Phase transition of Frustrated Ising model via D-wave Quantum Annealing Machine

Hayun Park\textsuperscript{1} and Hunpyo Lee\textsuperscript{1}

\textsuperscript{1}Department of Liberal Studies, Kangwon National University, Samcheok, 25913, Republic of Korea
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We study the frustrated Ising model on the two-dimensional $L \times L$ square lattice with ferromagnetic (FM) nearest-neighbor and antiferromagnetic diagonal-neighbor interactions using the D-wave quantum annealing machine (D-QAM) with 5000+ qubits composed on structure of the Pegasus graph. As the former Monte Carlo and mean field results, we find the FM to stripe order phase transition, through observations of the magnetization $M$, energy, magnetic susceptibility and structure factor. We also analyze probability which occurs any $M$ at a given interaction for many quantum annealing shots to estimate the shape of objective function $f$. The only one value of $M$ with specific phase is observed in the regions far from phase transition for many quantum annealing shots, while several values of $M$ with different possibilities are appeared in the regimes of phase transition. We guess that $f$ in the regimes of phase transition retains the multi-modal structure with several local minimums, due to the strong degeneracies caused by frustrations. Finally, we discuss fail of the quantum annealing simulations, through analysis of the number of the chains, defined as the same variable with $N$-qubits, as a function of $L$.

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I. INTRODUCTION

To search for an optimal solution from many possible candidates is one of the most important and challenging problems in the economics, computational science and machine learning communities. If many possible ones are expressed in a monotonous objective function $f$, it can be easily determined by minimizing (or maximizing) of $f$. On the other hand, most important and interesting problems appeared in computational science and machine learning calculation show the complex multi-modal structures in $f$ which processes several local minimums of plausible solutions. Therefore, various numerical approaches like a simulated annealing based on a stochastic method have been developing to avoid a trap of local minimums [1] [2].

Recently, another attempt to solve optimization problems has been performing on the D-wave quantum annealing machine (D-QAM) based on superconducting qubits [3]. A quantum annealing (QA) simulation is implemented on parameterized Hamiltonian of a transverse-field Ising model with binary quadratic form (BQF) modified from $f$ of the original optimization problem [3] [4]. It has not only described the unconventional phases in physical systems, but also have applied for various engineering applications such as green energy production and traffic signal optimization [5] [10]. On the other hand, more examinations and calculations on the D-QAM would be still required and highly beneficial, because they can provide more computation information and technique for an efficient utilization and application of D-QAM. In addition, there have been a few investigations via the D-QAM.

A frustrated Ising model on the two-dimensional (2D) square lattice at zero temperature $T$ is not only one of the good examples with several local traps in $f$, but also is an exactly unsolved and interesting system, which exhibits the exotic phases and phase transitions by competition among various orderings, contrary to the case of the Ising model with only nearest-neighbor interaction, where the exact result was known [11]. Furthermore, the standard Monte Carlo (MC) simulations have not been well performed at zero temperature $T$, because the values of the Boltzmann weight function $e^{-\Delta E/T}$ for acceptances of MC step are converged to zero ($e^{-\infty} = 0$) with decreasing $T$. Therefore, we believe that the frustrated Ising model would be a good applicant for analysis of the simulation results and techniques on the D-QAM.

In this paper, using the D-QAM with 5000+ qubits composed on structure of Pegasus graph in the amazon web services (AWS) we explore the frustrated Ising model on 2D $L \times L$ square lattice with competitions of between nearest-neighbor of ferromagnetic (FM) order and diagonal-neighbor of antiferromagnetic (AF) order, where the results were well known by the MC and mean field methods [12] [13]. The Hamiltonian is given as

$$H = -J_1 \sum_{<i,j>} \sigma_i^z \sigma_j^z + J_2 \sum_{<<i,j>>} \sigma_i^z \sigma_j^z, \quad (1)$$

where nearest- and diagonal-neighbors are denoted by $<i,j>$ and $<<i,j>>$, respectively. Here, we employ $J_1 > 0$ and $J_2 > 0$ which mean the preferences of FM and AF orderings, respectively. We confirm the FM to stripe order (SO) phase transition around $J_2/J_1 \approx 0.5$ from results of the magnetization $M$, energy per site $E$, magnetic susceptibility $\chi$ and structure factor $S(\tilde{q})$ for $L = 20$, through the QA simulation. These results consist with the former MC and mean field ones [12] [13]. We also analyze probability, which presents any value of $M$ at a given $J_2/J_1$ for many QA shots, to predict the shape of $f$. Finally, we discuss limitations of the D-QAM by break of the chains, via observation of the number of the chains with meaning of the same variable with $N$-qubits as a function of $L$.

