Quantum annealing of the random-field Ising model by transverse ferromagnetic interactions

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We introduce transverse ferromagnetic interactions, in addition to a simple transverse field, to accelerate the convergence of quantum annealing of the random-field Ising model. The conventional approach using only the transverse-field term is known to be plagued by slow convergence when the true ground state has strong ferromagnetic characteristics for the random-field Ising model. The transverse ferromagnetic interactions are shown to improve the performance significantly in such cases. This conclusion is drawn from the analyses of the energy eigenvalues of instantaneous stationary states as well as by the very fast algorithm of Bethe-type mean-field annealing adopted to quantum systems. The present study highlights the importance of a flexible choice of the type of quantum fluctuations to achieve the best possible performance in quantum annealing. The existence of such flexibility is an outstanding advantage of quantum annealing over simulated annealing.

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I. INTRODUCTION

Combinatorial optimization is one of the central problems in computer science [1]. A celebrated example is the traveling salesman problem, and many instances as well as this problem can be represented in terms of the Ising model, often with disorder or frustration [2]. In such cases, optimization corresponds to the search of the ground state of the disordered (frustrated) Ising model, a highly nontrivial task also from the viewpoint of physics.

Simulated annealing is a generic prescription suited for such purposes [3]. One introduces an artificial temperature variable to control the average energy through thermal fluctuations. By decreasing the temperature gradually from a very high initial value, one hopes to eventually reach the ground state in the zero-temperature limit.

This prescription of simulated annealing intrinsically restricts the control parameter only to the temperature. Also, the actual implementation of simulated annealing is typically realized by classical Monte Carlo simulations with time-dependent temperatures.

In contrast, quantum annealing makes use of quantum fluctuations to control the behavior of the relevant system [4–7]. Fluctuations of quantum nature are introduced artificially to the classical optimization problem represented by a disordered (frustrated) Ising model. One initially sets the coefficient of the quantum term very large so that the system searches very wide regions of the phase space for the optimal state. A gradual decrease of the coefficient of the quantum term yields an adiabatic evolution of the ground state starting from a trivial initial ground state, and hopefully leads to the nontrivial final ground state, which is the solution of the original optimization problem. We have some degrees of freedom in the choice of a type of quantum fluctuation. In addition, the implementation of quantum annealing can be made in a variety of ways including an exact numerical integration of the Schrödinger equation (for small systems), quantum Monte Carlo simulations [8,9], and Green's function Monte Carlo method [10].

Most studies of quantum annealing so far have put an emphasis on how fast quantum annealing performs, relatively to simulated annealing, with a single type of the quantum term in most cases, namely, the transverse-field term added to the classical Ising model representing the original optimization problem. Evidence has been accumulating to establish generic superiority of quantum annealing [4,11,12].

In the present paper we focus our attention on a different aspect of quantum annealing—flexibility in the choice of quantum terms. In particular, we investigate the random-field Ising model, for which quantum annealing with the conventional type of quantum term has been shown not to perform efficiently under certain circumstances [13]. We introduce additional terms of quantum nature—transverse interactions of a ferromagnetic type—by taking advantage of the flexibility in quantum annealing. The result shows a significant improvement, from which we conclude that the reduced efficiency of quantum annealing in comparison with simulated annealing reported in some cases may not necessarily reflect intrinsic limitations of quantum annealing. Rather, we expect that an appropriate choice of quantum terms would often accelerate significantly the convergence of quantum annealing to the ground state. This feature of flexibility is an outstanding advantage of quantum annealing.

We organize this paper as follows. In Sec. II, we first explain the basic ideas of conventional quantum annealing and quantum annealing using transverse ferromagnetic interactions. We then analyze the instantaneous ground state and the first excited state by numerical diagonalization. Advantages of transverse ferromagnetic interactions as a driving force of quantum annealing are pointed out. In Sec. III, quantum annealing by transverse ferromagnetic interactions is carried out for systems of large size using the Bethe approximation as an algorithm for practical implementation. We then present results of simulations and compare residual errors of

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conventional quantum annealing, quantum annealing by transverse ferromagnetic interactions, and simulated annealing. Section IV is devoted to our conclusion.

