

Quantum-thermal annealing with a cluster-flip algorithm

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(Received 9 March 2009; published 5 June 2009)

A quantum-thermal annealing method using a cluster-flip algorithm is studied in the two-dimensional spin-glass model. The temperature (T) and the transverse field (Γ) are decreased simultaneously with the same rate along a linear path on the T - Γ plane. We found that the additional pulse of the transverse field to the frozen local spins produces a good approximate solution with a low computational cost.

DOI: 10.1103/PhysRevE.79.065701

PACS number(s): 02.70.Ss, 02.70.Uu

An optimization problem frequently appears in many situations of science and technology [1]. All known algorithms need an exponentially long time to find the exact solution of nondeterministic polynomial problems. The traveling salesman problem, the satisfiability problem, and the ground-state search problem of spin glasses are the typical examples. It is important to develop an efficient algorithm that provides an approximate solution with a reasonable computational time. A standard method for such problems is the classical simulated-annealing (CA) method, which was proposed based on an analogy between optimization problems and statistical mechanics [2,3]. The idea of CA is to identify the cost function to be minimized with the energy in a statistical-mechanical system. We perform a numerical simulation to obtain the equilibrium state of this system. The temperature is artificially introduced into the system and gradually decreased toward zero. The thermal fluctuations enable the system to escape from the local minima of the cost function. At low temperatures, the system may stay with a high probability in the optimal state.

Quantum annealing (QA) is a novel algorithm proposed as an alternative of CA [4–7]. We use the quantum fluctuations instead of the thermal fluctuations. The quantum fluctuations are introduced by the additional energy term that is noncommutative with the cost function of the optimization problem. In the Ising-spin model, the transverse magnetic field (Γ) serves as this additional term. The additional term is initially set to take a large value, so that the initial state is disordered by the quantum fluctuations. It is gradually decreased with time, and it finally vanishes. Only the cost function term remains in the final state. It is expected that QA can find an approximate solution more efficiently than CA because of the quantum tunneling between the local minima. Analytical [8–10] and numerical [6,7,11] investigations support this scenario.

Although QA and CA have been studied a lot so far, hybrid methods of them have not attracted much attention. Lee and Berne [12] applied a method which carries out QA and CA alternately to the protein folding problem. Battaglia *et al.* [13] examined a similar method to the satisfiability problem. The present Rapid Communication aims to investigate quantum-thermal annealing (QTA) that carries out QA and CA *simultaneously*. In particular, we focus on the linear path on the transverse field (Γ) vs temperature (T) plane where these two parameters are lowered with keeping $\beta\Gamma$ constant

(Fig. 1), where $\beta=1/T$. To investigate QTA numerically in large systems, we used the path-integral Monte Carlo (PIMC) method with the cluster-flip algorithm (the cluster-flip PIMC) [14,15]. There are two reasons why the cluster-flip PIMC is suitable for QTA: first, the cluster-flip PIMC can simulate any Ising-spin system in the transverse field without not only the error due to Suzuki-Trotter mapping [16,17] but also the slowdown of relaxation known as the Wiesler freezing [18]. Second, the computational cost is independent of the temperature and the transverse field if keeping $\beta\Gamma$ constant.

The performance of QTA by the cluster-flip PIMC (the cluster QTA) is governed by the parameter $\beta\Gamma$. The residual error is small but the computational cost becomes larger when the value of $\beta\Gamma$ is large. To solve this dilemma, we introduce *the local transverse-field pulse process*. The main result of the present Rapid Communication is that the cluster QTA with the local pulse process exhibits the best performance in comparison among various annealing methods with regard to the residual energy and the computational cost.

Let us consider the transverse-field Ising model defined by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_{i=1}^N \sigma_i^x, \quad (1)$$

where σ_i^α ($\alpha=x, y, z$) are the Pauli matrices of the spin 1/2 operator at a site i . The first term corresponds to the cost function of the optimization problem we want to solve. The

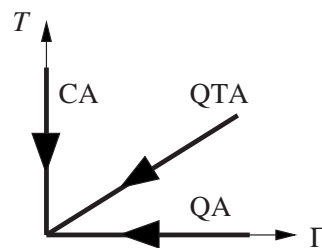


FIG. 1. Paths for three types of annealing method in the plane of the temperature and the transverse field. Note that when the quantum Monte Carlo method is applied to QA in practice, the QA path is lifted from the Γ axis because a small but nonzero temperature is introduced.

quenched random interaction J_{ij} follows the Gaussian distribution with the average 0 and the variance 1. We use, for the Monte Carlo simulation, a single configuration of random couplings on the 100×100 system with the periodic boundary condition. We confirmed that the results given below are consistent with similar simulations with other random configurations on 50×50 and 30×30 systems. The second term is the transverse field, which introduces the quantum fluctuation to the system.

