Quantum annealing, as currently implemented in hardware, cannot fairly sample all ground states. Graph minor embedding in a quantum annealer leads to biased sampling results. We demonstrate the influence of the embedding process on sampling results in a degenerate problem and analyze the details using perturbation theory. Our result also shows the relationship between the probabilities of ground states and the energy landscape between them.

Quantum annealing (QA) is a metaheuristic for solving combinatorial optimization problems using quantum effects. The hardware which implements QA has been developed, such as D-Wave quantum annealer. In some applications that have multiple solutions, such as SAT filter or machine learning, it is essential to attain all the ground states fairly. However, the standard QA cannot sample all ground states with equal probability and more sophisticated one might be necessary for fair sampling. Current versions of quantum annealers also sample all solutions unfairly.

Quantum annealer needs a certain transformation of problems for treating with them on the hardware, one of which is graph minor embedding. This is a process of mapping logical variables to physical qubits on the hardware graph. It is difficult to express an original problem on them directly, although the connectivity of graph which D-Wave quantum annealers has gradually increased. Then one can add auxiliary variables and ferromagnetic interactions called chain. For optimization purposes, chain strength is involved with the performance by QA.

The effect of embedding for sampling is more pronounced than for optimization. Although optimization aims to attain one of the ground states, sampling requires all of them ideally with equal probability. The graph minor embedding can have an influence on thermal and quantum sampling. Previous study demonstrates sampling performance of quantum annealer for problems with additional variables needless. We demonstrate the effect of embedding for sampling by QA in degenerate systems that needs auxiliary variables.

A Hamiltonian of transverse-field Ising model with $N$ spins is defined by

$$H(t) = -\left(1 - \frac{t}{\tau}\right) \sum_j \hat{\sigma}_j^z + \frac{t}{\tau} \hat{H}_0(\hat{\sigma}_j^z),$$

where $\hat{H}_0$ is a target Hamiltonian, and $\hat{\sigma}_j^x, \hat{\sigma}_j^z$ are $x$ and $z$ component of the Pauli operator. $\hat{H}(t)$ changes from $-\sum_j \hat{\sigma}_j^z$ at $t = 0$ to $\hat{H}_0$ at $t = \tau$. For large $\tau$, the system follows the instantaneous ground state more likely, leading to the nontrivial final ground state of $\hat{H}_0$.

We assume a five-spin system as shown in Fig.1 (a), whose target Hamiltonian is given by $\hat{H}_0 = -\sum_{i\neq j} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z$, where all interactions $J_{ij} = \pm 1$. This system has three ground states $|\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$, $|\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$, and $|\uparrow\uparrow\downarrow\downarrow\downarrow\rangle$, which are denoted by $|1\rangle$, $|2\rangle$, and $|3\rangle$ in order. As this model also has spin inversion symmetric ground states and the probabilities of the two spin-symmetric states are equal, we will attend to the three states mentioned above. In the embedded system shown in Fig.1 (b), the fifth and sixth spins correspond to the fifth spin in the original system and interact with each other at the chain strength $J_F(>0)$. This embedded model has the minimum number of spins for hardware graphs of D-Wave 2000Q and Advantage.

In general, the heuristic approach is often used to find a redundant embedding because it is difficult to find such a minor one of large-size or high-connective systems. We also do not consider any unembedding processes for excited states which have broken chains.

To account for the effects of embedding only in theoretical QA, we solve the Schrödinger equation directly. We evaluate unfairness of sampling results by the ratio of the probabilities $P_S/P_C$ that the ground states appear, where $S = |1\rangle$ and $C = |2\rangle, |3\rangle$. Fig.2 shows annealing time $\tau$ dependence on the ratio in $J_F \in \{0.5, 1.0, 1.5\}$. For sufficient large $\tau$, the ratio is non-zero in the embedded problem, although zero in the original problem. When $J_F = 1$ in particular, all the ground states can be attained fairly.

