Quantum Ferromagnetic Annealing

Sei Suzuki [1] and Hidetoshi Nishimori

Department of Physics, Tokyo Institute of Technology, 2-12-1 O-okayama, Meguro-ku, Tokyo 152-8551, Japan

Abstract

Quantum annealing by ferromagnetic interaction is investigated for random-field Ising ferromagnets and Ising spin-glasses, using the Bethe-type mean-field annealing scheme. The fact that there are rooms of choice of the type of quantum fluctuations is a prominent feature in quantum annealing which does not exist in classical simulated annealing. Results of mean-field annealing show that quantum annealing by ferromagnetic interaction lowers the energy of the obtained approximate ground state below that by conventional quantum annealing using only transverse field.

Key words: quantum annealing, transverse ferromagnetic interaction, random-field Ising model, Ising spin-glass

1. Introduction

It has been widely recognized that the Ising-spin representation plays a significant role in the study of interdisciplinary areas related to physics, information theory, computational theory, systems design technology, and so on [1]. In particular, low energy states of systems with thousands of Ising-spins with randomness are important quantities in a variety of situations. A lot of numerical methods have been developed so far to extract such states. Quantum annealing is one of the algorithms which uses quantum mechanics for the ground state search of classical Ising-spin systems [2–4].

Usually quantum annealing introduces the transverse field to the Ising representation of the problem to induce quantum fluctuations. A time-dependent Hamiltonian is composed of the transverse field and the Ising-spin Hamiltonian. The transverse field is initially so strong as to dominate the system, and is diminished with time. The time-dependent Hamiltonian becomes identical to the target Ising model finally. The ground state of the transverse field, namely the initial Hamiltonian, is trivial. If the initial state is chosen to be the ground state of the initial Hamiltonian, the final state becomes the ground state of the final Ising Hamiltonian approximately as far as the time-dependence of the Hamiltonian is mild enough. This consequence is guaranteed by the adiabatic theorem in quantum mechanics. Quantum annealing may be regarded as one of the algorithms of quantum computation. An experiment of three qubits has been carried out successfully [5]. Furthermore, an experiment using macroscopic materials has shown that quantum annealing can carry us to the target state more efficiently than thermal annealing, i.e. the classical counterpart of quantum annealing [6].

In the present paper, we propose quantum annealing using transverse-ferromagnetic interaction in addition to transverse field to accelerate convergence. The interaction between transverse components of spins gives tunneling effects involving multi-spins, which are ab-

[1] Corresponding author. E-mail: sei@stat.phys.titech.ac.jp

sent in the transverse field. Hence the transverse interaction is expected to yield additional acceleration effects to conventional quantum annealing by the transverse field.

In this paper we examine quantum annealing by transverse-ferromagnetic interaction applied to the random-field Ising model and Ising spin-glass model in two dimension with thousands of spins. To carry out quantum annealing, we introduce a procedure of the mean-field annealing on the basis of the Bethe-type approximation. In principle, the time evolution of quantum state is governed by the Schrödinger equation in quantum mechanics. However it is impossible to solve the Schrödinger equation for a large number of spins [7]. Following the dynamics of the mean-field annealing, the convergence of the final state to the true ground state is not always guaranteed since the adiabatic theorem is not available. Nevertheless, the mean-field annealing method is useful from the practical point of view because it yields approximate solutions quickly.

Previous studies on quantum annealing have paid attention to its efficiency of optimization in comparison with simulated annealing. Our study points out flexibility in the choice of quantum fluctuations. Such flexibility does not exist in simulated annealing, since one has only the thermal fluctuation controlled by the temperature. Within the procedure of mean-field annealing, we show that quantum annealing by the ferromagnetic interaction yields the state closer to the true ground state than quantum annealing by the transverse field. The results imply that quantum annealing can be improved further by choosing appropriate quantum fluctuations.

We organize the present paper as follows. Quantum ferromagnetic annealing as well as conventional quantum annealing are explained in sec. 2. The Bethe-type mean-field annealing is formulated in sec. 3. Section 4 is devoted to results of numerical simulation. This paper is concluded in sec. 5.

