Initialization, Entanglement and Scalability in Nuclear Spin Network Quantum Computers

Masahiro Kitagawa
kit@qc.ee.es.osaka-u.ac.jp
Graduate School of Engineering Science, Osaka University
Toyonaka, Osaka 560–8531 Japan
CREST, Japan Science and Technology Corporation

Abstract

Bulk-ensemble quantum computation using solution NMR is so far the most successful experimental scheme to demonstrate quantum algorithms. However the lacks of entanglement and scalability are often criticized. In this Talk, we present the initialization schemes which may restore entanglement, improve the scalability, and achieve the real quantum computation. Also we briefly introduce our research activities towards this goal.

1 Introduction

Bulk-ensemble NMR quantum computation was enabled by ingenious initialization schemes which make effective pure state[GC97] out of the thermal equilibrium state near the maximum entropy. It has been so far most successful in demonstrating quantum algorithms[VSB+00]. However, it has been criticized that the states used in NMR experiments are separable and therefore contain no entanglement[BCJ+99], and furthermore exponentially huge physical resources such as the number of molecules[LP01] or that of experiments are used. While separability itself does not immediately mean the equivalence to the classical computation as exponentially many coefficients may be involved to classically emulate NMR quantum computation[SC99], that the NMR quantum computation itself consumes exponentially huge physical resources certainly ruins the merit of quantum computation.

The simplest and the most extreme answer to this problem would be cooling all the spins down to the absolute zero $T = 0$K. Then the states of all molecular quantum computers would be initialized to $|0\rangle^{\otimes n}$, the real pure state. However it is not that simple. First of all, the absolute zero is never reached. We need the scenario which works not only at the absolute zero but also at very low to low temperature. That is, we still need some scheme to extract the pure state signal out of the mixed states. We will start with lowering temperature in existing initialization schemes. Secondly, 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. We have to decouple dipolar interactions by applying special pulse sequences such as WHH-4. Alternatively we may seek the possibility of refrigerating only spins without actually refrigerating materials[ITS+00, TTT01] or restore the liquid state after refrigeration.

2 Entanglement and Scalability in Effective Pure State Schemes

The exhaustive averaging requires $2^n - 1$ experiments and the reduced homonuclear version does $(2^n - 1)/n$ ones[VSB+00]. They require $\mathbf{EXP}(n)$ resources at the beginning and therefore are out of question as quantum computation. These schemes are apparently cheating 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 Hilbert space.

The logical labeling also suffers from the exponentially small population of effective pure state at room temperature. However if the origin of the problem is the extremely small polarization at room temperature, it is natural to seek the possibility of improving it by lowering the temperature.

Under the effective Hamiltonian of solution NMR,

$$H = -\sum_{i=0}^{n-1} \hbar\omega_i S_{zi} + \sum_{i=0}^{n-2} \sum_{j>i} \hbar\omega_{ij} S_{zi} S_{zj}$$

with $|\omega_k| >> |\omega_{ij}|$, the thermal equilibrium states can be well-approximated by the product density operator of the form $\rho = \bigotimes_{i=0}^{n-1} \rho_i$ with $\rho_i = p_i|0\rangle\langle 0| + q_i|1\rangle\langle 1|$ where $p_i = (1+\delta_i)/2$, $q_i = (1-\delta_i)/2$, $\delta_i = \tanh \alpha_i$, $\alpha_i = \hbar\omega_i/2k_BT$. They further reduce to independent identical distributions (i.i.d.) with $p_i = p$ for homonuclear system where $\omega_i \approx \omega$.

Unitary logical labeling transforms it into

$$\rho' = P(0) \underbrace{|0\rangle\langle 0|}_{n-m} \otimes [(1-\epsilon) \underbrace{I/2^m}_{m} + \epsilon \underbrace{|0\rangle\langle 0|}_{m}] + \sum_{j\neq 0} P(j) \underbrace{|j\rangle\langle j|}_{n-m} \otimes \underbrace{\rho_j}_{m}.$$

The first term is the conditional effective pure state. If ancilla bits are 0, then the rest of the qubits are in the effective pure state.

It turns out that within the subspace logically labeled by ancilla, the weight ϵ of the pure state is improved by lowering the temperature and the threshold for entanglement[BCJ+99] and even that for exponential speed-up[LP01] may be reached. However at these high polarizations (low temperatures), the population $P(0)$ of the subspace itself becomes exponentially small with n and therefore the scheme requires $\mathbf{EXP}(n)$ number of molecules.

