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SPECIAL TOPIC — Quantum computation and quantum simulation

# Quantum algorithm for a set of quantum 2SAT problems*

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We present a quantum adiabatic algorithm for a set of quantum 2-satisfiability (Q2SAT) problem, which is a generalization of 2-satisfiability (2SAT) problem. For a Q2SAT problem, we construct the Hamiltonian which is similar to that of a Heisenberg chain. All the solutions of the given Q2SAT problem span the subspace of the degenerate ground states. The Hamiltonian is adiabatically evolved so that the system stays in the degenerate subspace. Our numerical results suggest that the time complexity of our algorithm is $O(n^{3.9})$ for yielding non-trivial solutions for problems with the number of clauses $m = dn(n-1)/2$ ($d \lesssim 0.1$). We discuss the advantages of our algorithm over the known quantum and classical algorithms.

**Keywords:** adiabatic quantum computation, quantum Hamiltonian algorithm, quantum 2SAT problem

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## 1. Introduction

In 1990s, several quantum algorithms such as Shor's algorithm for factorization and Grover's algorithm for search[1] were found to have a lower time complexity than their classical counterparts. These quantum algorithms are based on discrete quantum operations, and are called quantum circuit algorithms.

Quantum algorithms of a different kind were proposed by Farhi *et al.*[2,3] In these algorithms, Hamiltonians are constructed for a given problem and the qubits are prepared initially in an easy-to-prepare state. The state of the qubits is then driven dynamically and continuously by the Hamiltonians and finally arrives at the solution state. Although quantum algorithms with Hamiltonians have been shown to be no slower than quantum circuit algorithms,[4,5] they have found very limited success. In fact, due to exponentially small energy gaps,[6] they often cannot even outperform classical algorithms. The random search problem is a rare exception, for which three different quantum Hamiltonian algorithms were proposed and they can outperform classical algorithms. But still these Hamiltonian algorithms are just as fast as Grover's.[2,7–9]

Recently, quantum Hamiltonian algorithms were found for a different problem, independent sets of a graph[10,11] and they can outperform their classical counterparts significantly. In this work, we apply it to a set of quantum 2-satisfiability (Q2SAT) problems, which have two groups of solutions in the form of product states and entangled states. We aim to find solutions in the form of entangled states. For a given Q2SAT problem, we construct a Hamiltonian whose ground states are all the solutions of the problem. Initially we prepare the system in a trivial product solution state, we then evolve it in the subspace of degenerate ground states by slowly changing the Hamiltonian parameters along a closed path. In the end we get a superposition of different solutions. Numerical calculation shows that the time complexity of our quantum algorithm is $O(n^{3.9})$ for problems with $m = dn(n-1)/2$ ($d \lesssim 0.1$), where $m$ is the number of clauses. There is a classical algorithm for the Q2SAT problem. Although its time complexity is better, it tends to find trivial product solutions.[12,15] The quantum algorithm in Ref. [16] can find entangled solutions but with a slower time complexity of $O(mn^2/\delta(n))$, where the energy gap $\delta(n)$ may be in the form of $n^{-g}$ ($g$ positive).

## 2. Quantum 2-satisfiability problem

The Q2SAT problem is a generalization of the well known 2-satisfiability (2SAT) problem.[12] The algorithm for 2SAT problem is widely used in scheduling and gaming.[13] Besides, 2SAT problem is a subset of $k$-satisfiability problem ($k$SAT). Since 2SAT problem is a P problem while $k$SAT problem for $k \geq 3$ is an NP complete problem, $k$SAT problem has a great importance in answering whether P = NP. Similarly, Q2SAT problem is a subset of quantum $k$-satisfiability problem (Q$k$SAT). It is expected that Q$k$SAT problem is more complex than $k$SAT problem, and that quantum algorithms perform better than classical algorithms in Q$k$SAT problem. Therefore, Q$k$SAT problem could become a breakthrough in answering whether P = BQP and BQP = NP.[14]

In a 2SAT problem, there are $n$ Boolean variables and $m$ clauses. Each clause of two Boolean variables bans one of the four possible assignments. For example, the clause $(\neg x_i \vee x_j)$

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bans the assignment $(x_i, x_j) = (1,0)$. The problem is to find an assignment for all the variables so that all the clauses are satisfied. For quantum generalization, we replace the boolean variables with qubits and the clauses with two-qubit projection operators. In a Q2SAT problem of $n$ qubits and $m$ two-qubit projection operators $\{\Pi_1, \Pi_2, \ldots, \Pi_m\}$, the aim is to find a state $|\psi\rangle$ such that projections of the state are zeros, i.e.,

$$\Pi_j|\psi\rangle = 0, \quad \forall j \in 1,2,\ldots,m. \tag{1}$$

When all the projection operators project onto product states, Q2SAT problems go back to 2SAT problems.