II. TRANSVERSE FERROMAGNETIC INTERACTIONS

A. Conventional approach

In the present paper we consider the problem of the ground-state search of the random-field Ising model (RFIM). The Hamiltonian

$$\mathcal{H}_{\rm pot}^{\rm RFIM} = -J\sum_{\langle ij\rangle}\sigma_i^z\sigma_j^z - \sum_i h_i\sigma_i^z, \tag{1}$$

where σ_i^z is the z component of the Pauli matrix, is regarded as the classical potential term in the context of quantum annealing. For this system, it is known that the conventional approach to quantum annealing using the transverse field as described below performs rather poorly when the interaction term in Eq. (1) is dominant relative to the random-field term [13]. We choose the two-dimensional square lattice and the random field is assumed to be either +1 or −1 with equal probability.

In the conventional approach, one adds a term of transverse field (TF) to Eq. (1),

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

which may also be regarded as the quantum kinetic energy, to induce quantum transitions between classical states. The strength of the quantum kinetic energy is controlled in the present paper by a linear function of time

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

with τ being the time assigned for annealing. The initial state is chosen to be the trivial ground state of the kinetic term $|\Psi(0)\rangle = \otimes_i[(|\uparrow\rangle_i + |\downarrow\rangle_i)/\sqrt{2}]$, where $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$ are the eigenstates of σ_i^z with the eigenvalues 1 and −1, respectively. It is expected intuitively that the system evolves adiabatically following the instantaneous ground state if τ is very large, reaching finally the nontrivial ground state of the potential term $\mathcal{H}_{\rm pot}^{\rm RFIM}$ at $t=\tau$ [14].

The quantitative criterion for such an adiabatic evolution is

$$\tau \gg \tau_c \equiv \frac{1}{\varepsilon_{\rm min}^2}\left|\left\langle \Psi_1\left(\frac{t}{\tau}\right)\left|\frac{d\mathcal{H}(t)}{d(t/\tau)}\right|\Psi_0\left(\frac{t}{\tau}\right)\right\rangle\right|_{\rm max}, \tag{4}$$

where $|\langle\Psi_1(t/\tau)|A|\Psi_0(t/\tau)\rangle|_{\rm max}$ denotes the maximum absolute value of the matrix element of A between the instantaneous ground state Ψ_0 and the first excited state Ψ_1. The denominator $\varepsilon_{\rm min}$ is the minimum energy gap between the instantaneous ground state and the first excited state. The residual error, the difference between the obtained approximate energy at $t=\tau$ and the true ground state energy of $\mathcal{H}_{\rm pot}^{\rm RFIM}$, is of $\mathcal{O}((\tau_c/\tau)^2)$ if the condition (4) is satisfied [15].

It is therefore important to find an improved quantum kinetic term to enhance the gap $\varepsilon_{\rm min}$ and suppress the transition matrix element $|\langle\Psi_1(t/\tau)|d\mathcal{H}(t)/d(t/\tau)|\Psi_0(t/\tau)\rangle|_{\rm max}$. Notice that the potential term $\mathcal{H}_{\rm pot}^{\rm RFIM}$ is given and fixed, and our degree of freedom lies in the choice of the quantum kinetic term. This flexibility is an outstanding feature of quantum annealing, which has not necessarily been fully exploited in existing studies using almost always the transverse-field term of Eq. (2).

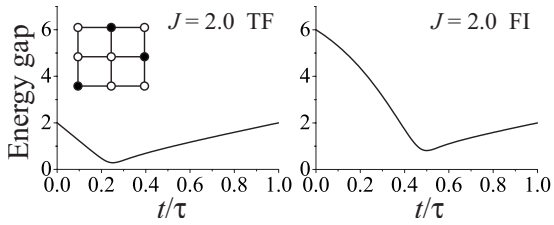

FIG. 1. Instantaneous energy gaps between the ground state and the first excited state of the time-dependent Hamiltonians for systems with $N=9$ spins. The coupling constant in $\mathcal{H}_{\rm pot}^{\rm RFIM}$ is set at $J=2.0$. We assume the two-dimensional square lattice with the open boundary condition. "TF" and "FI" in the figures correspond to the kinetic Hamiltonians $\mathcal{H}_{\rm kin}^{\rm TF}$ and $\mathcal{H}_{\rm kin}^{\rm FI}$, respectively. The configuration of random fields is depicted in the left panel, where open circles indicate $h_i=+1$ and filled ones indicate $h_i=-1$.

