An adiabatic quantum optimization for exact cover 3 problem*

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A perturbation method is applied to study the structure of the ground state of the adiabatic quantum optimization for the exact cover 3 problem. It is found that the instantaneous ground state near the end of the evolution is mainly composed of the eigenstates of the problem Hamiltonian, which are Hamming close to the solution state. And the instantaneous ground state immediately after the starting is mainly formed of low energy eigenstates of the problem Hamiltonian. These results are then applied to estimate the minimum gap for a special case.

Keywords: adiabatic quantum optimization, exact cover 3 problem, perturbation expansion

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1. Introduction

Quantum computation is widely believed to be able to provide a speedup for computationally hard problems.[1–3] Efficient quantum algorithms have been designed to solve computational problems such as factorization,[1] unstructured search,[2,4–8] etc. In the mean time, several quantum computational models have been proposed, one of which is the adiabatic quantum optimization (ADO) model.

The ADO model has attracted a lot of attention,[9–14] it was proposed by Farhi *et al.*[3] as a possible means for solving nondeterministic polynomial (NP) complete problems. There are some numerical studies of the ADO model for the NP-complete problems, reporting polynomial scaling of the minimum gap up to about 100 bits.[9,12] Meanwhile, counter examples were found in Refs. [10] and [11]. Later, it was shown that the size of the gap in those counter examples could be increased significantly by changing the adiabatic path or the initial Hamiltonian.[15]

In spite of this, there is no rigorous analytical result to characterize the performance of the ADO model for the NP-complete problems until recently. Little insight exists on the question of why the physical process can lead to extremely small gaps and hence demands an exponential evolution time. In Refs. [13] and [16], Amin *et al.* lifted the curtain on the question. But there are still many underlying elements left to be unveiled. In this paper, we investigate the ADO model for the exact cover 3 (EC3) problem, which is a well-known NP-complete problem in the computational regime.

The paper is organized as follows. In Section 2, we introduce the ADO model, and discuss how to map a classical EC3 problem onto it. In Section 3, we analyze how the instantaneous ground state immediately after the starting of the evolution is formed, and those near the end as well. In Section 4, the analytical results are applied to estimate the minimum gap for a special case. This paper is concluded in Section 5.

2. The ADO model

2.1. System Hamiltonian

In the ADO model, the Hamiltonian of the system is designed to evolve from an initial form $H_{\rm b}$, whose ground state is the initial state of the system, to a final Hamiltonian $H_{\rm p}$, whose ground state is the optimal solution to an optimization problem

$$H = (1-s(t))H_{\rm b} + s(t)H_{\rm p}, \quad s \in [0,1]. \tag{1}$$

According to the adiabatic theorem, the evolution time is determined by the minimum gap $g_{\rm m}$ between the ground state and the first excited state

$$T \propto \frac{1}{g_{\rm m}^2}. \tag{2}$$

We denote the ground state of the total Hamiltonian by

$$|G\rangle = \sum_z c_z |z\rangle, \tag{3}$$

where c_z are the complex probability amplitudes, and $|z\rangle$ ($z \in \{0,1\}^N$) is the computation basis. At the beginning of the evolution, $c_z = 1/2^{(N-1)}$, $|G\rangle$ is therefore a uniform superposition of all the computational states. At the end of the evolution, it is a superposition of all possible solution states.

2.2. The EC3 problem

The EC3 problem can be formalized in the following way. Consider N bits $x_1, x_2, ..., x_N$ which take values 0 or 1. An instance of EC3 consists of M triplets of bit indices $(i_{\rm c}, j_{\rm c}, k_{\rm c})$ (the clauses), where each clause is said to be satisfied if and only if one of the corresponding bits is 1 and the other two are 0. A solution of a particular instance of the EC3 problem is an

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assignment of the bits $X = (x_1, x_2, ..., x_N)$, which satisfies all the clauses. This problem can be assigned a cost function

$$f(x) = \sum_c (x_{i_c} + x_{j_c} + x_{k_c} - 1)^2 \tag{4}$$

such that each solution has zero cost and all other assignments have a positive cost. The goal is to find an assignment that has zero cost.