In this work we focus on a class of 2-QSAT problems, where all the projection operators are of an identical form

$$\Pi_j = |\Phi_j\rangle\langle\Phi_j|, \ |\Phi_j\rangle = \alpha|1_{a_j}0_{b_j}\rangle + \beta|0_{a_j}1_{b_j}\rangle, \quad \forall j, \tag{2}$$

where $|\alpha|^2 + |\beta|^2 = 1$ and $a_j, b_j$ label the two qubits acted on by $\Pi_j$. This is a special case of the restricted Q2SAT problems discussed by Farhi *et al.*,[16] i.e., where all the clauses are the same. These Q2SAT problems apparently have two solutions, $|\psi\rangle = |0\rangle\cdots|0\rangle$ and $|\psi\rangle = |1\rangle\cdots|1\rangle$, which are product states. We call them trivial solutions. We are interested in finding non-trivial solutions which are entangled.

A Q2SAT problem of $n$ qubits and $m$ two-qubit projections can be also viewed as a generalization of a graph with $n$ vertices and $m$ edges. As a result, in this work, we often refer to the Q2AT problem as a graph.

## 3. Previous algorithms

There are now several algorithms for Q2SAT problems. The algorithms proposed by Beaudrap *et al.* in Ref. [12] and Arad *et al.* in Ref. [15] are classical. The classical algorithm relies on that for every Q2SAT problem which has solutions, there is a solution that is the tensor product of one-qubit and two-qubit states,

$$|\psi_1\rangle = \prod_r |\psi_r\rangle \otimes \prod_{pq} |\psi_{pq}\rangle, \tag{3}$$

where $|\psi_r\rangle$ is the state of qubit $r$, $|\psi_{pq}\rangle$ is an entangled state of qubits $p$ and $q$, and the indices $r$ and $p,q$ do not overlap. This conclusion is drawn with the following proven fact. If a projection operator $\Pi_j$ projects onto an entangled state of qubits $a_j$ and $b_j$, then the solution has either of the following two forms:

$$|\psi_1\rangle = |\psi_{a_jb_j}\rangle \otimes |\text{rest}\rangle, \tag{4}$$

where $|\psi_{a_jb_j}\rangle$ is an entangled state of qubits $a_j$ and $b_j$, and

$$|\psi_1\rangle = |\psi_{a_j}\rangle \otimes |\psi_{b_j}\rangle \otimes |\text{rest}\rangle, \tag{5}$$

where $|\psi_{a_j}\rangle$ and $|\psi_{b_j}\rangle$ are single-qubit states. Based on this feature, we conclude that a qubit involved in only one projection operator has entanglement with the other qubit of this projection operator, and that a qubit involved in more than one projection operators has no entanglement with other qubits. To find a solution of the form in Eq. (3), one can use the strategy of Davis–Putman's algorithm for 2SAT problem. That is, we assign an initial state to a qubit, "propagate" the state to its adjacent qubits along projection operators, and finally find out the solution of this form. The above algorithm has a time complexity of $O(n+m)$, but it is impossible to find a solution where three or more qubits are entangled.

In the quantum algorithm of Ref. [16], Farhi *et al.* constructed a Hamiltonian

$$H = \sum_j \Pi_j, \tag{6}$$

where $\Pi_j$ is of the form in Eq. (2). There is one-to-one correspondence between the solutions of a Q2SAT problem and the ground states of its corresponding Hamiltonian. To see this, we consider a state $|\psi_2\rangle$. If a state $|\psi_2\rangle$ is a solution of the Q2SAT problem, then

$$H|\psi_2\rangle = \sum_j \Pi_j|\psi_2\rangle = 0, \tag{7}$$

and if $|\psi_2\rangle$ is not a solution, then

$$\langle\psi_2|H|\psi_2\rangle = \sum_j \langle\psi_2|\Pi_j|\psi_2\rangle > 0. \tag{8}$$