B. Transverse ferromagnetic interactions

We now try the following operator as the quantum kinetic term in place of $\mathcal{H}_{\rm kin}^{\rm TF}$ of Eq. (2):

$$\mathcal{H}_{\rm kin}^{\rm FI} = -\sum_i \sigma_i^x - \sum_{\langle ij\rangle}\sigma_i^x\sigma_j^x. \tag{5}$$

The time evolution of the system is governed by the time-dependent Hamiltonian similar to Eq. (3),

$$\mathcal{H}(t) = \left(1-\frac{t}{\tau}\right)\mathcal{H}_{\rm kin}^{\rm FI} + \frac{t}{\tau}\mathcal{H}_{\rm pot}^{\rm RFIM}. \tag{6}$$

In Eq. (5) the sum for interactions runs over the same pairs of sites as in the potential term (1). The ground state of Eq. (5) is the trivial ferromagnetic state in the x direction as in the conventional case. The overall symmetry (by the operation $\sigma_i^x \to -\sigma_i^x$) is broken by the transverse field term as is necessary to guarantee the uniqueness of the ground state. For simplicity we fix the coefficients to unity in Eq. (5) and do not try to optimize the ratio of the coefficients of the transverse field and interaction terms.

As a preliminary analysis, we have evaluated the characteristic time τ_c of Eq. (4) by direct diagonalization of $\mathcal{H}(t)$ for small systems. Figure 1 shows the energy gap between the instantaneous ground state and the first excited state for the two-dimensional square lattice system with nine spins ($N=9$) under the configuration of random fields indicated on the left panel. The interaction constant is $J=2.0$ and the open boundary condition is assumed. It is observed that the minimum value of the gap $\varepsilon_{\rm min}$ is larger for the case of transverse interactions (FI) on the right panel than for the transverse field (TF) case on the left panel: $\varepsilon_{\rm min}^{\rm FI}/\varepsilon_{\rm min}^{\rm TF}=2.89$. The absolute value of the matrix element appearing in Eq. (4) is depicted in Fig. 2. This quantity is also larger for FI than for

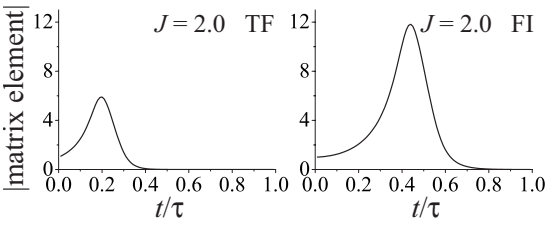

FIG. 2. Absolute values of the matrix element $|\langle\Psi_1(t/\tau)|d\mathcal{H}(t)/d(t/\tau)|\Psi_0(t/\tau)\rangle|$ for the system of Fig. 1.

TF, the ratio being 2.01. Thus the ratio of τ_c is $\tau_c^{\mathrm{FI}}/\tau_c^{\mathrm{TF}} = 2.01/2.89^2 = 0.24$. We therefore conclude that quantum fluctuations by transverse ferromagnetic interactions lead to much shorter characteristic time than the conventional counterpart for the present system. A similar tendency was observed for a larger system with $N=20$ and $J=2.0$.

The situation changes for $J=0.6$ as is seen in Fig. 3. The ratio of characteristic times is now $\tau_c^{\mathrm{FI}}/\tau_c^{\mathrm{TF}} = 1.21$, suggesting a slightly slower convergence under the transverse ferromagnetic interactions. Nevertheless, this deterioration by 21% may not be quite significant in comparison with the much larger gain of 76% (=1−0.24) for $J=2.0$.

In the next section we shall see the consequences of these observations from a different point of view.

III. MEAN-FIELD ANNEALING BY THE BETHE APPROXIMATION

Implementation of quantum annealing for large systems is often carried out by quantum Monte Carlo simulations based on the Suzuki-Trotter transformation [16]. In the present paper we instead make use of the method of mean-field annealing with the Bethe-type approximation [17]. The basic idea is to solve a set of equations for local magnetization iteratively. There are several reasons for the choice of this method. First, our main objective is to study the *relative* effectiveness of

