Excited state search using quantum annealing

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Abstract

Quantum annealing (QA) is one of the ways to search the ground state of the target Hamiltonian. Here, we analyze the performance of the QA to search the first excited state of the target Hamiltonian. In our scheme, the first excited state of the trivial Hamiltonian (such as transverse magnetic fields) is initially prepared and is adiabatically changed into the first excited state of the target Hamiltonian. As a comparison, we also consider another scheme to find the first excited state with non-adiabatic transitions from the ground state. By solving the Lindblad master equation, we evaluate the performance of each scheme under the effect of decoherence. Our conclusion is that the adiabatic scheme show better performance than the non-adiabatic scheme as long as the necessary evolution time to satisfy the adiabatic condition is shorter than the coherence time of the qubit. These results are important for applications such as quantum chemistry computation and post-quantum cryptography.
I. INTRODUCTION

Exploring new applications of noisy quantum devices is an important issue to work on for the development of quantum computing technologies. In recent years, a lot of groups have put intensive efforts into developing devices for quantum computing. For example, D-Wave Systems inc. has developed quantum devices based on quantum annealing (QA) [1], and released D-Wave 2000Q consisting of over two thousands of superconducting qubits [2]. In addition, several hardwares for quantum computing have been devised and developed [3–8]. Although it is unclear if such devices can resolve real world important issues, we cloud still use such devices to check whether these really provide us with the solutions of practical problems much faster than existing classical computers. For this purpose, it is important to look for the applications on such devices.

Quantum chemistry computation is considered as an application where quantum computation seems to have an advantage over classical computers [9]. The dynamics of molecules studied in quantum chemistry is governed by the second-quantized Hamiltonians. It requires exponentially large amount of memory to apply ab initio calculations on classical computers to the quantum chemistry computation, since the dimension of the Fock space grows exponentially as the number of the modes increases. Importantly, quantum computers cloud effectively represent the second-quantized Hamiltonians using qubits. Bravyi and Kitaev have developed a method to transform the second-quantized Hamiltonians to those of spin-1/2 systems, where the number of the spins is the same as that of the modes [10–12]. Thus, quantum computers can be used to analyze the molecule systems represented by spin-1/2 systems.

Excitation energy is an important physical property of molecule systems [13]. In order to explain (or predict) the spectroscopic and photochemical properties of molecules, the energy of the excited state as well as that of ground state is required. The simulation of the behavior of the excited states includes difficulties such as many classes of excited states, and hence methods for the calculation of the excited state are still under development in the quantum chemistry computation.

Excited state search also appears in post-quantum cryptography [14]. Some of the cryptograph base on the shortest vector problem, which belongs to the class of NP-hard [15]. Joseph et al. have investigated the performance of QA for the shortest vector problem, where
the solution of the problem is embedded in the first excited state of the problem Hamiltonian \[16\]. Their method prepares a ground state of an initial Hamiltonian, then causes quantum state transition to the first excited state.

In the present paper, we develop methods to calculate excited states based on quantum annealing \[17–19\], and compare performance of the methods. Quantum algorithms on the quantum circuit model to calculate the properties of excited states has been developed \[20–23\]. However, methods on QA to search excited states have not been studied well. We introduce two methods, adiabatic and non-adiabatic scheme, to obtain excited quantum states. While the idea of the latter method is the same as the method by Ref. \[16\], the former method for excited state search has not been investigated. In order to compare the methods, we apply them to the problem of finding the first excited state of the spin-star model, which is analytically tractable and has the similar type of interactions in the Hamiltonian to those in the Hamiltonians of the molecule systems \[24\]. To take noise into account, we adopt the Lindblad master equation \[23\], and compare the two schemes by numerically solving the master equation. We find that the adiabatic scheme has a better performance than the non-adiabatic scheme as long as the coherence time of the qubit is longer than the necessary evolution time to satisfy the adiabatic condition.

The remainder of this paper is organized as follows. In Sec. II, we introduce the adiabatic and non-adiabatic scheme to obtain excited estates based on quantum annealing. We show the Hamiltonian of the spin-star model in Sec. III. Section IV is devoted to explain protocol to apply the proposed methods to the spin-star model, and describing how to compare the methods. We show numerical results in Sec. V and give an interpretation to the results in Sec. VI. Finally, we conclude in Sec. VII.