Therefore, $|\psi_2\rangle$ is a solution of the Q2SAT problem if and only if it is a ground state of the Hamiltonian $H$. The state is initialized to

$$\rho_0 = \frac{1}{2^n}\mathbb{I}. \tag{9}$$

In each step of the algorithm, a projection operator $\Pi_j$ is selected and measured at random. If the result is 0, then do nothing, otherwise a Haar random unitary transfromation is applied,

$$\Lambda_{a_j}(\rho) = \int \mathrm{d}[U_{a_j}] U_{a_j}\rho U_{a_j}, \tag{10}$$

on one qubit $a_j$ of the two qubits $a_j$ and $b_j$ involved in $\Pi_j$. That is, the operation on the state in each step is

$$\mathcal{T}(\rho) = \frac{1}{m}\sum_j \mathcal{T}_j(\rho), \tag{11}$$

where

$$\mathcal{T}_j(\rho) = (1-\Pi_j)\rho(1-\Pi_j) + \frac{1}{2}\sum_{a_j,b_j} \Lambda_{a_j,b_j}(\Pi_j\rho\Pi_j). \tag{12}$$

Now set

$$T = \max\left\{\frac{49m^2n^2}{2c^2}, \frac{3mn^2}{2\epsilon}\right\}, \tag{13}$$

where $c(n)$ is the energy of the ground state and $\epsilon(n)$ is the energy gap between the ground state and the first excited state. It is assumed that $\epsilon(n) \approx n^{-g}$ ($g$ positive). After steps of length $T$, the algorithm has a probability of at least $2/3$ to produce a state $\rho_T$ whose fidelity with the solution is at least $2/3$. The quantum algorithm has a time complexity of at least $O(mn^2/\epsilon)$, and gives a non-trivial solution.

## 4. Our algorithm

Our algortihm follows the one proposed in Ref. [10]. For a Q2SAT problem of $n$ qubits and $m$ two-qubit projection operators $\{\Pi_1,\Pi_2,\ldots,\Pi_m\}$, we construct a Hamiltonian similar to Eq. (6)

$$H_0 = \Delta\sum_{j=1}^{m}\Pi_j, \tag{14}$$

where $\Delta$ is a positive real number and $\Pi_j$ is of the form in Eq. (2). Due to equations similar to Eqs. (7) and (8), solutions of the problem have one-to-one correspondence to the ground states of $H_0$. The above Hamiltonian can be re-written in terms of spin-1/2 operators $s^x, s^y, s^z$ as

$$\begin{aligned} H_0 \;=\; & \Delta\sum_{j=1}^{m}\Big\{-s^z_{a_j}s^z_{b_j}-\frac{1}{2}(1-2|\beta|^2)(s^z_{a_j}-s^z_{b_j}) \\ & +2\mathrm{Re}(\beta)\sqrt{1-|\beta|^2}(s^x_{a_j}s^x_{b_j}+s^y_{a_j}s^y_{b_j}) \\ & +2\mathrm{Im}(\beta)\sqrt{1-|\beta|^2}(s^x_{a_j}s^y_{b_j}-s^y_{a_j}s^x_{b_j})\Big\}, \end{aligned} \tag{15}$$

where we have replaced $|\alpha|$ with $\sqrt{1-|\beta|^2}$ and ignored the phase of $\alpha$. A constant is dropped from the Hamiltonian. We rotate all qubits along some axis $\boldsymbol{n}$,

$$s^{x,y,z}_{a_j}(t) = \exp\left(2\pi\mathrm{i}s^{\boldsymbol{n}}_{a_j}\frac{t}{T}\right)s^{x,y,z}_{a_j}\exp\left(-2\pi\mathrm{i}s^{\boldsymbol{n}}_{a_j}\frac{t}{T}\right), \tag{16}$$

where $s^{\boldsymbol{n}}_{a_j}=\boldsymbol{n}\cdot\hat{s}=n_xs^x_{a_j}+n_ys^y_{a_j}+n_zs^z_{a_j}$ is the spin operator along the direction of $\boldsymbol{n}$ and $t\in[0,T]$. Thus at time $t$ the Hamiltonian becomes

