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The quantum annealing and its application in a classical computer

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Combinatorial optimization is an inevitable task in various techniques of information processing. However this task is so hard that its complete achievement is almost impossible in practice. A lot of computational methods have been investigated to obtain an approximate solution for such a hard task. Some of effective methods originate in the concept of physics. For instance, the simulated thermal annealing method [1] is popular as a heuristic method which is inspired by the statistical mechanics.

In terms of physics, combinatorial optimization is represented by a disordered Ising spin Hamiltonian,

$$\mathcal{H} = -\sum_i J_i S_i^z - \sum_{ij} J_{ij} S_i^z S_j^z - \sum_{ijk} J_{ijk} S_i^z S_j^z S_k^z - \cdots, \tag{1}$$

where S_i^z is the Ising spin variable and J_i, J_{ij}, J_{ijk}, $\cdots$ are disordered coupling constants. The task imposed on us is to obtain the spin configuration of the ground state of this classical Hamiltonian. The quantum annealing method has been proposed originally by analogy with the simulated thermal annealing method [2, 3]. While the thermal annealing method introduces thermal fluctuations, the quantum annealing method exploits quantum fluctuations in order to achieve global optimization. It is known that thermal and quantum fluctuations cause similar changes in physical quantities of the Ising spin system. However, in spite of the resemblance, the mechanism of optimization is quite different. In the quantum annealing method, the solution is obtained from pursuing the time evolution of the quantum state vector governed by the Schrödinger equation. The optimization results from the adiabatic evolution of the quantum state [4]. Since the solution is obtained through quantum states, the quantum annealing method is a so-called quantum algorithm for classical problems.

For any algorithm, it is important to reveal its efficiency. In order to know how the accuracy of the solution improves with running time, the residual energy is an appropriate quantity to be investigated. The residual energy is defined by the energy difference between the approximate solution obtained using the algorithm and the true solution. Small residual energy corresponds to high accuracy. It has been predicted for the quantum annealing method that the residual energy decreases with time, τ, as $E_{\rm res} \sim 1/(\ln \tau)^6$ [5]. However this has not been confirmed numerically. In contrast, we have shown another scaling law of the residual energy given by

$$E_{\rm res} \sim \frac{1}{\tau^2}, \tag{2}$$

which has been supported by numerical calculations [6]. Since theoretical grounds of these two formulas are different, they are not in contradiction. The latter is valid for $\tau \to \infty$, while the former is predicted for finite τ region. The behavior of residual energy in wide time region should be clarified numerically in future. Note here that eq. (2) means that the residual energy decreases qualitatively faster due to the quantum adiabatic evolution algorithm in comparison with logarithmic behavior due to the thermal annealing algorithm, $E_{\rm res} \sim 1/(\ln \tau)^\zeta$ with $1 \leq \zeta \leq 2$.

One aspect of the quantum annealing method lies in possibility of implementation in classical computers. In order to carry out the algorithm, we have to calculate time evolution of a quantum state. If we do it straightforwardly, the number of bases increases exponentially with system size and thus the simulation is limited to small sizes. So far the quantum Monte-Carlo method has been applied to carry out the algorithm for problems of large size. It has been reported that the quantum Monte-Carlo method succeeds in obtaining results better than those from the thermal annealing method in optimization of

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some disordered Ising models [7]. However, in quantum Monte-Carlo method, the state evolves stochastically by means of Markovian Monte-Carlo process. The dynamics of Markovian process is different from the real-time dynamics in quantum mechanics. Hence it has been also reported that the quantum Monte-Carlo method fails in optimization of another model [8].

In order to simulate the quantum annealing method ideally, calculation of the real-time evolution of a quantum state is needed. In our study, we propose application of the density matrix renormalization group method (DMRG) for numerical implementation of the quantum annealing method. DMRG has been developed in study of one-dimensional quantum systems in solid state physics. It was arranged for calculation of real-time evolution of quantum states recently [9]. It is a unique method which enables to simulate the real-time quantum dynamics in systems of large size.

We studied one-dimensional disordered Ising model with periodic boundary condition in practice. The interaction was assumed to act between pairs of nearest neighbor spins, and longitudinal magnetic field was considered to remove trivial degeneracy of the ground state. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{i=1}^{N-1} J_{ii+1} S_i^z S_{i+1}^z - J_{N1} S_N^z S_1^z - h \sum_{i=1}^{N} S_i^z. \tag{3}$$

The coupling constants, J_{ii+1}, were randomly selected from $[-1, 1]$. The sign of coupling constant between spins at both edges, J_{N1} was arranged so as to introduce frustration to the system. Due to the presence of frustration and the magnetic field, the problem finding the ground state of this model is non-trivial.

DMRG calculations were performed for the system up to $N = 80$ sites. The solution obtained from quantum annealing method is a superposition of classical states. We found that the solution becomes close to a classical state with increasing running time. We checked that the asymptotic classical state is the true ground state of the Hamiltonian, eq. (3), up to $N = 32$ sites. Hence it is reasonable to conclude that the solution from the quantum annealing approaches the true one even in $N = 80$ case. Furthermore we found that the residual energy decreases as inverse square of the running time for long running time. The residual energy here was measured from the energy of the asymptotic classical state. This behavior of the residual energy is consistent with eq. (2) which is mentioned in ref. [6].

The results of simulation mean that DMRG calculation produces not only the correct solution but asymptotic feature of the solution expected for long running time at least for the present model. The problem of one-dimensional model we studied is a simple but non-trivial combinatorial optimization problem. Although application to more complicated models is in progress, success of simulated quantum annealing method using DMRG is promised for one-dimensional periodic problems.

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