2. Quantum ferromagnetic annealing

We consider the following Ising-spin Hamiltonian.

$$\mathcal{H}_{\text{pot}} = -\sum_{<ij>} J_{ij}\sigma_i^z\sigma_j^z - \sum_i h_i\sigma_i^z, \tag{1}$$

where σ_i^z is the z-component of the Pauli spin operator. We suppose that coupling constants $\{J_{ij}\}$ and magnetic fields $\{h_i\}$ are given and they may be inhomogeneous generally. The purpose of quantum annealing is to obtain the ground state and/or the ground-state energy of this potential Hamiltonian, $\mathcal{H}_{\text{pot}}$. In the conventional quantum annealing, the kinetic Hamiltonian is introduced by the transverse field.

$$\mathcal{H}_{\text{kin}}^{\text{QA}} = -\sum_i \sigma_i^x, \tag{2}$$

where σ_i^x is the x-component of the Pauli spin operator.

The time-dependent Hamiltonian is made from $\mathcal{H}_{\text{kin}}$ and $\mathcal{H}_{\text{pot}}$ as

$$\mathcal{H}(t) = \left(1 - \frac{t}{\tau}\right)\mathcal{H}_{\text{kin}}^{\text{QA}} + \frac{t}{\tau}\mathcal{H}_{\text{pot}}, \tag{3}$$

where τ, the time scale of annealing procedure, is supposed to be given. This time-dependent Hamiltonian evolves from the kinetic Hamiltonian, $\mathcal{H}_{\text{kin}}^{\text{QA}}$ at $t = 0$ to the potential Hamiltonian, $\mathcal{H}_{\text{pot}}$, at $t = \tau$ linearly with time. Its change with time, namely the gradient with respect to time, is milder for larger τ.

For the initial condition of the state vector, we take the ground state of the initial Hamiltonian, which is written as $|\Psi(0)\rangle = \bigotimes_i \left[(|\uparrow\rangle_i + |\downarrow\rangle_i)/\sqrt{2}\right]$, where $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$ are the eigenstates of σ_i^z with the eigenvalues $+1$ and -1, respectively. The time evolution of the state vector $|\Psi(t)\rangle$ is governed, in principle, by the Schrödinger equation in quantum mechanics. Then the quantum adiabatic theorem guarantees that the final state, $|\Psi(\tau)\rangle$ converges to the ground state of the final Hamiltonian for $\tau \to \infty$ as far as the ground eigenstate of $\mathcal{H}(t)$ does not cross with excited states (Note that level crossing is avoided as far as a peculiar symmetry is absent.). The ground state of the final Hamiltonian is nothing but the objective of quantum annealing. In practice, since solving the Schrödinger equation in classical computers is limited to systems with small number of spins, we need to resort to a different rule of dynamics in order to implement quantum annealing in large systems. In our study, we employ the rule of mean-field annealing, which is explained in the next section. Unfortunately the adiabatic theorem is not available in the mean-field annealing. However this method has the advantage that it enables us to implement quantum annealing for large systems with low computational costs (i.e., time and memory).

Now we propose quantum ferromagnetic annealing, namely quantum annealing by the transverse-ferromagnetic interaction. The kinetic Hamiltonian of quantum ferromagnetic annealing is given by

$$\mathcal{H}_{\mathrm{kin}}^{\mathrm{QFA}} = -\sum_i \sigma_i^x - \sum_{<ij>} \sigma_i^x \sigma_j^x. \tag{4}$$

Although different relative strengths of the field and interaction may yield different results, we set both strengths to unity for simplicity since tuning of relative strength is not our primary purpose. Generally we can consider ferromagnetic interactions associating more than three spins. We focus our attention on the two-spin interaction in this paper. The ground state of $\mathcal{H}_{\mathrm{kin}}^{\mathrm{QFA}}$ is identical with that of $\mathcal{H}_{\mathrm{kin}}^{\mathrm{QA}}$. Everything of annealing procedure is done in the same way with conventional quantum annealing except that $\mathcal{H}_{\mathrm{kin}}^{\mathrm{QA}}$ is replaced by $\mathcal{H}_{\mathrm{kin}}^{\mathrm{QFA}}$.