$$\begin{aligned} H(t) \;=\; & \Delta\sum_{j=1}^{m}\Big\{-s^z_{a_j}(t)s^z_{b_j}(t)-\frac{1}{2}(1-2|\beta|^2)\left[s^z_{a_j}(t)-s^z_{b_j}(t)\right] \\ & +2\sqrt{1-|\beta|^2}\Big[\mathrm{Re}(\beta)(s^x_{a_j}(t)s^x_{b_j}(t)+s^y_{a_j}(t)s^y_{b_j}(t)) \\ & +\mathrm{Im}(\beta)(s^x_{a_j}(t)s^y_{b_j}(t)-s^y_{a_j}(t)s^x_{b_j}(t))\Big]\Big\}. \end{aligned} \tag{17}$$

It is obvious that the eigen-energies of $H(t)$ do not change with $t$ and the corresponding eigenstates can be obtained by rotating those of $H_0$. Specifically, the energy gap $\delta(n)$ between the ground states and the first excited states does not change with $t$. We are interested in the adiabatic rotation, where $T$ is big enough. In this case, according to Ref. [17], if the initial state $|\psi(0)\rangle$ lies in the subspace spanned by the degenerate ground states $\{|\psi_k(0)\rangle\}$, i.e., $|\psi(0)\rangle=\sum_k c_k|\psi_k(0)\rangle$, then the final state $|\psi(T)\rangle$ lies in the subspace spanned by the ground states $\{|\psi_k(T)\rangle\}$ as well. Specifically, we have

$$|\psi(T)\rangle = \sum_{kl}c_kU_{kl}|\psi_l(0)\rangle, \tag{18}$$

where

$$U \;=\; P\left[\exp\left(\mathrm{i}\int_0^T\mathrm{d}tA(t)\right)\right], \tag{19}$$

$$A_{kl}(t) \;=\; \mathrm{i}\langle\psi_l(t)|\frac{\mathrm{d}}{\mathrm{d}t}|\psi_k(t)\rangle. \tag{20}$$

Here $A$ is the non-Abelian gauge matrix that drives the the dynamics in the subspace of the degenerate ground states. For the special case $\alpha=\beta=\sqrt{2}/2$, the gauge matrix has the following form:

$$A_{kl}(t) = \mathrm{i}\pi\langle\psi_l|\sum_{a=1}^{n}(s^+_a-s^-_a)|\psi_k\rangle. \tag{21}$$

Here is our algorithm.

- Choose a trivial solution of the Q2SAT problem as the initial state $|\psi(0)=|00\cdots00\rangle$ and set $H(0)=H_0$.
- Adiabatically rotate all qubits along some axis $\hat{n}$ from $t=0$ to $t=T$. During this rotation, the Pauli matrices $s^{x,y,z}_{a_j}$ of the qubit $a_j$ evolve according to Eq. (16) and the Hamiltonian of the system $H(t)$ evolves according to Eq. (17).
- Make measurement at the end.

As shown in Ref. [3], the time complexity of a quantum adiabatic algorithm is proportional to the inverse square of the energy gap $\delta(n)$ between the ground states and the first excited states. So, the time complexity of our algorithm depends on how the energy gap $\delta(n)$ scales with $n$. Here we consider a special case to estimate the energy gap and examine how it is influenced by the coefficient $|\beta|$. In this special case, the spins form a one-dimensional chain and couple to their two neighbors. We assume that $\beta$ is a positive real number. The special case is in fact the well known Heisenberg chain and has been thoroughly studied. Its Hamiltonian is

$$\begin{aligned} H_0 \;=\; & \Delta\sum_i\Big[-s^z_is^z_{i+1}-\frac{1}{2}(1-2|\beta|^2)(s^z_i-s^z_{i+1}) \\ & +2|\beta|\sqrt{1-|\beta|^2}\left(s^x_is^x_{i+1}+s^y_is^y_{i+1}\right)\Big]. \end{aligned} \tag{22}$$

Its eigen-energies form a band $E_k$ and can be analytically found.[18] We examine two limits. When $\beta\to0$, $E_k\to\Delta(1/2-2|\beta|\cos k)$, thus the gap approaches a constant, $\delta(n)\to\Delta/2$. When $\beta=\sqrt{2}/2$, $E_k=\Delta(1+\cos k)$, the gap $\delta=0$ if the chain is infinitely long. In our problem, due to that the chain has a finite length $n$, the wave vector $k$ is actually discrete and we have $\delta(n)\sim O(n^{-2})$. As a result, we expect our algorithm to have the worst performance when $|\beta|$ approaches $\sqrt{2}/2$. According to the above analysis, we mainly investigate the performance of our algorithm at $\beta=\sqrt{2}/2$, and regard it as the worst performance.

