Consideration on Quantum Simulation of Adaibatic Quantum Computation in SAT Problem

Shigeru Nakayama[1] and Ichiro Iimura[2]

[1]Graduate School of Science and Enginnering, Kagoshima University, Japan
[2]Dept. of Administration, Faculty of Administration, Prefectural University of Kumamoto, Japan

1 Introduction

Adiabatic quantum computation[1] was proposed as a quantum algorithm with adiabatic evolution to solve combinatorial optimization problem. Then it has been applied to many problems like Deutsch problem and Deutsch·Jozsa problem[2]. Among them, satisfiability problem (SAT) has been tried to be solved by using adiabatic quantum computation[3]. Adiabatic quantum computation has been actively studied to solve NP-complete problems.

This paper demonstrates the idea of adiabatic computation to solve function optimization problem. Then, this idea is extended to adiabatic quantum computation to keep the solution on the ground state in time evolution of discrete expression of Schrödinger equation. Moreover, the paper shows detailed numerical calculation of the computer simulation in which the adiabatic quantum computation is applied to 1-SAT problem with two literals. Energy gaps are also discussed in relation to transfer of observation probabilities. We show quantum simulation of solving a simple SAT problem, modify the adiabatic quantum computation, and propose a method to solve 1-SAT problem with two literals more efficiently with higher observation probability.

2 Satisfiability(SAT) Problem

Satisfiability(SAT) is the problem of finding the variables for a given Boolean formula written using only AND, OR, NOT, variables(literals), and parentheses(clauses) to be satisfiable as TRUE. A litetal is a valuable or the negation. A clause has more than one literal.

The k-SAT problem includes k literals in one clause. For example, the formula (x_1) AND (x_2) is satisfiable because one can find the values $(x_1) = true(1)$ and $(x_2) = true(1)$, which make (x_1) AND (x_2) $true(1)$. According to the Cook–Levin theorem, the Boolean satisfiability problem with $k \geq 3$ is NP-complete.

3 Adiabatic Quantum Computation

3.1 Discrete expression of Schrödinger equation

SAT problem is to find the state vector $|\psi(t)\rangle$ where the eigenvalue (energy) of time-independent Hamiltonian H is minimized by using the adiabatic quantum computation. Adiabatic quantum computation uses the Schrödinger equation.

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H |\psi(t)\rangle . \tag{1}$$

The continuous differential equation must be converted into discrete expression for computer simulation.

$$|\psi(t+\Delta)\rangle = e^{-iH\Delta} |\psi(t)\rangle , \tag{2}$$

where Plank constant is used as $\hbar = 1$ for simplicity, and Δ is a differential time contributing to a phase scaling parameter on the right hand side of eq. (2).

3.2 Hamiltonian and unitary transform

Adiabatic quantum computation introduces a step parameter s ranging from 0 to 1. Then, the Hamiltonian H can be written as

$$H(s) = (1-s)H_i + sH_f, \tag{3}$$

as a function of step parameter s, where H_i is Hamiltonian of the initial state independent of any problem and H_f is Hamiltonian of the final state depending on a given problem. When the step parameter s is gradually changed from 0 to 1, the Hamiltonian will be changed from the initial Hamiltonian to final Hamiltonian.

Therefore, the state vector $\left|\psi^{(h)}\right\rangle$ gradually changes with each step by unitary transform as follows;

$$\left|\psi^{(h)}\right\rangle = e^{-i(1-s)H_i\Delta - isH_f\Delta} \left|\psi^{(h-1)}\right\rangle \tag{4}$$

where an integer parameter h $(1 \leq h \leq j+1)$ is calculated from $s = h/(j+1)$, j is the number of repetition steps, and $U^{(h)}$ is a unitary transform for adiabatic quantum evolution written as,

$$U^{(h)} = e^{-i(1-s)H_i\Delta - isH_f\Delta}. \tag{5}$$

In the case of 1-SAT problem with two literals, the number of repetition steps is used as $j = 4$ in our numerical simulation, and Δ is a phase scaling parameter used as $\Delta = 1$ required for adiabatic quantum evolution.

$U_{SM}^{(h)} = e^{-i(1-s)H_i}$ has non-diagonal elements and is unitary transform for state mixing between interacting states. This causes diversification of the solutions. On the other hand, $U_{PS}^{(h)} = e^{-isH_f}$ has only diagonal elements and is unitary transform for phase shifting where the phase of a state with high cost is shifted very much and that of a state with low cost is not shifted much. This results in intensification for searching solutions.

3.3 Hamiltonian modified by nonlinear step functions

We modify the linear step parameter s to a nonlinear step function $p(s)$ changing from 0 to 1. Hamiltonian can

be written as

$$H(s) = (1 - p(s))H_i + p(s)H_f, \tag{6}$$

where we introduce a nonlinear step function $p(s)$ changing from 0 to 1. The nonlinear step function must be monotonic to fulfill both $p(0) = 0$ and $p(1) = 1$. In the case of linear step function,

$$p(s) = s. \tag{7}$$

Although the step function $p(s)$ is originally used as a linear function[1, 2], we propose the nonlinear step function and did the computer simulation to solve 1-SAT problem. Here, we propose the cubic step function,

$$p(s) = 4(s - 1/2)^3 + 1/2, \tag{8}$$

and compare the linear step function with the cubic step function.