The paper is organized as follows: Section [1] gives a
FIG. 1. (a) Frustrated lattice on two-dimensional $4 \times 4$ square lattice with nearest-neighbor and diagonal-neighbor interactions of ferromagnetic (FM) order with $J_1 > 0$ and antiferromagnetic order with $J_2 < 0$, respectively. (b) The embedding with 16-sites on Perasus graph which topologically consists with (a) lattice of open boundary condition (OBC). (c) The embedding with 36-sites of OBC. (d) The embedding with 16-sites on Perasus graph which topologically consists with (a) lattice of periodic boundary condition. Here, the chains expressed as the same variables with $N$-qubits on the Pegasus graph are marked as the dotted line.

In Section III, we discuss various results on the frustrated 2D square lattice Ising model at $T = 0$ and limitation of the D-QAM by chops of the chains with different $N$-qubits. Finally, we present the conclusions in Section IV.

II. ANNEALING METHOD

For our QA simulation we use the D-QAM with 5000+ qubits composed on structure of Pegasus graph in the AWS. The QA is performed on the transverse field Ising model with BQF based on superconducting qubits. Therefore, $f$ needs to be converted into the BQF in the first QA step. On the other hand, this transformation process is not necessary in our QA simulation, because $f$ was already expressed as BQF of Ising spins.

Next QA step is to map the 2D $L \times L$ square lattice into the architecture of the Pegasus graph on the D-QAM with 5000+ qubits. Figs. 1(a) and (b) show an example of $4 \times 4$ square lattice with (red) nearest- and (blue) diagonal-neighbors interactions and an embedding with 16-site spins on the Pegasus graph with open boundary condition (OBC), respectively. Here, the chains expressed as the same variables should essentially introduce in the embedding, because the original lattice is topologically in discord with the architecture of Pegasus graph.

The quality of the QA calculations mainly suffer with increasing the number of the chains and $N$, due to high possibilities of a break of chain. Therefore, to find the embedding with the smallest number of the chains in many possibilities of embeddings is an important process for qualities of the QA simulations. We employ the iterative embedding algorithm offered in the D-QAM with 5000+ qubits of the AWS.

Finally, the QA is performing on BQF which is defined as

$$\text{BQF} = f + \sum_{i=1}^{L^2} g(i),$$

where $g(i)$ is a constraint for the optimal solution. The detailed procedures of the QA process are following. (i) Initially, we randomly select $g(i)$ to find the specious solution in many shots. (ii) After determining the specious solution, we adjust $g(i)$ to search for more optimal solution, through consulting the former configuration and constraint. (iii) We perform the QA with modified $g(i)$ again and find the specious solution which is closer to optimal solution. (iv) In the end the total energy is converged into the lowest one with the optimal solution, after doing several (ii) and (iii) processes. We perform the QA shots of 10000 times to find the configurations with meaning of the same variables should essentially introduce in the embedding, because the original lattice is topologically in discord with the architecture of Pegasus graph.

Note that the chains are composed as $N$-qubits, where $N$ is the number of qubits. The chains on the Pegasus graph are marked as the dotted line in Figs. 1(b), (c) and (d). As the results shown in Figs. 1(b) with $L = 4$ and (c) with $L = 6$ in OBC, the number of the chains and $N$ are increasing with increasing the size of $L$ in the original lattice. In addition, the number of the chains and $N$ in periodic boundary condition (PBC) are more than those in OBC, respectively, as results displayed in Figs. 1(b) with OBC and (d) with PBC. The qualities of the QA calculations mainly suffer with increasing the number of the chains and $N$, due to high possibilities of a break of chain. Therefore, to find the embedding with the smallest number of the chains in many possibilities of embeddings is an important process for qualities of the QA simulations. We employ the iterative embedding algorithm offered in the D-QAM with 5000+ qubits of the AWS.

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FIG. 3. (Color online) (Left) Structure factors for (a) $J_2/J_1 = 0.38$, (b) 0.46 and (c) 0.54. FM, coexisting and stripe order (SO) phases are observed in (a), (b) and (c), respectively.

the lowest energy in final $g(i)$, and obtain all measured quantities from the configurations with the lowest energy.

III. RESULT

We use the 2D $L \times L$ square lattice with $L = 20$ for the results shown in Fig. 2, Fig. 3 and Fig. 4. We first plot $M$ and $E$ as a function of $J_2/J_1$ in Fig. 2(a). The FM phase with spin alignments is clearly observed below $J_2/J_1 = 0.46$ in the results of $M$. The phase transition, where $M$ rapidly drops, is shown at $J_2/J_1 \approx 0.5$. $E$ displays the highest energy around phase transition with $J_2/J_1 \approx 0.5$. We also present $\chi$ expressed as $\chi = \frac{1}{2} \left< M^2 \right> - \left< M \right>^2$ in Fig. 2(b). We confirm that the magnetic fluctuations are rapidly increasing around phase transition, because the FM and AF orderings are strongly competing.