This is because the states of the type $\{|0\rangle^{\otimes n/2}|1\rangle^{\otimes n/2}\}$ chosen as the background to span the effective pure subspace with the signal state $|0\rangle^{\otimes n}$ are no longer typical. They were typical at room temperature where $\delta \approx \alpha \approx 10^{-5} << 1$.

3 Logical Labeling with Typical Sequences[Kit01]

We have generalized the logical labeling scheme[GC97] to arbitrary temperature by using typical sequences $\{|0\rangle^{\otimes np}|1\rangle^{\otimes nq}\}$ as the background and the most probable state $|0\rangle^{\otimes n}$ as

the signal state, where np is treated as an integer for simplicity. Then the population $P(0)$ of the subspace spanned by these states is larger than $1/\sqrt{2\pi n}$ at any temperature, which scales very well.

The weight of the pure state, ϵ, can be raised above the threshold for entanglement by lowering the temperature. The entanglement is restored without requiring exponentially many molecules. However, ϵ never reaches the threshold for exponential speed-up[LP01]. This is the limit of using single signal state because any state is subject to exponentially small population for increasing n at finite temperature.

Our generalization has revealed that the number of qubits available is given by $m \approx nH(p)$ where $H(p) = -p\log p-(1-p)\log(1-p)$ is the entropy. We loose qubits by lowering the temperature. The counter-intuitive nature of the logical labeling is the consequence of using the most typical states as the background which does not emit the signal.

4 Typical Sequences as Signal States[Kit01]

The last two considerations naturally lead 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 state.

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 total population of the signal states is $P(x \in \mathcal{A}) = 2^{-nH(p)}|\mathcal{A}| \approx 1/\sqrt{2\pi npq}$, which scales very well.

One way of doing this is the unitary Schumacher compression 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 number of qubits available is $m \approx n[1 - H(p)]$, which is very reasonable since we gain qubits by lowering the temperature and all qubits are available in the limit of absolute zero ($p = 1$).

The scheme includes [SV99] but is not limited to it. Various algorithms in classical data compression or source coding may be applied.

5 Conclusions

We have shown that existing effective pure state schemes can not reach the regime where genuine entanglement is involved. We have generalized the logical labeling scheme to arbitrary temperature and have shown that our scheme enables entanglement at very low temperature. However we have also shown that any effective pure state schemes including ours can never reach the genuine quantum computation regime where exponential speed-up

is enabled without requiring exponentially many resources other than Hilbert space. Finally we have proposed the new initialization scheme which uses the typical states as signal state and enables the genuine quantum computation by nuclear spin network quantum computers.

References

[BCJ+99] S. L. Braunstein, C. M. Caves, R. Jozsa, N. Linden, S. Popescu, and R. Schack, Phys. Rev. Lett. **83**, pp.1054-1057 (1999).

[GC97] N. Gershenfeld and I. L. Chuang, Science **275**, pp.350-356 (1997).

[ITS+00] M. Iinuma, Y. Takahashi, I. Shaké, M. Oda, A. Masaike, T. Yabuzaki, and H. M. Shimizu, Phys. Rev. Lett. **84**, pp.171-174 (2000).

[Kit01] M. Kitagawa, submitted to Phys. Rev. Lett. (2001).

[LP01] N. Linden and S. Popescu, Phys. Rev. Lett. **87**, 047901 (2001).

[SC99] R. Schack and C. M. Caves, Phys. Rev. **A 60**, pp. 4354-4362 (1999).

[SV99] L. J. Schulman and U. Vazirani, in Proc. 31'st STOC, ACM Press, 1999.

[TTT01] K. Takeda, T. Takegoshi, and T. Terao, Chem. Phys. Lett. **345**, p.166 (2001).

[VSB+00] L. M. K. Vandersypen, M. Steffen, G. Breyta, C. S. Yannoni, R. Cleve, and I. L. Chuang, Phys. Rev. Lett. **85**, pp.5452-5455 (2000).

[VYSC99] L. M. K. Vandersypen, C. S. Yannoni, M. H. Sherwood, and I. L. Chuang, Phys. Rev. Lett. **83**, pp.3085-3088 (1999).