II. ADIABATIC AND NON-ADIABATIC SCHEME FOR EXCITED STATES

We propose two methods to obtain excited states of spin-1/2 systems, namely adiabatic scheme and non-adiabatic scheme.

The adiabatic scheme, which is known as adiabatic quantum computation, is based on the adiabatic theorem \[25\]. Let us consider a problem of finding an \(n\)-th excited state of a problem Hamiltonian. Assuming that there are no crossings for the \(n\)-th energy level of the total Hamiltonian during the annealing process, we can obtain the \(n\)-th excited state of the
problem Hamiltonian with a high fidelity by evolving the \( n \)-th excited state of the driver Hamiltonian sufficiently slowly in the absence of noise. Under noisy environment, as we increase the evolution time, the decoherence is more significant, resulting in a low fidelity. Hence, there should be an optimal evolution time in order to obtain the highest fidelity in the noisy environment.

The non-adiabatic scheme could provide us with a way to obtain the desired excited state by inducing the transitions from the ground state to the other states. In the present paper, we prepare the ground state of the trivial initial Hamiltonian such as the conventional transverse-field term, then non-adiabatically change the parameters of the Hamiltonian so that the final state should have some overlap with the desired state due to the Landau–Zener transition. It is worth mentioning that, while the adiabatic scheme could provide the excited state with a high fidelity without any decoherence due to the adiabatic theorem, there is no guarantee for the non-adiabatic scheme to obtain the desired state with a high fidelity.

### III. SPIN-STAR MODEL

In this section, we introduce the spin-star model \cite{24}. It is worth mentioning that this model contains both \( XX \) and \( YY \) interactions unlike the conventional Ising type model that only contains \( ZZ \) interactions. Importantly, considerable attention has been attracted to such \( XX \) and \( YY \) interactions in the field of QA, because the typical Hamiltonian in the quantum chemistry (that is one of the practical applications in the QA) contains such terms.

We show the Hamiltonian of the spin-star model with a uniform longitudinal field, i.e. without detuning. Under the uniform longitudinal filed \( h/2 \), the Hamiltonian of the spin-star model is given by

\[
\hat{H}_P = \frac{h}{2} \sum_{i=0}^{N} \hat{\sigma}_i^z + J \sum_{i=1}^{N} (\hat{\sigma}_i^+ \hat{\sigma}_{i-1}^- + \hat{\sigma}_i^- \hat{\sigma}_{i+1}^+),
\]

(1)

where the spin at the zeroth site corresponds to the central spin and the others to the satellite spins. The Pauli operators acting on site \( i \) are denoted as \( \sigma_i^x, \sigma_i^y, \) and \( \sigma_i^z \). The creation and annihilation operators are \( \sigma_i^\pm = \sigma_i^x \pm i\sigma_i^y \). The Hamiltonian \((1)\) can be rewritten using the angular momentum coupling of the satellite spins as

\[
\hat{H}_P = \frac{h}{2} \hat{\sigma}_0^z + h \hat{S}^z + J(\hat{\sigma}_0^+ \hat{S}^- + \hat{\sigma}_0^- \hat{S}^+),
\]

(2)
where the $z$ component of the total angular momentum is defined as \( \hat{S}^z \equiv \sum_{i=1}^N \hat{\sigma}_i^z / 2 \), and the $x$ and $y$ components are defined similarly. The spin ladder operators for the total angular momentum are defined as \( \hat{S}^\pm \equiv \hat{S}^x \pm i \hat{S}^y \).

We analytically show the eigensystem of the spin-star Hamiltonian with the uniform longitudinal field. The eigenstate of the Hamiltonian (2) can be represented by using the Dicke states \( |S,S^z\rangle \), which are simultaneous eigenstates of the square of the total angular momentum \( \hat{S}^2 \equiv (\hat{S}^x)^2 + (\hat{S}^y)^2 + (\hat{S}^z)^2 \) and the $z$ component of the total angular momentum \( \hat{S}^z \). The variables in the Dicke states take discrete values, \( S = N/2, N/2 - 1, \ldots \) and \( S^z = -S, -S + 1, \ldots, S - 1, S \). Firstly, we can confirm that the eigenstates of the problem Hamiltonian for \( -S + 1 \leq S^z \leq S - 1 \) are given as

\[
|\psi^+_{S^z}\rangle = \frac{1}{\sqrt{2}} |\downarrow \rangle |S,S^z\rangle + \frac{1}{\sqrt{2}} |\uparrow \rangle |S,S^z - 1\rangle, \\
|\psi^-_{S^z}\rangle = \frac{1}{\sqrt{2}} |\downarrow \rangle |S,S^z\rangle - \frac{1}{\sqrt{2}} |\uparrow \rangle |S,S^z - 1\rangle,
\]

and the eigenvalues are

\[
E_{S^z}^\pm = \hbar \left( S^z - \frac{1}{2} \right) \pm J \sqrt{S(S + 1) - S^z(S^z - 1)}. 
\]