In PIMC, the transverse-field Ising model is mapped to the classical Ising model with an additional imaginary-time dimension by the Suzuki-Trotter formula [16,17,19]. The partition function at the inverse temperature β is expressed as

$$Z_M = \text{Tr} \exp \left[\sum_{m=1}^M \left(\frac{\beta}{M} \sum_{\langle ij \rangle} J_{ij} S_i^{(m)} S_j^{(m)} + \gamma \sum_{i=1}^N S_i^{(m)} S_i^{(m+1)} \right) \right], \quad (2)$$

where M is the length along the extra dimension (Trotter number) and $S_i^{(m)}$ ($= \pm 1$) denotes a classical Ising spin at a site i on the m th Trotter slice. The boundary condition along the imaginary-time direction is periodic, i.e., $S_i^{(m+M)} = S_i^{(m)}$. The nearest-neighbor interaction between adjacent Trotter slices,

$$\gamma = \frac{1}{2} \ln \left(\coth \frac{\beta \Gamma}{M} \right), \quad (3)$$

is ferromagnetic. The mapped classical system is equivalent to the original quantum system in the limit of the infinite Trotter number. As far as the Trotter number is finite, the error of quantum-classical mapping appears. To suppress the error at low temperature, one has to choose a large Trotter number. When the Trotter number is large, the simulation suffers from the Wiesler freezing [18], where the spin-flip probability becomes very small and the spin state freezes in a practical computational time.

The cluster-flip algorithm proposed in Refs. [14,15] solves the problems of the standard PIMC. The idea of the present algorithm is to make an update global in the imaginary-time direction and local in the real space. We create clusters only in the imaginary-time direction in the same manner as the Swendsen-Wang method [20]. Each cluster is updated according to the local molecular field from the neighboring sites. Since the correlated cluster in the imaginary-time direction is flipped by one update trial, the Wiesler freezing does not occur. Moreover, one can take the infinite limit of the Trotter number by replacing dynamics of clusters themselves to that of domain walls between clusters. It follows that the error of the Suzuki-Trotter mapping disappears. We can identify the spin states of the mapped classical system by the location of the domain walls and the spin state on the lowest Trotter slice. The computational cost of the cluster-flip PIMC is proportional to $\beta \Gamma$, which is the average number of domain walls in the imaginary-time direction at one site. This is contrasted with the standard single-flip PIMC where the computational cost is governed by the Trotter number M .

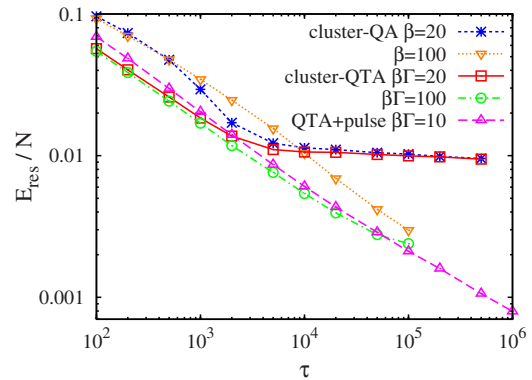


FIG. 2. (Color online) Annealing time τ dependence of the minimum residual energy per site for a 100×100 two-dimensional Ising spin glass. The cluster QTA is performed with $\beta \Gamma = 20$ and 100 . Correspondingly, the cluster QA is done with $\beta = 20$ and 100 . The broken curve with upper triangles is the data obtained by the cluster QTA with the local pulse process performed with $\beta \Gamma = 10$. The initial value of the transverse field is chosen to be $\Gamma_0 = 1$ in all cases. Each annealing method is tried at least 100 times.

In QTA, we employ the schedule of the transverse field given by

$$\Gamma(t) = \Gamma_0 (1 - t/\tau), \quad (4)$$

where Γ_0 is the initial value and τ is the annealing time. The Monte Carlo step t moves from $t=0$ to $t=\tau$. We decrease the transverse field and the temperature simultaneously while keeping $\beta \Gamma$ constant. Note that the convergence annealing schedule for QTA is the inverse-logarithmic law of the temperature and the transverse field [21], which is slower than the power-law schedule for QA. However, the system surely converges to the desired optimal state in the infinite time limit. We also consider the standard annealing schedule of QA for comparison, in which the transverse field is decreased as Eq. (4) with the temperature fixed at a sufficiently low value.

The initial cluster states in QTA and QA are made by giving the position of domain walls by the Poisson process with the mean value $\beta \Gamma$. If the number of generated domain walls, n_{dw} , is odd, one of the domain walls is removed to obey the periodic boundary conditions along the imaginary-time direction. Since the expectation value of σ^x is $n_{\text{dw}}/\beta \Gamma$ in the infinite limit of the Trotter number, the initial state corresponds to the all-up state along the x axis.