3. Mean-field annealing with the Bethe-type approximation

In mean-field annealing, the Hamiltonian is changed under a certain schedule as the self-consistent calculation is repeated. Originally, this method with the simplest Weiss-type approximation was discussed in ref. [8]. We generalize it to the Bethe-type approximation in order to improve the performance. In the Bethe approximation, a cluster composed of a center site i and neighboring sites j is treated rigorously. The time-dependent Hamiltonian of the cluster is written as

$$\mathcal{H}^{(i)}(l) = \left(1 - \frac{l}{\tau}\right) \mathcal{H}_{\mathrm{kin}}^{\mathrm{QA,QFA}\ (i)} + \frac{l}{\tau} \mathcal{H}_{\mathrm{pot}}^{(i)}, \tag{5}$$

$$\mathcal{H}_{\mathrm{kin}}^{\mathrm{QA}(i)} = -\sigma_i^x - \sum_{j \in \mathcal{S}(i)} \sigma_j^x, \tag{6}$$

$$\mathcal{H}_{\mathrm{kin}}^{\mathrm{QFA}(i)} = -\sigma_i^x \sum_{j \in \mathcal{S}(i)} \sigma_j^x - \sigma_i^x - \sum_{j \in \mathcal{S}(i)} (1 + \sum_{k \in \mathcal{S}(j) \setminus i} m_k^x) \sigma_j^x, \tag{7}$$

$$\mathcal{H}_{\mathrm{pot}}^{(i)} = -\sigma_i^z \sum_{j \in \mathcal{S}(i)} J_{ij} \sigma_j^z - h_i \sigma_i^z - \sum_{j \in \mathcal{S}(i)} (h_j + \sum_{k \in \mathcal{S}(j) \setminus i} J_{jk} m_k^z) \sigma_j^z, \tag{8}$$

where we denote the set of neighboring sites of i by $\mathcal{S}(i)$ and suppose that $\mathcal{S}(j) \setminus i$ indicates $\mathcal{S}(j)$ except for i. The diagonalization of $\mathcal{H}^{(i)}(l)$ is numerically performed, so as to obtain the expectation values of spin operators, m_i^x, m_j^x, m_i^z and m_i^z, with respect to the ground state of the cluster. The same calculations are performed, shifting the center site i. After the whole system has been scanned, the discrete time step l is increased by one. Note that the integral run-time τ is given and fixed.

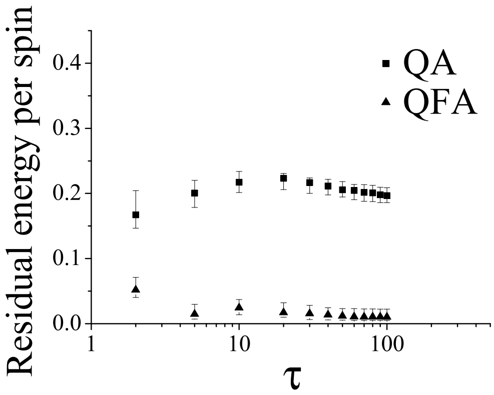

Fig. 1. Residual energies after quantum ferromagnetic annealing and conventional quantum annealing within mean-field annealing scheme for the random field Ising model with $J = 2.0$ on the 100×100 two-dimensional square lattice. Symbols indicate median values of over 80 samples. Error bars show the twentieth largest/smallest values.

4. Results

We use two examples in order to compare quantum ferromagnetic annealing and conventional quantum annealing. The first is the random field Ising model, which is represented by eq. (1) with the uniform ferromagnetic coupling constant $J_{ij} = J$. We give $+1$ or -1 with the same probability for the random field h_i. The second is the spin-glass model which is represented by eq. (1). We give $+1$ or -1 randomly for both J_{ij} and h_i. For both of the two models, we assume the two-dimensional square lattice, and mean-field annealing is carried out for 80 instances of random configurations.