Secondly, for \( S^z = -S \), the eigenstate is

\[
|\psi^-_{-S}\rangle = |\downarrow \rangle |S,-S\rangle 
\]

and the eigenvalue is

\[
E_{-S}^- = -\hbar \left( S + \frac{1}{2} \right).
\]

Finally, the eigenstate for \( S^z = S \) is given as

\[
|\psi^+_{S}\rangle = |\uparrow \rangle |S,S\rangle,
\]

and the eigenvalue is

\[
E_{S}^+ = \hbar \left( S + \frac{1}{2} \right).
\]

IV. SETUP FOR COMPARISON OF ADIABATIC AND NON-ADIABATIC SCHEME

We compared the performance of adiabatic and non-adiabatic scheme based on the fidelity, that is, the overlap between the target quantum state and the final state after performing the proposed methods. Let us consider the problem of finding the first excited state
of the spin-star model. The fidelity is defined as

$$F(T) = |\langle \psi_{-S+1} | \Psi(T) \rangle|^2,$$  \hspace{1cm} (10)

where $|\psi_{-S+1}\rangle$ is the eigenstate of the spin-star model in the maximum angular momentum space $S = N/2$ given by Eq. (4), and $|\Psi(T)\rangle$ is a result of quantum annealing whose evolution time is $T$.

We calculate the final state after performing the proposed methods by solving the Lindblad master equation. The detail of the form of the Lindblad operator strongly depends on the choice of the physical systems, and there are many research about the decoherence during the quantum annealing. Here, we adopt a simple phenomenological depolarizing model described in Ref. [26]. The Lindblad master equation used in the present paper is given as

$$\frac{d\rho(t)}{dt} = -i[\hat{H}(t), \rho(t)] + \frac{1}{T_1} \sum_{i=1}^{N} \sum_{\alpha=x,y,z} (\hat{\sigma}_i^{\alpha} \rho(t) \hat{\sigma}_i^{\alpha} - \rho(t) \hat{\sigma}_i^{\alpha} \rho(t) \hat{\sigma}_i^{\alpha}),$$  \hspace{1cm} (11)

where $\rho(t)$ is a density matrix of the quantum state at time $t$, $T_1$ is a relaxation time that corresponds to the inverse of the strength of the decoherence, and $\hat{H}(t)$ is a total Hamiltonian of quantum annealing given as

$$\hat{H}(t) = t \hat{H}_P + \left(1 - t \frac{1}{T}\right) \hat{V}.$$  \hspace{1cm} (12)

Here, the problem Hamiltonian $\hat{H}_P$ is the Hamiltonian of the spin-star model in Eq. (I), and the operator $\hat{V}$ is a driver Hamiltonian that introduces quantum effects into the system, and induces transitions between the quantum states.

In the case of the non-adiabatic scheme, we adopt the usual transverse-field term as the driver Hamiltonian, $\hat{V} = -\sum_{i=1}^{N} \hat{\sigma}_i^{x}$. Firstly, we prepare the ground state of the transverse-field term at the beginning of the quantum annealing, $|\Psi(0)\rangle = |+ \cdots +\rangle$, where the quantum state $|+\rangle$ represents the eigenstate of $\hat{\sigma}_i^{x}$ with the eigenvalue $+1$. Secondly, let this state evolve by the Lindblad master equation in Eq. (11). Finally, we calculate the fidelity given by Eq. (10). In order to find the best evolution time that maximizes the fidelity, we repeat the above procedure for various evolution times. We confirmed that there exists the optimal total evolution time $T$ to maximize the fidelity. Also, we confirmed that in the limit of of small or large $T$, the fidelity converges to a finite small value.

