Initialization, Entanglement and Scalability in Bulk-Ensemble NMR Quantum Computation

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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. However, the states used in NMR experiments are separable and therefore contain no entanglement[BCJLPS99] and furthermore exponentially huge physical resources such as the numbers of molecules[LP01] or experiments are used. In this Paper, we present the initialization schemes which may restore entanglement, improve the scalability, and achieve the real quantum computation.

The simplest answer to this problem would be cooling all spins down to $T = 0$K. Then the states of all molecular quantum computers would be initialized to $|0\rangle^{\otimes n}$. However it is not that simple. First of all, $T = 0$K is never reached. We need the scenario which works not only at 0K. 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. Alternatively we may seek the possibility of refrigerating spins without actually refrigerating materials[ITSOMYS00].

Logical Labeling with Typical Sequences

The exhaustive averaging 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 Hilbert space.

The logical labeling[GC97] 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. We have generalized the logical labeling [GC97] to arbitrary temperature by using typical sequences $\{|0\rangle^{\otimes np}|1\rangle^{\otimes nq}\}$ as the background (np is treated as an integer for simplicity) and the most probable state $|0\rangle^{\otimes n}$ as the signal state.

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

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

The first term is the conditional effective pure state and its population $P(0) > 1/\sqrt{2\pi n}$ scales very well.

The entanglement is restored if p is large enough. However, the population ϵ of the effective pure state still decreases exponentially with n. This is the limit of using single signal state since 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 lose qubits by lowering the temperature. The counter-intuitive nature of the logical labeling is the consequence of using the most typical states as the signal-less background.

Typical Sequences as Signal States

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.

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 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 $T = 0$.

The scheme includes [SV99] but is not limited to it.

References

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