In order to define an adiabatic quantum algorithm for EC3, we need to choose $H_{\rm p}$ and $H_{\rm b}$. To get $H_{\rm p}$, we change the above cost function by replacing x_i with $x_i = (1 - \sigma_i^z)/2$, where σ_i^z is the Pauli-Z operator on the i-th qubit. The problem Hamiltonian is obtained as

$$H_{\rm p} = MI - \frac{1}{2}\sum_{i=1}^{N} B_i \sigma_i^z + \frac{1}{4}\sum_{i,j=1}^{N} J_{ij}\sigma_i^z\sigma_j^z, \tag{5}$$

where B_i is the number of clauses that involve bit i, J_{ij} is the number of clauses in which bits i and j participate together, M is the total number of clauses, and I is the identity operator. For $H_{\rm b}$, we make the conventional choice

$$H_{\rm b} = \frac{1}{2}NI - \frac{1}{2}\sum_{i=1}^{N}\sigma_i^x, \tag{6}$$

where σ_i^x is the Pauli-X operator on the i-th qubit.

3. Analysis by perturbation expansion

In the earlier works, it was known that the instantaneous ground state changes from a large superposition of computational states to a small superposition of computational states suddenly at the critical point where a quantum phase transition occurs, and slowly at other time intervals.[11,13,16] Therefore, the instantaneous ground states immediately after the starting and near the end of the adiabatic evolution carry much information about the instantaneous ground states immediately before and after the transition. In the following, the instantaneous ground state near the end of the adiabatic evolution is analyzed, along with that immediately after the starting.

3.1. The ground state near the end

For convenience, the Hamiltonian near the end of the evolution is modified as

$$H_\gamma = \gamma H_{\rm b} + H_{\rm p}, \tag{7}$$

where $0 < \gamma \ll 1$. We can use a perturbation expansion in γ, taking $H_{\rm p}$ as the unperturbed Hamiltonian, to calculate the eigenstates of H. Upon perturbation, the energy eigenvalue and the eigenstate become

$$E(\gamma) = E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \cdots, \tag{8}$$

$$|G(\gamma)\rangle = |G^{(0)}\rangle + \gamma|G^{(1)}\rangle + \gamma^2|G^{(2)}\rangle + \cdots. \tag{9}$$

For simplicity, it is assumed that the problem has a unique solution, therefore the ground state of $H_{\rm p}$ is a nondegenerate state $|f\rangle$, where f is the final solution. To the 0-th order in γ, $|G^{(0)}\rangle = |f\rangle$. The first-order correction has $E^{(1)} = 0$, because the operators in $H_{\rm b}$ each flip only one qubit. The lowest order nonzero term is therefore the second-order one.

In order to figure out the components that contribute to the instantaneous ground state significantly, we introduce a threshold small number ϵ. If $|c_z| > \epsilon$, the component $|z\rangle$ is thought to be significant. Let us introduce a set

$$S = \{|z\rangle : |c_z| > \epsilon\}. \tag{10}$$

Define the number of different qubits in a state $|z\rangle$ from the final solution state $|f\rangle$ to be $d_z = ||z - f||$, i.e., the Hamming distance. Since $H_{\rm b}$ is a linear function of σ_i^x, it can only generate single qubit flips. To include $|z\rangle$ into $|G\rangle$, we need to apply $H_{\rm b}$ at least m times. Therefore, $|c_z| = {\rm O}(\gamma^{d_z})$. By requiring $\gamma^{d_z} > \epsilon$, it is found

$$d_z < \delta \equiv \frac{\log\epsilon}{\log\gamma}. \tag{11}$$

This indicates that, if $|z\rangle$ is significant, then it should be close to the final solution state in the Hamming distance. If $d_z < \delta$, $|z\rangle$ is believed to be δ-close to the final solution state. Therefore, the set S can be rewritten as

$$S = \{|z\rangle : d_z < \delta\}, \tag{12}$$

which consists of the states that are δ-close to the final solution state. It is clear now that the instantaneous ground state near the end of the evolution is mainly composed by the eigenstates included in S.

3.2. The ground state immediately after the starting

Again, the perturbation method is applied. Now the system Hamiltonian becomes

$$H_\lambda = H_{\rm b} + \lambda H_{\rm p}, \tag{13}$$

and the perturbation expansion is performed around $H_{\rm b}$. Since $H_{\rm b}$ is diagonal in the Hadamard basis, we need to carry out the perturbation expansion on that basis. The instantaneous ground state can be expanded on the Hadamard basis as

$$|G\rangle = \sum_z b_z|\pi(z)\rangle, \tag{14}$$

where $|\pi(z)\rangle = H^{\otimes n}|z\rangle$ is the Hadamard basis, with H being the Hadamard transformation.

