Efficient Initialization Scheme for Real Quantum Computation using NMR

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Introduction

Bulk-ensemble NMR quantum computation was enabled by ingenious initialization schemes which make effective pure state[GC97, CFH97] out of the thermal equilibrium state near the maximum entropy. It has been so far most successful in demonstrating quantum algorithms[VSB+01]. However, the states used in NMR experiments are separable and therefore contain no entanglement[BCJ+99] and furthermore exponentially huge physical resources such as the numbers of molecules[LP01] or experiments are used. In this Paper, we present the initialization scheme which may achieve the real quantum computation.

The simplest answer to this problem would be cooling all the spins down to T=0K. Then the states of all quantum computers would be initialized to $|0\rangle^{\otimes n}$. However it is not that simple. If the material is simply cooled, it is frozen to the solid in which the dipolar interactions make the computational basis including $|0\rangle^{\otimes n}$ non-stationary. It might be avoided by decoupling dipolar interactions by applying special pulse sequences although it would be too tedious and busy.

We are seeking alternative possibility of cooling spins without actually freezing materials[ITS+00, TTT01]. The spin temperature might be cooled down to mK but never to 0K. Therefore we still need some scheme to extract the pure state (zero entropy) signal out of the low temperature mixed states (low entropy). That is the main topics of the Paper.

Conventional Effective Pure State

The exhaustive averaging[KCL98] which requires 2^n-1 experiments is out of question from the computational complexity viewpoint and will never be used for the real quantum computation. By real quantum computation, we mean the exponential speed-up over classical computation without requiring exponentially huge physical resources other than the size of Hilbert space itself.

The logical labeling[GC97] also suffers from the exponentially small signal and in turn requires exponentially many molecules. This is the limit of using single signal state since any state is subject to exponentially small population for increasing n at finite temperature.

Under the effective Hamiltonian of homonuclear solution NMR, the thermal equilibrium states can be well-approximated by the density operator $\rho^{\otimes n}$ with $\rho=p|0\rangle\langle 0|+q|1\rangle\langle 1|$ (*i.i.d.*) where $p=(1+\delta)/2$, $q=1-p$ and $\delta=\tanh(\hbar\omega/2k_BT)$.

The logical labeling [GC97] have been generalized to arbitrary temperature by using typical sequences $\{|0\rangle^{\otimes np}|1\rangle^{\otimes nq}\}$ as the background state only to lose available qubits $nH(p)$ by lowering the temperature[Kit01], where $H(p)=-p\log p-(1-p)\log(1-p)$ is the entropy. This is the consequence of wasting the most typical states as the signal-less background.

Typical Sequences as Multiple Signal States

The lesson of generalized logical labeling naturally leads to the conclusions; (a) we should use as many signal states as possible, (b) all signal states should give the same result, and (c) the typical states should be used as signal state rather than background[Kit01].

Each of the typical states $\mathcal{A}=\{|0\rangle^{\otimes np}|1\rangle^{\otimes nq}\}$ has the probability of $2^{-nH(p)}$ and the number of the typical states is $|\mathcal{A}|=\binom{n}{np}\approx 2^{nH(p)}/\sqrt{2\pi npq}$. If all the typical states give the same result, the signal strength is proportional to the population $P(x\in\mathcal{A})=2^{-nH(p)}|\mathcal{A}|\approx 1/\sqrt{2\pi npq}$, which scales well.

One way of doing this is the unitary Schumacher compression[Sch95] S which transforms the thermal equilibrium state into

$$\rho' = \sum_{x=0}^{|\mathcal{A}|-1} 2^{-nH(p)} \underbrace{|x\rangle\langle x|}_{nH(p)} \otimes \underbrace{|0\rangle\langle 0|}_{n[1-H(p)]} + \sum_{y\notin\mathcal{A}} P(y) S \underbrace{|y\rangle\langle y|}_{n} S^\dagger.$$

The difference in typical states are compressed into nH-qubits and the redundant $n(1-H)$ qubits are initialized to the same signal sub-state. We gain qubits by lowering the temperature and all qubits are available in the limit of T=0.

Although the scalable initialization by some kind of data compression algorithm ("*algorithmic cooling*") has been first suggested by Schulman and Vazirani[SV99], the discussion based on typical sequences may shed more light on the problem.

Demonstration of Initialization by Compression

Although we are working towards spin-cooled[TTT01] solution NMR, it is still under fundamental development and not

yet available. Also currently the number of qubits n cannot be increased to the extent where the law of large numbers or the asymptotic equipartition property (A.E.P.) come into effect. Therefore we have used the exhaustive averaging to prepare the pseudo low temperature state of n=4 and p=3/4, the equal mixture of the pseudo typical states, $|0001\rangle$, $|0010\rangle$, $|010\rangle$ and $|1000\rangle$. After application of the simple compression circuit, it has been transformed into the equal mixture of $|0000\rangle$, $|0001\rangle$, $|0010\rangle$ and $|0011\rangle$, in which the leading two qubits are successfully initialized to $|00\rangle$. However, the compression circuit is not claimed to be efficient.

Compression Circuit for Initialization

The data compression algorithm (circuit) for the initialization of NMR quantum computers is subject to the special requirements: a) no clean qubit is initially available, and, b) no state reduction by strong measurement is available, c) the total computational complexity must be polynomial(n). The first requirement makes the application of existing classical (or even quantum) compression algorithms very difficult since they use clean workspace for granted. Only after the initialization, the clean qubits are made available. This is the special requirement for initialization algorithm only. The second requirement is specific to the NMR implementation.

The third requirement of course prohibits the use of exhaustive averaging of n-qubits. However, the exhaustive averaging of log($poly$(n))-qubits which requires only $poly$(n) experiments is not prohibited. Similarly, the selective readout conditioned on the state of log($poly$(n))-qubit ancilla[Kit98] requires at most $poly$(n) experiments and therefore is allowed. In either way, log($poly$(n)) clean qubits are available within $poly$(n) overhead.

By careful application of the above observations and Draper's QFT-based in-place addition[Dra00], we have developed efficient initialization scheme which requires at most $O(n^5)$ steps and $\log n$ uninitialized ancilla qubits. It is based on the Schumacher compression circuit of Cleve and DiVincenzo[CD96] which requires $O(n^3)$ steps and $2\sqrt{n} + \log n$ clean work qubits. The details of the quantum circuit will be presented elsewhere[KK02].

Obviously the strict space saving requirement has significantly increased the steps. The other in-place initialization algorithm [SV99] claims much attractive $O(n \log n)$ steps while it is not an error-free compression nor implemented in quantum circuit. Although there might be a room for further improvements in our circuit, it is sufficient as a proof of NMR quantum computation without exponentially huge resource.

Summary

In summary, we have investigated the initialization problem of NMR quantum computers and have developed the efficient initialization scheme which enables real quantum computation using NMR.

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