Next we present $S(\vec{q})$ with different $J_2/J_1$ in Figs. 3(a)-(c). $S(\vec{q})$ is defined as

$$S(\vec{q}) = \sum_{i,j} \sigma_i^z \sigma_j^z e^{i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)},$$

where $\vec{R}_{i,j}$ is the relative position of two spins and $\vec{q}$ is the wave vector in reciprocal space. It not only supplies information of the spatial configurations in the real space, but also can be directly compared to the results measured by the neutron diffuse scattering spectrum. The strong intensity is clearly seen at $S(\vec{q} = (0,0))$ with FM phase in Fig. 3(a) with $J_2/J_1 = 0.38$. It is disappeared at $S(\vec{q} = (0,0))$ with increasing $J_2/J_1$ and spread out from $\vec{q} = (0,0)$ to $(\pi,0)$ in Fig. 3(b) with $J_2/J_1 = 0.46$. These results mean the coexistence phase around phase transition. In the end it is only observed at $(\pi,0)$ with SO phase in Fig. 3(c) with $J_2/J_1 = 0.54$ of the strong diagonal AF interaction.

In the following we analyze probability, where any value of $M$ is observed for the QA shots of 10000 times, to predict the shape of $f$ for $J_2/J_1 = 0.26, 0.46$ and 0.78. The only one value of $M$ in the regions with PM and SO phases of $J_2/J_1 = 0.26$ and 0.78 respectively, while those spread out as several $M$ around phase transition with $J_2/J_1 = 0.46$.

FIG. 4. (Color online) Probability where any $M$ is observed for the QA shots of 10000 times for $J_2/J_1 = 0.26$, 0.46 and 0.78. The possibilities indicate only one value of $M$ in the regimes with PM and SO phases of $J_2/J_1 = 0.26$ and 0.78 respectively, while those spread out as several $M$ around phase transition with $J_2/J_1 = 0.46$.

Finally, we discuss fail of the QA simulations happened by breaks of the chains, through measurement of the number of the chains with several $N$-qubits as a func-
FIG. 5. (Color online) The numbers of the chain as a function of $L$ in both OBC and PBC for (a) 2-qubits, (b) 3-qubits, (c) 4-qubits and (d) 5-qubits.

The numbers of the chain as a function of $L$. The results are shown in Figs. 5(a)-(d). The numbers of the chains in both OBC and PBC are commonly increasing with increasing $L$ in the chains composed of 2-qubits in Fig. 5(a). The numbers of the chain in PBC are rapidly increasing with increasing $L$ in the chains with $N$-qubits, while they in OBC are not largely increasing till $L = 30$ in Figs. 5(b)-(d). We confirm that the QA simulations have been well performed on the sizes smaller than $L = 30$ in OBC, while they have not been only worked on the sizes smaller than $L = 16$ in PBC. In the end we stress that 2-qubits in the chains are not well broken, while $N$-qubits more than 2-qubits in those are easily separated.

IV. CONCLUSION

Via the D-QAM with 5000+ qubits composed on structure of Pegasus graph in the AWS, we investigate the frustrated Ising model on the 2D $L \times L$ square lattice at $T = 0$, where frustrations are present by AF diagonal-neighbor interaction. We confirm FM to SO phase transition, which consists with the former MC and mean field results, through measurements of the $M$, $E$, $\chi$ and $S(\vec{q})$. We also analyze probability which happens the particular $M$ at a given $J_2/J_1$ for many QA shots. The possibilities indicate only one $M$ in the regimes with FM and SO phases far from phase transition. We think that the deep global minimum might be observed in $f$ of these regions. On the other hand, those spread out as several $M$ around phase transition. Owing to the strong degeneracies caused by frustrations, we guess that several local traps with plausible solutions in $f$ might extensively appear around phase transition. Finally, we discuss limitation of the D-QAM with 5000+ qubits, through analysis of the number of the chains, which are defined as the same variables with $N$-qubits on architecture of the Pegasus graph, as a function of $L$.

We would like to note that the QA simulations on D-QAM are limited as the 2D lattice with small $L$ because of breaks of the chains, unlike the MC and mean field approaches which can consider one with large $L$ [12, 13]. Therefore, we have not discussed the type of phase transition and the critical exponents, appeared in the former MC and mean field results, in our manuscript [12, 13].

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