## 5. Numerical simulation

In our numerical simulation, we focus on the special case where

$$|\Phi_j\rangle = \frac{1}{\sqrt{2}}(|0_{a_j}1_{b_j}\rangle+|1_{a_j}0_{b_j}\rangle). \tag{23}$$

For this case, the Hamiltonian takes a simple form

$$H_3 = \Delta\sum_{j=1}^{m}(s^x_{a_j}s^x_{b_j}+s^y_{a_j}s^y_{b_j}-s^z_{a_j}s^z_{b_j}). \tag{24}$$

This Hamiltonian commutes with the total angular momentum along the $z$ axis $[H_3, \sum_{a=1}^{n} s_a^z] = 0$. The graph for each Hamiltonian is generated as follows. We first fix $n$, the number of vertices (or qubits), and then generate edges between each pair of vertices with the probability $d$. As a result, the number of edges $m \approx dn(n-1)/2$. In our numerical calculation, we choose $d = 0.1$. We randomly generate 10000 graphs for $n = 5$ to $n = 11$, 1000 for $n = 12$, $n = 13$ and $n = 14$, and 100 for $n = 15$. The corresponding Hamiltonians are diagonalized numerically and the energy gap $\delta$ is extracted. The average of the energy gap $\delta$ is plotted in logarithm scale in Fig. 1. Fitted by least squares method, we get

$$\log\left(\left\langle \frac{1}{\delta^2} \right\rangle\right) = 3.8634\log(n) - 7.2048, \tag{25}$$

with correlation coefficient $r = 0.995$. This shows that the inverse square of the energy gap $\langle 1/\delta^2 \rangle \approx O(n^{3.9})$ and the time complexity $t \approx O(n^{3.9})$ according to Ref. [3]. Such a time complexity is better than that of the quantum algorithm in Ref. [16], which is of $O(n^{5.9})$ for $m \approx dn(n-1)/2$ and $1/\delta \approx O(n^{1.9})$.

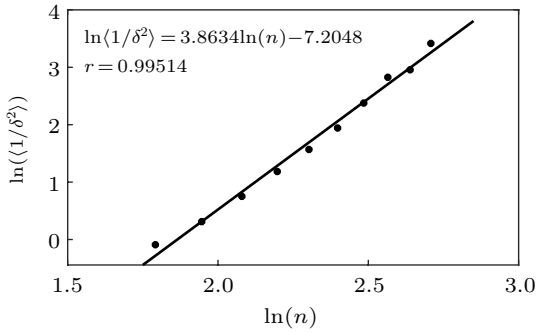



**Fig. 1.** The relation between the average of the inverse square of energy gaps of randomly generated problems and the number of qubits. The $x$-axis is the logarithm of the number of qubits, $\log(n)$, and the $y$-axis is the logarithm of the average of the inverse square of the energy gap, $\log(\langle 1/\delta^2 \rangle)$. The line is fitted by least squares method.

Shown in Fig. 2 is the distribution of the inverse square of energy gaps $1/\delta^2$ for a group of randomly generated graphs with $n = 11$. The distribution shows that few graphs lead to a large inverse square of the gap, but most problems correspond to small inverse square of the gap near the average. Thus it is reasonable that we use the average of the inverse square of the energy gap to compute the time complexity.

