$ with probability p_0 and in $|1\rangle$ with $p_1 = 1 - p_0$. The population of $|0\rangle^{\otimes n}$ becomes exponentially small with n. But the population of the typical ensemble $\mathcal{A}$ in which the number of $|0\rangle$'s is np_0 and that of $|1\rangle$'s is np_1 is $\binom{n}{np_0} p_0^{np_0} p_1^{np_1} \sim 1$. Since the number of elements of $\mathcal{A}$ is $\binom{n}{np_0} \sim 2^{nH}$, we can express the states in $\mathcal{A}$ with only nH qubits, where $H = -p_0 \log p_0 - p_1 \log p_1$ is the entropy. Therefore we can make remaining $n(1-H)$ qubits set to the same state, $|0\rangle^{\otimes n(1-H)}$.

Such a process can be regarded as Schumacher compression, and the polynomial time algorithm is already known [4]. The algorithm can be performed with inequality judgings and additions. The required time is $O(n^3)$ while $n + \lceil \log n \rceil$ clean ancillary qubits are needed. However, restriction specific to initialization is that the number of ancillary qubits must be less than or equal to log[poly(n)]. The known algorithm [4] does not satisfy it. The in-place algorithm based on the different principle has been proposed, which claims $O(n \log n)$ steps but allows some errors [5]. Efficient in-place algorithm without error has not been known.

In Ref. [4], n ancillary qubits are used for addition. But, addition can be executed without ancillary qubits by using quantum Fourier transform (QFT) [6].

QFT of $|a\rangle$ and $|a+b\rangle$ are expressed as $|\phi(a)\rangle$ and $|\phi(a+b)\rangle$ respectively. Then $|\phi(a)\rangle$ can be transformed into $|\phi(a+b)\rangle$ by phase shifts without ancillary qubits.

This addition requires $O(n^2)$ steps; $O(n^2)$ for QFT's and $O(n)$ for phase shifts.

Next, we consider inequality judging. When a number b is subtracted from a,

$$|0\rangle|b\rangle \xrightarrow{-a} \begin{cases} |0\rangle|b-a\rangle & (b \geq a) \\ |2^{n+1} - (a-b)\rangle = |1\rangle|x\rangle & (b < a) \end{cases} \tag{1}$$

that is, if $b < a$, the most significant qubit is changed from $|0\rangle$ to $|1\rangle$, else unchanged. We can use the most significant qubit for inequality judging. Therefore inequality judging is performed with an ancillary qubit and $O(n^2)$ steps (for addition).

In Ref. [4], both addition and inequality judging are performed with $O(n)$ operations and $O(n)$ ancillary qubits. But here they are carried out with $O(n^2)$ operations with no or one ancillary qubit. Therefore we can perform Schumacher compression with $O(n^4)$ steps and $\lceil \log n \rceil$ ancillary qubits. It satisfies conditions required for initialization algorithm.

In Fig. 1, we show an example of circuit in the case of $n = 4$, $p_1 = 1/4$. In this case, typical states are $|0001\rangle$, $|0010\rangle$, $|0100\rangle$, $|1000\rangle$. They are compressed into $|0000\rangle$, $|0001\rangle$, $|0010\rangle$, $|0011\rangle$ with one ancillary qubit. Also the simulation result of the circuit in Fig. 1 is shown in Fig. 2

By initialization, thermal equilibrium state is transformed into

$$\begin{aligned} \rho' =& Q(0) \underbrace{|0\rangle\langle 0|}_{\text{ancilla}} \otimes \Bigg(\sum_x 2^{-nH(p_0)} \underbrace{|0\rangle\langle 0|}_{n[1-H]} \otimes |x\rangle\langle x| \\ &+ \sum_{y \notin \mathcal{A}} P(y) S |y\rangle\langle y| S^\dagger \Bigg) + \sum_{j \neq 0} Q(j) \underbrace{|j\rangle\langle j|}_{\text{ancilla}} \otimes \rho_j \end{aligned} \tag{2}$$

where $Q(x)$ is probability which ancillary qubit's state is $|x\rangle$. Therefore in the block where ancillary qubits is $|0\rangle$, $n[1-H]$ qubits are initialized. This is the similar situation as effective pure state by logical labeling [7]. Consequently, the signal from a particular block can be extracted

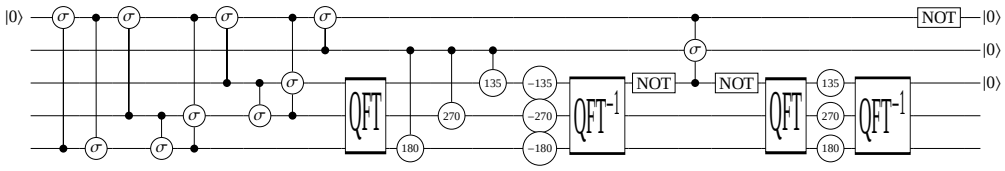

Figure 1: Example of circuit in the case of $n = 4$, $p_1 = 1/4$. The most significant qubit is an ancillary qubit initialized to $|0\rangle$.

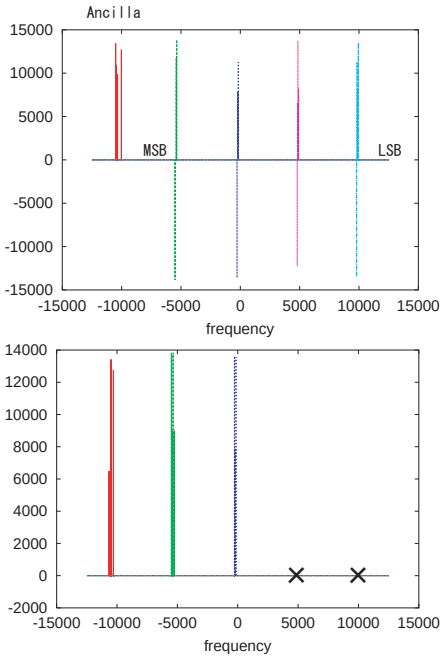

Figure 2: The simulation result of circuit in Fig. 1. top: the spectra of typical states (most left qubit is ancillary qubit initialized to $|0\rangle$). bottom: the spectra after compression. The last two qubits are with no signal because they are completely random and next two qubits are initialized to $|00\rangle$.

in at most n experiments by the method similar to Ref. [8]. Accordingly, total cost is $O(n^5)$ and $\lceil \log n \rceil$ uninitialized ancillary qubits.

In conclusion we have developed the efficient initialization algorithm for NMR quantum computation. We show that the cost required by this algorithm is $O(n^5)$ steps and $\lceil \log n \rceil$ ancillary qubits. That does not require exponential cost. Therefor, true quantum computation becomes possible in NMR quantum computer.

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