For the adiabatic scheme, we cannot use the conventional driver Hamiltonian (that is designed to find the ground state), but need to choose a suitable Hamiltonian, depending
on which excited state we want to find. More specifically, the first excited state of the conventional transverse-field term is degenerate, which makes it difficult to achieve the target first excited state of the problem Hamiltonian after the adiabatic scheme. The proper superposition of the degenerate first excited state could be derived from the backward unitary evolution of the target state based on the Hamiltonian \[ \hat{H} \] (12). However, it is generally impossible to obtain the proper superposition without knowing the target state. In order to resolve the issue, we adopt the following inhomogeneous transverse field as the driver Hamiltonian:

\[
\hat{V} = -b\hat{\sigma}_0^x - \sum_{i=1}^{N} \hat{\sigma}_i^x.
\] (13)

Here, the parameter \( b \), which takes a real value between zero and unity, determines the difference between the eigenvalue of the first excited state and that of the ground state. This also determines the difference between the eigenvalue of the second excited state and that of the first excited state. The eigenvalue of the first excited state is \( E_1 = E_0 + b(E_2 - E_0) \), where \( E_0 = -N - b \) and \( E_2 = -N - b + 2 \) are the eigenvalues of the ground state and second excited state, respectively. We can use the non-degenerate first excited state as the initial state. Also, we let the state evolve by the Lindblad master equation in the Eq. (11) for a time \( T \), and calculate the fidelity \( F(T) \). By sweeping \( T \), we find the maximum fidelity with an optimized evolution time \( \tau \).

In order to compare the two schemes (adiabatic and non-adiabatic one), we consider two sets of parameters where the energy difference between the first excited state and ground state of the target Hamiltonian is different. The energy difference between the first excited state and the ground state is \( h - J\sqrt{N} \) from Eqs. (5) and (7). We adopt the strength of longitudinal field as the reference scale of energy, and so we set \( h = 1 \). We consider two cases with \( J = 1/(2\sqrt{N}) \) and \( J = 9/(10\sqrt{N}) \) where the ground state and the first excited state are well detuned from the other excited states. In the former case, the energy of the first excited state is much more detuned from that of the ground state than the latter case. In the latter case, the first excited state is close to the resonance with the ground state. We refer to the former and latter cases as \textit{detuned} and \textit{nearly-degenerate} cases, respectively.

We used QuTiP [27] to solve the Lindblad master equation (11), multidimensional arrays of NumPy [28] as containers of data, and the Brent’s method implemented in SciPy [29] to find the maximum fidelity. All the figures for numerical results were generated using...
V. RESULTS

Firstly, we show the maximum fidelity as a function of the relaxation time $T_1$. Figure 1a represents the results for the detuned case. The total number of the spins is six, consisting of five satellite spins and one central spin. The maximum fidelity increases as the relaxation time increases for all the data. Regardless of the value of $b$, the maximum fidelities for the adiabatic scheme are greater than the fidelity for the non-adiabatic scheme. While the fidelity for the non-adiabatic scheme does not reach unity, those for the adiabatic scheme converge to unity as the relaxation time gets longer, so that we can obtain the target state with a high probability by using the adiabatic scheme. In contrast, Fig. 1b shows that the maximum fidelities are almost the same for both schemes for a large value of $T_1$ in the nearly-degenerate case.

![Graph](image1.png)

(a) Detuned case  
(b) Nearly-degenerate case

FIG. 1. Maximum fidelity as a function of relaxation time for detuned case (a) and nearly-degenerate case (b). The thick solid line represents the maximum fidelity obtained from the non-adiabatic scheme. The thin lines show the maximum fidelities for the adiabatic scheme with the parameters, namely $b = 0.1$ (solid), $b = 0.5$ (dashed), and $b = 0.9$ (dotted).

Secondly, we plot the optimized evolution time $\tau$ where the fidelity is maximized. Figure 2a (2b) corresponds to the detuned (nearly-degenerate) case. We can see that the optimal evolution time for the non-adiabatic scheme to get the best fidelity is almost constant for
both cases, whereas the optimal evolution times for the adiabatic scheme increase as the relaxation time increases except for $b = 0.5$ in the nearly-degenerate case.