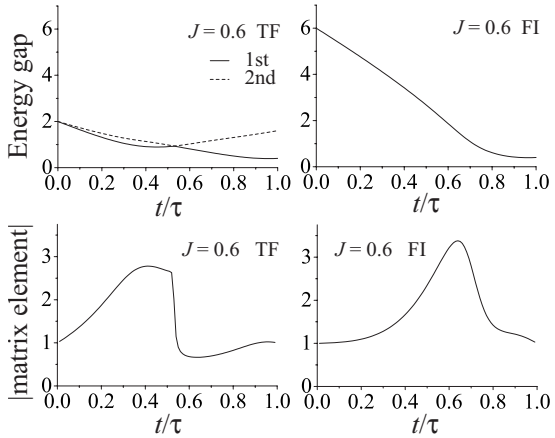

FIG. 3. Instantaneous energy gaps (upper panel) and absolute values of the matrix element (lower panel) for the random-field configuration of Fig. 1 with $J=0.6$. The energy gap between the second excited state and the ground state is also plotted in the panel for TF. The abrupt change of the matrix element in the TF panel is due to level crossing of the first and second excited states.

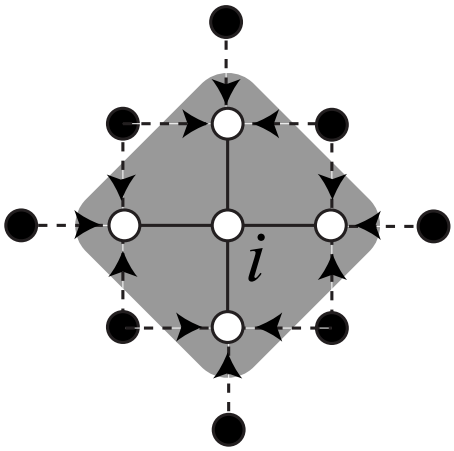

FIG. 4. In the Bethe approximation one focuses on a site i and its immediate neighbors. All other site variables are replaced with their averages.

transverse ferromagnetic interactions and transverse field as the quantum kinetic energy. The present approximation is likely to affect both approaches to a similar degree, and therefore the relative performance is expected to be largely unchanged by the introduction of approximation. Second, the mean-field annealing is much faster than quantum Monte Carlo. The former may therefore be suitable for practical purposes under appropriate circumstances. Third, we can follow the ground state directly in the mean-field annealing without introducing small but finite temperatures as in quantum Monte Carlo. Lastly, the implementation of quantum Monte Carlo involving transverse ferromagnetic interactions is a little more complicated than the case of simple transverse field only, whereas mean-field annealing can be formulated easily for both cases.

A. Bethe approximation

To achieve the best possible results within mean-field-type methods, we employ the Bethe approximation in place of a simple single-body mean-field theory. One focuses on a site i and approximates the Hamiltonian involving i by the cluster Hamiltonian (see Fig. 4)

$$\mathcal{H}^{(i)}(t) = \left(1 - \frac{t}{\tau}\right)\mathcal{H}_{\mathrm{kin}}^{(i)} + \frac{t}{\tau}\mathcal{H}_{\mathrm{pot}}^{(i)}, \tag{7}$$

$$\mathcal{H}_{\mathrm{pot}}^{(i)} = -J\sigma_i^z \sum_{j\in\mathcal{S}(i)} \sigma_j^z - h_i\sigma_i^z - \sum_{j\in\mathcal{S}(i)} \left(h_j + J\sum_{k\in\mathcal{S}(j)\backslash i} m_k^z\right)\sigma_j^z, \tag{8}$$

$$\mathcal{H}_{\mathrm{kin}}^{(i)} = -\sigma_i^x \sum_{j\in\mathcal{S}(i)} \sigma_j^x - \sigma_i^x - \sum_{j\in\mathcal{S}(i)} \left(1 + \sum_{k\in\mathcal{S}(j)\backslash i} m_k^x\right)\sigma_j^x, \tag{9}$$

where j is a neighboring site of i and k is a neighbor of j excepting i. For this Hamiltonian one calculates the ground-state expectation values of σ_i^z, σ_j^z, σ_i^x, and σ_j^x, giving m_i^z, m_j^z, m_i^x, and m_j^x, respectively. The same process is repeated by shifting the center site i of the cluster. After scanning the

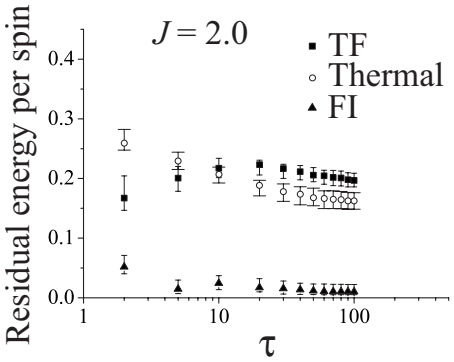

FIG. 5. Residual energy for the random field Ising model with $J=2.0$ averaged over 80 configurations of random fields. Filled squares and triangles indicate the results of quantum annealing by transverse field (TF) and by transverse interaction (FI), respectively. Open circles are for simulated annealing.

whole system, one updates the time variable. The same idea applies to the conventional quantum annealing, in which one drops the transverse interaction term.