Next, we analyze the influence of graph minor embedding on sampling results in detail using perturbation theory. Following previous approaches using perturbation theory has done. We define the Hamiltonian around the final time as $\hat{H}(\tau) = \hat{H}_0 + \lambda \hat{V}$, where $\lambda > 0$ is a sufficient small coefficient and $\hat{V}$ is a driver Hamiltonian, which is recognized as
a perturbation for the target Hamiltonian $\hat{H}_0$. As mentioned above, we focus on transverse-field $V = -\sum_{i,j} J_{ij}$. Given $d$ ground states $|n^{(0)}\rangle$ of $\hat{H}_0$ with energy $E_n^{(0)}$, the eigenstate $|n\rangle$ and eigenergy $E_n$ of $\hat{H}\langle n|$ are expanded as $|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \ldots$, $E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$ for small $\lambda$. Let $\hat{P}_1$ be a project operator onto the first-level degenerate eigenspace of $\hat{H}_0$. The first-order perturbation satisfies the following equation in the degenerate level, $E_n^{(1)} |n^{(0)}\rangle = \hat{P}_1 \hat{V} \hat{P}_1 |n^{(0)}\rangle$, where the first-order energy correction $E_n^{(1)}$ and the zero-order state correction $|n^{(0)}\rangle$.

When the first-order perturbation has degeneracy, the second-order perturbation has to be considered. Let $\hat{P}_2$ be a project operator to the degenerate subspace of $\hat{P}_1 \hat{V} \hat{P}_1$. The second-order perturbation satisfies the following in the degenerate level,

$$E_n^{(2)} |n^{(0)}\rangle = \hat{P}_2 \hat{W} \hat{P}_2 |n^{(0)}\rangle,$$

where $\hat{W} = \hat{V} \hat{Q} \frac{1}{E_n^{(0)} - \hat{H}_0} \hat{Q} \hat{V}$,

and $\hat{Q} = 1 - \hat{P}_1$. Solving this equation attains the second-order energy correction $E_n^{(2)}$ and the zero-order state correction $|n^{(0)}\rangle$. The probability that ground states appear at the final time can be calculated from the eigenvector for the minimal eigenvalue of $\hat{P}_2 \hat{W} \hat{P}_2$. We confirmed that the analysis by perturbation theory corresponds to the direct solution of the Schrödinger equation in $t = 1000$ as shown in Fig.3 (a).

In the embedded model,

$$-\hat{P}_2 \hat{W} \hat{P}_2 = \begin{bmatrix}
\frac{2 J_F + 5}{J_F + 2} & 0 & 0 & 0 & 1 \\
0 & \frac{4 J_F + 1}{J_F} & 0 & 0 & 0 \\
1 & \frac{4 J_F + 1}{J_F} & 0 & 0 & 0 \\
0 & 0 & 1 & \frac{2 J_F + 5}{J_F + 2} & 0 \\
0 & 0 & 0 & \frac{4 J_F + 1}{J_F} & 0 \\
0 & 0 & 0 & 0 & \frac{4 J_F + 1}{J_F}
\end{bmatrix},$$

and equation (3), (4) show that chain strength $J_F$ changes energy gap $E_n^{(0)} - \hat{H}_0$ between the nearest ground states. As shown in Fig.3 (b), the probabilities of ground states are determined by the ratio of energy gap $\Delta E_S/\Delta E_C$, where $\Delta E$ is the average energy gap between the other nearest ground states. When $\Delta E_S/\Delta E_C > 1$, the ground state $S$ exists in a sharper valley than the ground states $C$, and hence $P_{S,1} < P_{C,2}, P_{C,3}$.

