Extended Abstracts of the 2020 International Conference on Solid State Devices and Materials, VIRTUAL conference, 2020, pp647-648

Direct estimation of the energy gap between the ground state and excited state with quantum annealing

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Abstract

Quantum chemistry is one of the important applications of quantum information technology. Especially, an estimation of the energy gap between a ground state and excited state of a target Hamiltonian corresponding to a molecule is essential in medical areas. In the previous approach, an energy of the ground state and that of the excited state are estimated separately, and the energy gap can be calculated from the subtraction between them. Here, we propose a direct estimation of the energy gap between the ground state and excited state of the target Hamiltonian with quantum annealing. The key idea is to combine a Ramsey type measurement with the quantum annealing. This provides an oscillating signal with a frequency of the energy gap, and a Fourier transform of the signal let us know the energy gap. Based on typical parameters of superconducting qubits, we numerically investigate the performance of our scheme when we estimate an energy gap between the ground state and first excited state of the Hamiltonian. We show robustness against non-adiabatic transitions between the ground state and first-excited states. Our results pave a new way to estimate the energy gap for quantum chemistry.

1. Introduction

Quantum annealing (QA) has been studied as a way to solve combinational optimization problem [1,2] where the goal is to minimize a cost function. Such a problem is mapped into a finding of a ground state of Ising Hamiltonians that contain the information of the problem. QA is designed to find an energy eigenstate of the target Hamiltonian by using adiabatic dynamics. So, by using the QA, we can find the ground state of the Ising Hamiltonian for the combinational optimization problem.

Recently, it was shown that the QA can be also used for quantum chemistry calculations [3,4]. Important properties of molecules can be investigated by the second quantized Hamiltonian of the molecules. Especially, the energy gap between the ground state and excited states is essential information for such a study [3]. The second quantized Hamiltonian can be mapped into the Hamiltonian of qubits [4]. Importantly, not only the ground state but also the excited state of the Hamiltonian can be prepared by the QA [5]. By measuring suitable observable on such states prepared by the QA, we can estimate the eigenenergy of the eigenstates. In the conventional approaches, we need to perform two separate experiments to estimate an energy gap between the ground state and the excited state. In the first (second) experiment, we measure the eigenenergy of the ground (excited) state prepared by the QA. From the subtraction between the estimation of the eigenenergy of the ground state and that of the excited state, we can obtain the information of the energy gap.

Here, we propose a way to estimate an energy gap between the ground state and excited state in a more direct manner. The key idea is to use the Ramsey type measurement where a superposition between the ground state and excited state acquires a relative phase that depends on the energy gap [7]. By performing a Fourier transform of the signal from the Ramsey type experiments, we can estimate the energy gap. We numerically study the performance of our protocol to estimate the energy gap between the ground state and first excited state. We show robustness of our scheme against non-adiabatic transitions between the ground state and first excited state.

2. Estimation of the energy gap between the ground state and excited state based on the Ramsey type measurement

$$H_{\mathrm{QA}} = (1-\frac{t}{T})H_{\mathrm{D}} + \frac{t}{T}H_{\mathrm{P}} \quad (1)$$

$$H_{\mathrm{R}} = H_{\mathrm{P}} \quad (2)$$

$$H_{\mathrm{RQA}} = \frac{t-(T+\tau)}{T}H_{\mathrm{D}} + (1-\frac{t-(T+\tau)}{T})H_{\mathrm{P}} \quad (3)$$

where H_{QA} denotes the Hamiltonian that are used in the standard QA, H_{D} denotes the driving Hamiltonian that are typically chosen as the transverse magnetic field terms, H_{P} denotes the target (or problem) Hamiltonian whose energy gap we want to know, H_{R} denotes the Hamiltonian for the Ramsey type evolution, and H_{RQA} denotes the Hamiltonian that are used in a reverse QA [8]. Firstly, prepare an initial state of $|\varphi_0\rangle=(|E_0^{(D)}\rangle+|E_1^{(D)}\rangle)/\sqrt{2}$ where $|E_0^{(D)}\rangle$ ($|E_1^{(D)}\rangle$) denotes the ground (excited) state of the driving Hamiltonian. Secondly, let this state evolve by the Hamiltonian of H_{QA} from t=0 to t=T, and we obtain a state of $(|E_0^{(P)}\rangle+e^{-i\theta}|E_1^{(P)}\rangle)/\sqrt{2}$ if the dynamics is adiabatic where $|E_0^{(P)}\rangle$ ($|E_1^{(P)}\rangle$) denotes the ground (excited) state of the target Hamiltonian and θ denotes a relative phase acquired during the dynamics. Thirdly, let the state evolve by the Hamiltonian

of H_R for a time τ, and we obtain $(|E_0^{(P)}\rangle + e^{-i\Delta E\tau - i\theta}|E_1^{(P)}\rangle)/\sqrt{2}$ where $\Delta E = E_1^{(P)} - E_0^{(P)}$ denotes an energy gap and $E_0^{(P)}$ ($E_1^{(P)}$) denotes the eigenenergy of the ground (first excited) state of the target Hamiltonian. Fourthly, let this state evolve by the Hamiltonian of H_{RQA} from $t=T+\tau$ to $t=2T+\tau$, and we obtain a state $(|E_0^{(D)}\rangle + e^{-i\Delta E\tau - i\theta'}|E_1^{(D)}\rangle)/\sqrt{2}$ if the dynamics is adiabatic where θ' denotes a relative phase acquired during the dynamics.. Fifthly, we readout the state by using a projection operator of $|\varphi_0\rangle\langle\varphi_0|$, and the projection probability is $P_\tau = (1 + \cos(\Delta E\tau + \theta'))/2$, which is an oscillating signal with a frequency of the energy gap. Finally, we repeat the above five steps by sweeping τ, and obtain several values of P_τ. We can perform the Fourier transform of P_τ such as