For comparison, the same Bethe-type mean-field annealing was tested for simulated annealing using thermal fluctuations. In this case the kinetic term $\mathcal{H}_{\mathrm{kin}}^{(i)}$ is dropped and temperature is introduced to calculate the thermal expectation value m_i^z of σ_i^z. The same linear annealing schedule $T=T_0(1-t/\tau)$ was used with a sufficiently high initial temperature T_0.

B. Results

We have applied the method above described to the random-field Ising model with the system size 100×100 in two dimensions. The residual energy was calculated as the difference between the obtained approximate energy and the true ground-state energy estimated by a well-established algorithm [18].

Figure 5 shows the result for $J=2.0$ averaged over 80 samples, and Fig. 6 is the histogram of the residual energy at $\tau=100$. It is clearly seen that quantum annealing by transverse ferromagnetic interactions is far more superior to the other methods. Simulated annealing and the conventional transverse-field quantum annealing perform almost similarly,

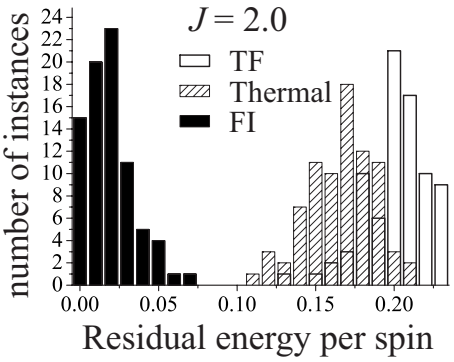

FIG. 6. Histogram of the residual energy at $\tau=100$. The parameters are the same as in Fig. 5.

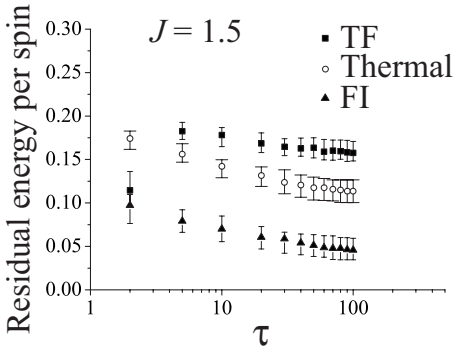

FIG. 7. Residual energy for $J=1.5$. Other conditions are the same as in Fig. 5.

the former being slightly better probably owing to the difference in the effects of our approximation to thermal and quantum annealing. A similar situation is found for $J=1.5$ in Fig. 7. The difference between various methods diminishes as J decreases further (see Figs. 8 and 9).

Our method works efficiently for large J, in which the true ground state is either exactly or close to the ferromagnetic state. The introduction of transverse ferromagnetic interactions does not necessarily improve the result for the cases of disordered ground states. This observation is to be compared with the finding of Sarjala *et al.* [13] who showed by quantum Monte Carlo simulations that quantum annealing by the conventional method is less efficient than simulated annealing when the ground state is strongly ferromagnetic. We may conclude that their consequence does not necessarily reflect intrinsic features of quantum annealing. Sophisticated implementations of quantum annealing can significantly improve the performance. The same may apply to the problem of 3-satisfiability (3-SAT), in which quantum annealing was observed to give less efficient results than simulated annealing [19].

IV. CONCLUSION

We have discussed the effect of the introduction of transverse ferromagnetic interactions to quantum annealing of the random-field Ising model. The exact diagonalization study on small systems revealed that transverse ferromagnetic interactions shorten the characteristic time τ_c from the value

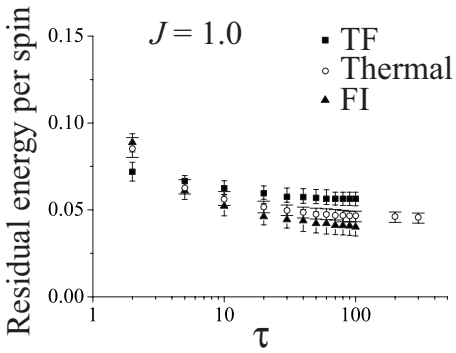

FIG. 8. Residual energy for $J=1.0$.