4 Hamiltonian of 1-SAT Problem

4.1 Initial and final Hamiltonians of 1-SAT problem

We use an example 1-SAT instance with 2 variables and 2 clauses of $(NOT(x_1))\ AND\ (NOT(x_2))$, which has one solution, $x_1 = false(0)$ and $x_2 = false(0)$. For a given instance, the cost $c(x_1x_2)$ of an assignment x_1, x_2 is the number of clauses it does not satisfy.

In matrix form [3], the initial Hamiltonian H_i is implemented with elementary quantum gates by use of the Walsh-Hadamard transform with elements $W_{r.s} = 2^{-n/2}(-1)^{r.s}$, where $H^{(0)} = WDW$ and D is a diagonal matrix with the value for state r given by the sum of the bits, i.e, the element $D_{r,r}$ is just a count for the number of bits equal to 1 in state r.

$$H_i = W \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} W = \frac{1}{2} \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix}. \tag{9}$$

The initial Hamiltonian H_i is independent of any SAT problem. This Hamiltonian makes a state mixing factor in the amplitude of each state, then it results in the diversification of solution candiates.

The final Hamiltonian H_f is a diagonal matrix depending on the SAT problem instance. In the 1-SAT problem of $(NOTx_1)\ AND\ (NOTx_2)$, each diagonal element has each cost $c(x_1x_2)$ such as $c(00) = 0$, $c(01) = 1$, $c(10) = 1$, and $c(11) = 2$. Therefore, the final Hamiltonian H_f is given by

$$H_f = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}. \tag{10}$$

This Hamiltonian introduces a phase shift factor in the amplitude of assignment i depending on its associated cost $c(i)$, where the higher cost results in more phase shift.

4.2 Quantum Adiabatic Evolution in 1-SAT problem

According to Hogg[3], the initial superposition state with all equal probability amplitudes,

$$\left|\psi^{(0)}\right\rangle = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle), \tag{11}$$

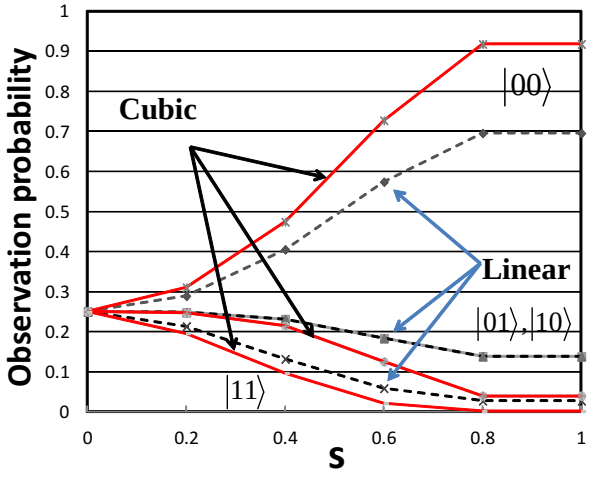

Fig. 1. Observation probabilities of four state vectors as a parameter of step parameter s in the linear and cubic step functions.

is also used in 1-SAT problem with 2 literals.

Therefore, we should make the observation probability of the state vector $|00\rangle$ as high as possible from 25% in the initial state $|\psi_0\rangle$. The initial state $\left|\psi^{(0)}\right\rangle$ with equal superposition state is evolved by applying the unitary transform as follows:

$$\left|\psi^{(h)}\right\rangle = e^{-i(1-p(s))H_i\Delta - ip(s)H_f\Delta}\left|\psi^{(h-1)}\right\rangle, \tag{12}$$

where an integer parameter h $(1 \le h \le j+1)$ is calculated from $s = h/(j+1)$. Here, the repetition number $j = 4$ is used in our numerical simulation and Δ is a phase scaling parameter required for time evolution used as $\Delta = 1$.

In adiabatic quantum computation, the observation probability of each state vector at each step can be calculated from taking the square of the absolute value of the probability amplitude. At the last step $s = 1(h = 5)$, the observation probability of the $|00\rangle$ state is 91.76% as shown in Fig. 1. On the other hand, we could not increase the observation probability in the linear step function $p(s) = s$. We get the final observation probability 69.54% of finding the solution as shown in Fig. 1.

5 Conclusion

In this paper, we proposed the nonlinear cubic step function $p(s) = 4(s - 0.5)^3 + 0.5$ instead of the linear step function $p(s) = s$ in the adiabatic quantum computation to effectively solve 1-SAT problem. We could obtain the higher observation probability of finding the solution by using the nonlinear cubic step function.

References

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