Figure 2 shows minimum residual energies of QTA and QA by the cluster-flip PIMC against the annealing time τ . The minimum residual energy is defined by the difference between the lowest energy in all the Trotter slices and the ground-state energy. The ground-state energy was obtained by the spin-glass server [22]. The parameters $\beta \Gamma$ for QTA and β for QA are set at $\beta \Gamma = \beta = 20$ or $\beta \Gamma = \beta = 100$. The initial value of the transverse field is chosen at $\Gamma_0 = 1$ in all cases. Every simulation is repeated at least 100 times.

As common to QTA and QA, when $\beta \Gamma$ or β is small, the residual energy rapidly decays for small τ , while it is almost saturated for large τ . The change in the residual energy curve from a rapid decay to a slow decay is understood as a cross-

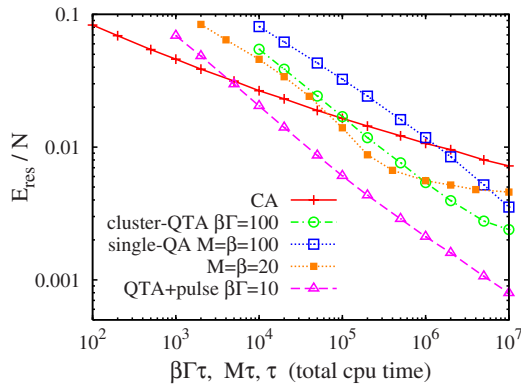


FIG. 3. (Color online) Comparison of the minimum residual energies per site obtained by the cluster QTA, single QA, and CA. The abscissa is the computational cost (total CPU time) which is defined by the annealing time τ multiplied by $\beta\Gamma$ for the cluster QTA, τ multiplied by M for the single QA, and τ for CA. The initial temperature for CA is $T_0=3$ and the initial transverse field for the other methods is set $\Gamma_0=1$.

over from the intrinsic curve of QA to the curve of QA with strong thermal disturbances [23]. The cluster QTA with $\beta\Gamma=100$ preserves the large decay rate longer than that with $\beta\Gamma=20$. Since the thermal fluctuation is less effective when $\beta\Gamma$ is large, the rapid decay is attributed to QA at zero temperature. On the contrary, the thermal fluctuation begins to dominate the dynamics as τ becomes large. The system finds itself at the finite temperature after the long Monte Carlo steps. This is because the rate of nonadiabatic transition is suppressed and the excitation occurs due to very small but finite thermal fluctuations. We observed that the similar crossover takes place also in the QA by the single-flip PIMC (see data of $M=\beta=20$ in Fig. 3), as it has been recognizable in Fig. 1 of Ref. [11].

For large τ , after the crossover takes place, the final state of the cluster QTA is a classical state in which no domain wall is present at all. Such a state loses the quantum fluctuations represented by $n_{dw}/\beta\Gamma$. Once a spin falls into a classical state which minimizes the cost function locally, it can hardly escape from the local minimum. Therefore, we introduce the local pulse process.

The local pulse process is applied to a real-space site when there is no domain wall along the imaginary-time direction at this site. What is done in this process is to reinitialize the cluster state, so that it contains $\beta\Gamma$ domain walls on average as in the disordered initial state. The other sites are left untouched. This process is physically interpreted as an application of the on-site transverse-field pulse. The pulse process destroys classical states by creating domain walls and induces extra quantum fluctuations. It helps the spin state to escape from the local minimum. An increase in energy caused by this process is on the order of unity because it is applied locally. It is noted that every site always has at least two domain walls during the whole annealing process. However, this constraint does not matter for the spin-glass model we have investigated. Because of the global spin-flip symmetry, the final spin state is expected to contain both the ground state and its spin-flip state. For the system without the spin-flip symmetry, we might need to stop the pulse process at some time.

The broken curve connecting upward triangles in Fig. 2 shows the performance of the cluster QTA with the local pulse process. Even if we choose $\beta\Gamma=10$, the residual energy continues to decay without the crossover. We found that the parameter $\beta\Gamma=10$ is almost optimal for the cluster QTA with the pulse process. If $\beta\Gamma$ is larger than 10, a larger computational cost is needed to obtain the same residual energy. On the other hand, the smaller $\beta\Gamma$ causes insufficient quantum fluctuations which raise the residual energy. The additional cost of computation by the pulse process is only about the factor of 0.2 of the whole computational time. It is because the pulse process is not always applied and the reinitialization of the cluster state does not cost as much as the update.