The Hamiltonian $H_{\rm p}$ is a bilinear function of σ_i^z; hence, it can generate single- and two-qubit flips in the Hadamard basis. To include a state $|\pi(z)\rangle$ into the superposition $|G\rangle$, we need to apply $H_{\rm b}$ at least $w/2$ times, where w is the Hamming weight of z. This leads to $b_z = {\rm O}(\lambda^{w/2})$. By requiring that $\lambda^{w/2} > \epsilon$, it can be found

$$w < w_{\rm c} \equiv \frac{\log(1/\epsilon)}{\log(1/\lambda)}. \tag{15}$$

Let $\Delta E_{\rm b}$ and $\Delta E_{\rm p}$ be the uncertainties of $H_{\rm b}$ and $H_{\rm p}$, respectively. According to the uncertainty principle, we have

$$\Delta E_{\rm b}\Delta E_{\rm p} \geq \frac{1}{2}\langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle. \tag{16}$$

Note that

$$H_{\rm b}|\pi(z)\rangle = w|\pi(z)\rangle, \tag{17}$$

i.e., $|\pi(z)\rangle$ is an eigenstate of $H_{\rm b}$ with eigenvalue $E_{\rm b} = w$. Therefore, we have $\Delta E_{\rm b} \sim w$ for the ground state $|G\rangle$ by using Eq. (15). The uncertainty principle requires $\Delta E_{\rm p} \sim \langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle/2w_{\rm c}$, leading to $E_{\rm p} < \langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle/2w_{\rm c}$. As discussed above, here the set S becomes

$$S = \left\{|z\rangle : E_{\rm p} < \frac{1}{2}\langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle/w_{\rm c}\right\}, \tag{18}$$

which consists of the eigenstates of $H_{\rm p}$ whose eigenvalues are less than $\langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle/2w_{\rm c}$, and the instantaneous ground state immediately after the starting is mainly composed by the eigenstates in S.

4. The gap of a special case

Here, a simple case is considered. Suppose that $g_{\rm m}$ is much smaller than the separation of the two crossing levels from other energy levels, then the slow evolution of the system close to the anticrossing will be restricted to only those levels. The system Hamiltonian can then be approximately rewritten in the two-state subspace as

$$H = (\varepsilon\sigma_z + g_{\rm m}\sigma_x)/2, \tag{19}$$

where $\varepsilon = 2E(s - s^*)$, s^* is the transition point, and E is an energy scale characterizing the anticrossing. By using Eq. (19), it can be shown that for $\varepsilon \gg g_{\rm m}$,

$$g_{\rm m} = \varepsilon|\langle G(+\varepsilon)|G(-\varepsilon)\rangle|, \tag{20}$$

where $|G(\pm\varepsilon)\rangle$ denote the ground states before and after the anticrossing. Here $\varepsilon \gg g_{\rm m}$ ensures that the above perturbation expansion is valid, therefore the results of Section 3 hold. This means that $g_{\rm m}$ is determined by the complex amplitudes of the eigenstates that are δ-close to the final solution state and of the eigenstates of $H_{\rm p}$ whose eigenvalues are less than $\langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle/2w_{\rm c}$. It can be shown

$$g_{\rm m} \leq \sqrt{\frac{|S^+|}{|S^-|}}, \tag{21}$$

where $|S|$ denotes the cardinality of set S, and $S^{\pm}$ correspond to set S at the coordinates $\pm\varepsilon$. The equality happens when all states in S^+ also belong to S^-. This indicates that if the problem Hamiltonian happens to have an exponentially large number of low energy states that have large Hamming distances to the correct solution, the resulting gap will then be exponentially small.

5. Conclusion

To conclude, we have applied a perturbation method to study the structure of the instantaneous ground state in the ADO model for the EC3 problem. It is found that the instantaneous ground state near the end of the evolution is mainly composed by the eigenstates that are δ-close to the final solution state, and the instantaneous ground state immediately after the starting is mainly composed by the eigenstates of $H_{\rm p}$ whose eigenvalues are less than $\langle {\rm i}[H_{\rm b}, H_{\rm p}]\rangle/2w_{\rm c}$. These results are then used to estimate the minimum gap for a simple case.

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