$$f(\omega) = \sum_{n=1}^{N} (P_{\tau_n} - 0.5) e^{-i\omega\tau_n} \qquad (4)$$

where $\tau_n = t_{min} + (n-1)/((N-1)(t_{max} - t_{min}))$ denotes a time step, t_{min} (t_{max}) denotes a minimum (maximum) time to be considered, and N denotes the number of the steps. The peak in $|f(\omega)|$ shows the energy gap ΔE.

To check the efficiency, we perform the numerical simulations to estimate the energy gap between the ground state and first excited state, based on typical parameters for superconducting qubits. We choose the following Hamiltonians.

$$H_D = \sum_{i=1}^{L} \frac{\lambda_i}{2} \sigma_x^{(i)} \qquad (4)$$

$$H_P = \sum_{i=1}^{L} \frac{\omega_i}{2} \sigma_z^{(i)} + \sum_{i=1}^{L-1} g\, \sigma_z^{(i)} \sigma_z^{(i+1)} + g'\, (\sigma_+^{(i)} \sigma_-^{(i+1)} + hc) \qquad (5)$$

where λ_i denotes the amplitude of the transverse magnetic fields of the i-th qubit, ω_i denotes the frequency of the i-th qubit, and g (g') denotes the Ising (flip-flop) type coupling strength between qubits. The initial state is |1>|-> where |1> (|->) is an eigenstate of σ_z (σ_x) with an eigenvalue of +1 (-1). In the Fig. 1, we plot the Fourier function $f(\omega)$ against ω for this case. We have a peak around $\omega = 1.067$GHz, which corresponds to the energy gap ΔE of the problem Hamiltonian in our parameter. So this result shows that we can estimate the energy gap by using our scheme.

Also, we have a smaller peak of around $\omega = 0$ in the Fig.1, and this comes from non-adiabatic transitions between the ground state and first excited state. If the dynamics is perfectly adiabatic, the population of both the ground state and first excited state should be 1/2 at t=T. However, in our parameters with T=150 (75) ns, the population of the ground state and excited state is around 0.6 (0.7) and 0.4 (0.3) at t=T, respectively. In this case, the probability at the readout step should be modified as $P_\tau = (a + b\cos(\Delta E\tau + \theta'))$ where the parameters a and b deviates from 1/2 due to the non-adiabatic transitions. This induces the peak of around $\omega = 0$ in the Fourier function $f(\omega)$. As we decrease T, the dynamics becomes less adiabatic, and the peak of $\omega = 0$ becomes higher while the target peak corresponding the energy gap ΔE becomes smaller as shown in the Fig. 1. Importantly, we can still identify the peak of the energy gap for the following reasons. First, there is a large separation between the peaks. Second, the non-adiabatic transitions do not affect the peak position. So our scheme is robust against the non-adiabatic transition between the ground state and first excited state. This is stark contrast with a previous scheme that is fragile against such non-adiabatic transitions [6].

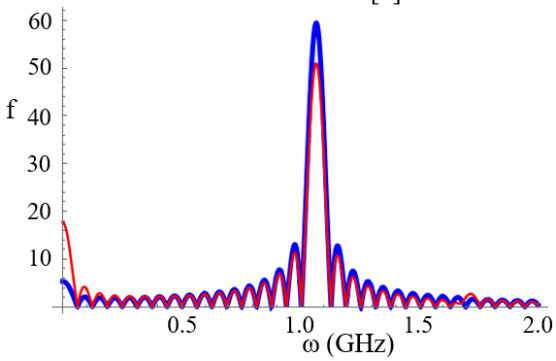

Fig. 1 Fourier function against a frequency. Here, we set parameters as $\lambda_1/2\pi$=1 GHz, $g/2\pi$=0.5 GHz, $\omega_1/2\pi$=0.2 GHz, ω_2/ω_1=1.2, g'/g=2.1, λ_2/λ_1=10.7, L=2, N=10000, t_{min}=0, and t_{max}=100 ns. Also, we set T=150 (75) ns for the blue (red) plot.

5. Conclusions

In conclusion, we propose a scheme that allows the direct estimation of an energy gap of the target Hamiltonian by using quantum annealing (QA). While a ground state of a driving Hamiltonian is prepared as an initial state for the conventional QA, we prepare a superposition between a ground state and the first excited state of the driving Hamiltonian as the initial state. Also, the key idea in our scheme is to use a Ramsey type measurement after the quantum annealing process where an information of the energy gap is encoded as a relative phase between the superposition. The readout of the relative phase by sweeping the Ramsey measurement time duration provides a direct estimation of the energy gap of the target Hamiltonian. Our scheme paves an alternative way to estimate the energy gap of the target Hamiltonian for applications of quantum chemistry.

Acknowledgements

This presentation is partly based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan. This work was also supported by Leading Initiative for Excellent Young Researchers MEXT Japan, JST presto (Grant No. JPMJPR1919) Japan.

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