![Graph showing optimal evolution time as a function of relaxation time for detuned case and nearly-degenerate case.](image)

**FIG. 2.** Optimal evolution time as a function of relaxation time for detuned case (a) and nearly-degenerate case (b). The thick solid line represents the optimal evolution time for the non-adiabatic scheme. The thin lines show the optimal evolution time for the adiabatic scheme with the parameters, namely $b = 0.1$ (solid), $b = 0.5$ (dashed), and $b = 0.9$ (dotted).

**VI. DISCUSSION**

We showed that the adiabatic scheme can achieve a fidelity that is equal or higher than that for the non-adiabatic scheme in Fig. 1. In the detuned case, the maximum fidelity for the adiabatic scheme is always higher than that for the non-adiabatic scheme. In contrast, for the nearly-degenerate case, the non-adiabatic scheme achieves as high fidelity as the adiabatic scheme. This behavior can be understood from the minimum gap between the instantaneous first excited state and the ground state. In the detuned case, the gap is greater than the nearly-degenerate case. The large gap suppresses the quantum state transition from the ground state to the first excited state, and causing the low fidelity for the non-adiabatic scheme. In the nearly-degenerate case, it is possible to move the large amount of population in the ground state to the first excited state by adjusting the evolution time. Although the gap for the nearly-degenerate case is smaller than the detuned case, the adiabatic scheme can obtain as high fidelity as the non-adiabatic scheme. Accordingly, we conclude that the
adiabatic scheme is better than the non-adiabatic scheme in terms of the achievable fidelity.

The optimal evolution time for the non-adiabatic scheme is almost independent of the relaxation time in both cases (Fig. 2). The optimal evolution time is of the order of 10, which is much smaller than the relaxation time we investigated. Since the induced noise hardly affects the system in this regime, the optimal evolution time is almost independent of $T_1$.

The optimal evolution time for the adiabatic scheme strongly depends on the value of $b$. This behavior is determined by the relaxation time and the minimum energy gap between the ground state and first excited state. When the gap is sufficiently large, and thus the evolution time to satisfy the adiabatic condition is smaller than the relaxation time shown in the Fig. 2, the optimal evolution time is almost independent of the relaxation time. This is due to the same reason for the optimal evolution time for the non-adiabatic scheme described above. In contrast, when the evolution time to satisfy the adiabatic condition is greater than the relaxation time, the optimal evolution time is determined by the competition between the diabatic transition from the first excited state and the relaxation of the quantum state. In this regime, the optimal evolution time increases as the relaxation time increases. Once the relaxation time becomes longer than the necessary evolution time for the adiabatic process, the optimized evolution time becomes independent of the relaxation time.

VII. CONCLUSION

The major aim of the present paper is to show the advantage of the adiabatic scheme against the non-adiabatic scheme when we search the excited state of the Hamiltonian. To quantify the performance, we adopt a fidelity between the state obtained from the dynamics and the first excited state of the target Hamiltonian. As the example to quantify the performance, we consider the spin-star model that contains flip-flop interaction terms, which provides us with a non-trivial excited state unlike the Ising Hamiltonian. To take the noise into account, we adopt a Lindblad master equation that represents the depolarizing noise. We implemented the numerical simulation to study the performance of each scheme. We conclude that the adiabatic scheme can achieve a higher fidelity than the non-adiabatic scheme if the energy gap between the target energy level and the other levels is large, while the fidelity of the adiabatic scheme is still comparable with that of the non-adiabatic scheme.
even when such a gap becomes small.

Such a search of the excited state is one of the important topics of quantum chemistry. In order to apply our proposal to the excited state search, it is necessary to realize the non-stoquastic Hamiltonian in QA device, since the Hamiltonian for the quantum chemistry computation can include $XX$ interactions as well as $ZZ$ interactions that cause the negative sigh problem in the quantum Monte Carlo method. In the current technology, only a few qubit can be coupled each other via the non-stoquastic Hamiltonian. However, it is expected that more sophisticated technique of the fabrication would be applied to the qubits in the future so that we could use a better device for the QA, which will lead us to realize the practical applications of the quantum chemistry using QA. It is also worth mentioning that D-Wave machine uses only DC magnetic fields, and accordingly it cannot prepare the excited state with microwave $\pi$ pulses. On the other hand, there is another type of quantum annealing that uses microwave (or radio frequency) driving fields such as Refs. [31, 32], and this kind of architecture is suitable for our scheme. Our theoretical proposals would be useful to provide one of the examples to check whether such future QA devices outperform the classical computers.

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