Figure 3 shows the residual energy against the computational cost. We performed not only the cluster QTA but also CA and QA by the single-flip PIMC (single QA) on the same sample. In CA, we chose a completely random spin configuration as an initial state and the temperature is decreased linearly from the initial value, $T_0=3$, to zero. As for the single QA, the initial spin configuration is completely random in the $(2+1)$ -dimensional space. The inverse temperature β is fixed to the Trotter number M according to Ref. [11], and the initial value of the transverse field is set at $\Gamma_0=1$. These initial values for T and Γ are almost optimized so as to obtain the lowest residual energy. The residual energy in the single QA is obtained from the lowest energy among all the Trotter slices. The computational cost is defined by τ multiplied by $\beta\Gamma$ for the cluster QTA, τ multiplied by M for the single QA, and τ for CA, which roughly correspond to the total CPU time.

Apparently the decay rate of CA (solid curve) is slower than others. The single QA and the cluster QTA with and without the pulse process have similar decay rates. However, the cluster QTA with the pulse process achieves the highest efficiency compared with other methods. It is clearly observed both in Figs. 2 and 3 that the crossover appears when a value of $\beta\Gamma$ or β is small. We consider that it appears much later in case when $\beta\Gamma$ is large. The crossover prevents us from obtaining a lower residual energy. We must choose a large value of $\beta\Gamma$ in order to avoid the crossover. However, we must pay much computational cost in turn. The cluster QTA with the local pulse process is the solution of this dilemma. We put the quantum fluctuations not to the whole system but only to the spin that is frozen earlier. This is the main reason why we can achieve the lower residual energy very efficiently.

In conclusion, we investigated QTA implemented by the cluster-flip PIMC and revealed that the local transverse-field pulse improves the performance of QTA. In practice, we showed that QTA with the pulse process gives the best performance with respect to the residual energy and the computational cost, compared to CA, QA, and QTA without the pulse process. Although we have considered only the two-dimensional Ising spin glass, it is noteworthy that QA by the single-flip method was reported not to be better than CA in a satisfiability problem [13]. Whether QTA by the cluster-flip method works well in such a harder optimization problem is the future problem.

The authors are grateful to G. E. Santoro and H. Nishimori for helpful discussions. S.M. is supported by the Japan Society for the Promotion of Science. S.S. acknowledges

support by Grant-in-Aid for Scientific Research (Grant No. 20740225) from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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- [1] M. R. Garey and D. S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness* (Freemann, San Francisco, 1979).
- [2] S. Kirkpatrick, S. D. Gelett, and M. P. Vecchi, *Science* **220**, 671 (1983).
- [3] V. Černý, *J. Optim. Theory Appl.* **45**, 41 (1985).
- [4] T. Kadowaki and H. Nishimori, *Phys. Rev. E* **58**, 5355 (1998).
- [5] G. E. Santoro, R. Martoňák, E. Tosatti, and R. Car, *Science* **295**, 2427 (2002).
- [6] A. Das and B. K. Chakrabarti, *Quantum Annealing and Related Optimization Methods*, Lecture Notes in Physics Vol. 679 (Springer, Berlin, 2005).
- [7] G. E. Santoro and E. Tosatti, *J. Phys. A* **39**, R393 (2006).
- [8] S. Morita and H. Nishimori, *J. Phys. A* **39**, 13903 (2006).
- [9] S. Morita and H. Nishimori, *J. Phys. Soc. Jpn.* **76**, 064002 (2007).
- [10] S. Suzuki, *J. Stat. Mech.: Theory Exp.* (2009) P03032.
- [11] R. Martoňák, G. E. Santoro, and E. Tosatti, *Phys. Rev. B* **66**, 094203 (2002).
- [12] Y.-H. Lee and B. J. Berne, *J. Phys. Chem. A* **104**, 86 (2000).
- [13] D. A. Battaglia, G. E. Santoro, and E. Tosatti, *Phys. Rev. E* **71**, 066707 (2005).
- [14] T. Nakamura and Y. Ito, *J. Phys. Soc. Jpn.* **72**, 2405 (2003).
- [15] T. Nakamura, *Phys. Rev. Lett.* **101**, 210602 (2008).
- [16] H. F. Trotter, *Proc. Am. Math. Soc.* **10**, 545 (1959).
- [17] M. Suzuki, *Prog. Theor. Phys.* **46**, 1337 (1971).
- [18] A. Wiesler, *Phys. Lett. A* **89**, 359 (1982).
- [19] D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge University Press, Cambridge, England, 2000), Chap. 8.
- [20] R. H. Swendsen and J.-S. Wang, *Phys. Rev. Lett.* **58**, 86 (1987).
- [21] Since $\beta\Gamma$ and γ in Eq. (2) are constant, the convergence proof by Ref. [8] can be applied straightforwardly and yield inverse-logarithmic law of the temperature and the transverse field.
- [22] Spin-glass server, http://www.informatik.uni-koeln.de/ls_juenger/research/sgs/sgs.html
- [23] D. Patane, A. Silva, L. Amico, R. Fazio, and G. E. Santoro, *Phys. Rev. Lett.* **101**, 175701 (2008).