We have demonstrated experimentally and analytically that graph minor embedding influences sampling degenerate ground states by QA. Our toy model results show that the probability distribution of ground states in the embedded problem is different from that in the original problem. We use perturbation theory to analyze the probabilities of ground states and confirm that the analysis corresponds to our numerical result. We also found the relationship between the energy landscape between ground states and the probabilities. Although we deal with minimal embedding, different embeddings will vary sampling results in QA. For quantum annealers as open quantum systems, we expect to attain similar results to the present case of isolated systems, except for the effects of external bath \(^{19}\) and control errors.\(^{20}\)

**Acknowledgments** We would like to thank the fruitful discussion with Masayuki Yamamoto and Manaka Okuyama. This work was financially supported by JSPS KAKENHI Grant Nos. 20H02168, 19H01095, 18J20396 and 18H03303, partly supported by JST-CREST (No. JPJMIKRI402), the Next Generation High-Performance Computing Infrastructures and Applications R&D Program of MEXT and by MEXT-Quantum Leap Flagship Program Grant Number JPMSZ102352099.

---

1) T. Kadokawa and H. Nishimori: Physical Review E 58 (1998) 5355.
2) M. W. Johnson, P. Bunyk, F. Maibam, E. Tolkacheva, A. J. Berkley, E. M. Chapple, R. Harris, J. Johansson, T. Lanting, I. Perminov, E. Ladizinsky, T. Oh, and G. Rose: Superconductor Science and Technology 23 (2010) 065004.
3) R. Harris, M. W. Johnson, T. Lanting, A. J. Berkley, J. Johansson, P. Bunyk, E. Tolkacheva, E. Ladizinsky, T. Oh, F. Cinata, I. Perminov, P. Spear, C. Enderud, C. Rich, S. Uchaikin, M. C. Thom, E. M. Chapple, J. Wang, B. Wilson, M. H. S. Amin, N. Dickson, K. Karimi, B. Macready, C. J. S. Truncik, and G. Rose: Physical Review B 82 (2010) 024511.
4) S. A. Weaver, K. J. Ray, V. W. Marek, A. J. Mayer, and A. K. Walker: Journal on Satisfiability, Boolean Modeling and Computation 8 (2012) 129.
5) M. Azinović, D. Herr, B. Heim, E. Brown, and M. Troyer: SciPost Physics 2 (2017) 013.
6) G. E. Hinton: Neural Computation 14 (2002) 1771.
7) S. M. A. Eslami, N. Heess, C. K. I. Williams, and J. Winn: International Journal of Computer Vision 107 (2014) 155.
8) Y. Matsuda, H. Nishimori, and H. G. Katzgraber: New Journal of Physics 11 (2009) 073021.
9) M. S. Konz, G. Mazzola, A. J. Ochoa, H. G. Katzgraber, and M. Troyer: Physical Review A 100 (2019) 030303.
10) S. Mandrž, Z. Zhu, and H. G. Katzgraber: Physical Review Letters 118 (2017) 070502.
11) N. Dattani, S. Szalay, and N. Chancellor: arXiv:1901.07636 [quant-ph] (2019).
12) K. Boothby, P. Bunyk, J. Raymond, and A. Roy: arXiv:2003.00133 [quant-ph] (2020).
13) V. Choi: Quantum Information Processing 7 (2008) 193.
14) J. Marshall, A. Di Gioacchino, and E. G. Rieffel: Physical Review Research 2 (2020) 032020.
15) J. Marshall, G. Mossi, and E. G. Rieffel: arXiv:2103.07036 [quant-ph] (2021).
16) J. Cai, W. G. Macready, and A. Roy: arXiv:1406.2741 [quant-ph] (2014).
17) E. Pelofske, G. Hahn, and H. Djidjev: 2020 International Conference on Rebooting Computing (ICRC), December 2020, pp. 34–41.
18) L. M. Sieberer and W. Lechner: Physical Review A 97 (2018) 052329.
19) T. Kadokawa and M. Ohzeki: Journal of the Physical Society of Japan 88 (2019) 061008.
20) N. Chancellor, P. J. D. Crowley, T. Duric, W. Vinci, M. H. Amin, A. G. Green, P. A. Warburton, and G. Aeppli: arXiv:2006.07685 [quant-ph] (2021).