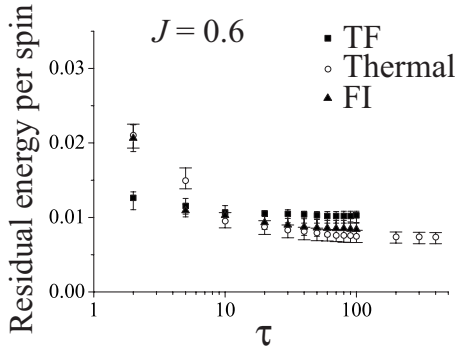

FIG. 9. Residual energy for $J=0.6$.

given by the conventional transverse field when the interaction constant J is large. Then we compared residual energies after quantum annealing by transverse ferromagnetic interactions with those by conventional quantum annealing using transverse field and simulated annealing for large systems. In order to carry out quantum and thermal annealing in larger systems, we employed the method of mean-field annealing based upon the Bethe-type approximation. The results of mean-field annealing showed that quantum annealing by transverse ferromagnetic interactions is far more efficient than the other two schemes for large J. This implies that the previously reported fact on the reduced efficiency of conventional quantum annealing for the ferromagnetic ground state is not an intrinsic feature of quantum annealing, but a better efficiency than simulated annealing can be obtained by exploiting an appropriate quantum effect. It is important to make use of the room of choice of quantum fluctuations to extract the best performance in quantum annealing. Such flexibility is an outstanding character of quantum annealing that does not exist in simulated annealing. It may also be interesting to take into account many-body interactions of the form $-\sigma_{i_1}^x \sigma_{i_2}^x \cdots \sigma_{i_n}^x$ in the mean-field quantum annealing.

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[1] M. R. Garey and D. S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness* (Freeman, San Francisco, 1979).
[2] J. J. Hopfield and D. W. Tank, Science **233**, 625 (1986).
[3] S. Kirkpatrick, C. D. Gelett, and M. P. Vecchi, Science **220**, 671 (1983).
[4] T. Kadowaki and H. Nishimori, Phys. Rev. E **58**, 5355 (1998).
[5] *Quantum Annealing and Related Optimization Methods*, edited by A. Das and B. K. Chakrabarti (Springer, Heidelberg, 2005).
[6] G. E. Santoro and E. Tosatti, J. Phys. A **39**, R393 (2006).
[7] A. B. Finnila, M. A. Gomez, C. Sebenik, C. Stenson, and J. D. Doll, Chem. Phys. Lett. **219**, 343 (1994).
[8] T. Kadowaki, Ph.D. thesis, Tokyo Institute of Technology, (1998); e-print arXiv:quant-ph/0205020.
[9] R. Martoňák, G. E. Santoro, and E. Tosatti, Phys. Rev. B **66**, 094203 (2002).
[10] L. Stella and G. E. Santoro, Phys. Rev. E **75**, 036703 (2007).
[11] G. E. Santoro, R. Martoňák, E. Tosatti, and R. Car, Science **295**, 2427 (2002).
[12] R. Martoňák, G. E. Santoro, and E. Tosatti, Phys. Rev. E **70**, 057701 (2004).
[13] M. Sarjala, V. Petäjä, and M. Alava, J. Stat. Mech.: Theory Exp. (2006) 1008.
[14] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, e-print arXiv:quant-ph/0001106.
[15] S. Suzuki and M. Okada, J. Phys. Soc. Jpn. **74**, 1649 (2005).
[16] M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976); See also *Quantum Monte Carlo Methods in Condensed Matter Physics*, edited by M. Suzuki (World Scientific, 1993), and references cited therein.
[17] Mean-field annealing with the simplest Weiss-type approximiation for quantum systems has been first discussed in K. Tanaka and T. Horiguchi, Electron. Commun. Jpn., Part 3 **83**, 84 (2000).
[18] M. Alava, P. Duxbury, C. Moukarzel, and H. Rieger, *Phase Transitions and Critial Phenomena*, edited by C. Domb and J. L. Lobowitz (Academic, San Diego, 2001), Vol. 18.
[19] D. A. Battaglia, G. E. Santoro, and E. Tosatti, Phys. Rev. E **71**, 066707 (2005).