Although our algorithm is quantum, we can still simulate it on our classical computer when the graph size is not very large. In our simulation, we choose the direction $\hat{n}$ to be along the $y$-axis. In this simple case, we have explicitly how the spin operators rotate

$$\begin{cases} s_{a_j}^x(t) = s_{a_j}^x \cos(2\pi t/T) + s_{a_j}^z \sin(2\pi t/T), \\ s_{a_j}^y(t) = s_{a_j}^y, \\ s_{a_j}^z(t) = -s_{a_j}^x \sin(2\pi t/T) + s_{a_j}^z \cos(2\pi t/T). \end{cases} \tag{26}$$

In our numerics, we choose $T = \pi/(50\delta^2)$ for randomly-generated graphs with $n$ from 8 to 14. We simulate the evolution of the system by the fourth-order Runge–Kutta method, and calculate the module square of the coefficients, i.e., probability, of the final state on all the possible ground states. The probability of the trivial states for graphs with $n$ from 8 to 14 and the probability distribution for a graph with $n = 14$ are shown in Fig. 3. It can be seen that after the adiabatic evolution, we do not return to the trivial state but reach a non-trivial state with a high probability. Such an ability to find a non-trivial solution is better than that of the classical algorithm proposed in Refs. [12,15].

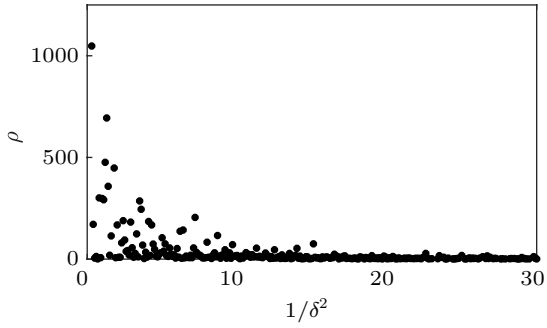



**Fig. 2.** The distribution of the inverse square of energy gaps for 10000 randomly generated problems with $n = 11$. The $x$-axis is the inverse square of the energy gap, $1/\delta^2$, and the $y$-axis is the number $\rho$ of problems whose energy gap is within $[1/\delta^2 - 0.1, 1/\delta^2]$.

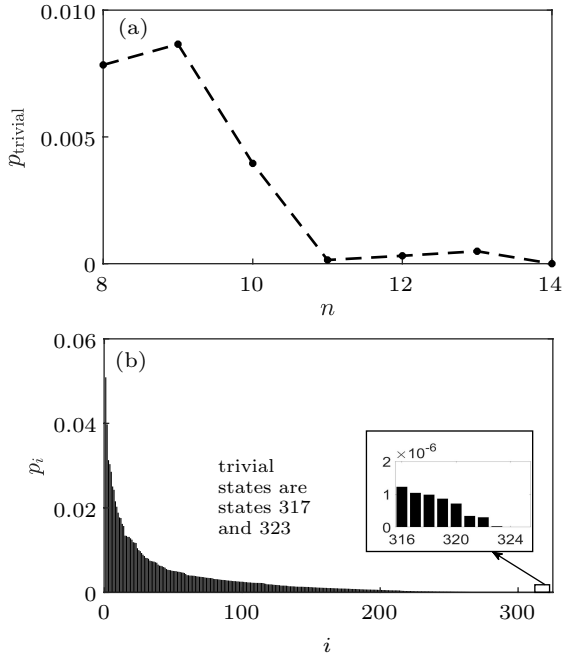



**Fig. 3.** (a) The probability of trivial states of a randomly generated Q2SAT problem after the adiabatic evolution for different $n$. The dashed line is guide for the eyes. (b) The probability distribution of a randomly generated Q2SAT problem on all its ground states after the adiabatic evolution for $n = 14$. The $x$-axis is the index of all the ground states. The $y$-axis is the probabilities of the ground states in the final state. The ground states are indexed according to their probabilities in the descending order. The indexes of the trivial states are 317 and 323.

For our algorithm to work, a large number of solutions are required. However, when $d > 0.1$, the number of solutions decreases significantly. In that case, the state remains on trivial states with a high probability after the adiabatic evolution,

and our algorithm thus does not work any more. Numerical results show that for $n = 14$ and $d > 0.15$, our algorithm fails with a non-negligible probability.

## 6. Conclusion

A quantum adiabatic algorithm for the Q2SAT problem is proposed. In the algorithm, the Hamiltonian is constructed so that all the solutions of a Q2SAT problem are its ground states. A trivial product-state solution is chosen as the initial state. By rotating all the qubits, the system evolves adiabatically in the subspace of solutions and ends up on a non-trivial state. Theoretical analysis and numerical simulation show that, for a set of Q2SAT problems, our algorithm finds a non-trivial solution with time complexity better than the existing algorithms.

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