Figure 1 shows residual energies, namely energies after quantum ferromagnetic annealing and conventional quantum annealing measured from the true ground energy, for the random field Ising model with $J_{ij} = J = 2.0$. The true ground energy was obtained by an algo-

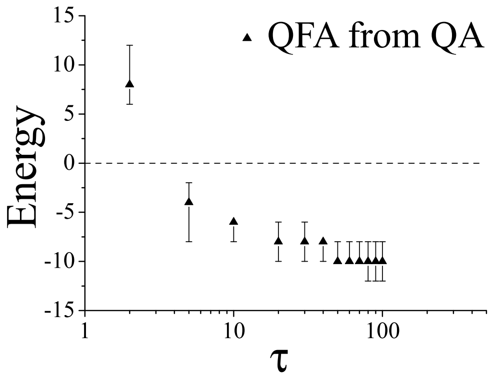

Fig. 2. Energies after quantum ferromagnetic annealing measured from energies after conventional quantum annealing for the spin-glass model on the 50×50 two-dimensional square lattice.

rithm described in ref. [9]. Clearly residual energy after quantum ferromagnetic annealing is lower than that after conventional quantum annealing. In the present condition of system parameters, the ground state is completely ferromagnetic. It has been shown by quantum Monte-Carlo simulations that conventional quantum annealing does not always work well for the ferromagnetic ground state and residual energy of quantum annealing is higher than that of simulated annealing [10]. Our result shows that such a deteriorated efficiency for the ferromagnetic ground state is not an intrinsic feature of quantum annealing but can be overcome by means of the transverse-ferromagnetic interaction. In fact, by comparison of quantum ferromagnetic annealing with simulated annealing within the same mean-field annealing scheme, it is shown that quantum ferromagnetic annealing performs much better [11].

Figure 2 shows energies after quantum ferromagnetic annealing measured from energies after conventional quantum annealing. We find that quantum ferromagnetic annealing always yields lower energy than conventional quantum annealing except for a very short τ. This result verifies that the transverse-ferromagnetic interaction improves quantum annealing as well for disordered ground states. For disordered ground states, several studies have shown that conventional quantum annealing works better than simulated annealing in Monte-Carlo simulations [10,12–14]. Hence quantum ferromagnetic annealing should be even more efficient than simulated annealing in the Monte-Carlo regime.

5. Conclusion

We proposed quantum ferromagnetic annealing for random Ising models. We showed, using the Bethe-type mean-field annealing scheme, that quantum ferromagnetic annealing lowers the energy of the final state than conventional quantum annealing for the ferromagnetic ground state of random field Ising model and the disordered ground state of the spin-glass model. The present study sheds light on the flexibility in the choice of driving force of quantum annealing. This is a prominent feature over simulated annealing. Making use of this flexibility, one can attain the ground state search more efficiently than conventional quantum annealing.

References

[1] H. Nishimori, *Statistical Physics of Spin Glasses and information processing: An Introduction*, (Oxford, 2001).

[2] *Quantum Annealing and Related Optimization Methods*, Eds. A. Das and B. K. Chakrabarti (Springer, Heidelberg, 2005).

[3] T. Kadowaki and H. Nishimori, Phys. Rev. E **58**, 5355 (1998).

[4] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, quant-ph/0001106.

[5] M. Steffen, W. van Dam, T. Hogg, G. Breyta, and I. Chuang, Phys. Rev. Lett. **90**, 67903 (2003).

[6] J. Brooke, D. Bitko, T. F. Rosenbaum, and G. Aeppli, Science **284**, 779 (1999).

[7] S. Suzuki and M. Okada, in ref. [2] ; J. Phys. Soc. Jpn. **74**, 1649 (2005).

[8] K. Tanaka and T. Horiguchi, Electron. Commun. Jpn. Pt. 3 **83** 84 (2000).

[9] M. Alava, P. Duxbury, C. Moukarzel, and H. Rieger, *Phase Transitions and Critial Phenomena* vol. 18, ed. C. Domb and J. L. Lobowitz (2001, San Diego, CA: Academic).

[10] M. Sarjala, V. Petäjä, and M. Alava, J. Stat. Mech., 1008 (2006).

[11] S. Suzuki, H. Nishimori, and M. Suzuki, in preparation.

[12] T. Kadowaki, Thesis, quant-ph/0205020.

[13] G. E. Santoro, R. Martoňák, E. Tosatti, and R. Car, Science **295**, 2427 (2002).

[14] R. Martoňák, G. E. Santoro, and E. Tosatti, Phys. Rev. B **66**, 94203 (2002).