

Nonequilibrium work performed in quantum annealing

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Abstract. Quantum annealing is a generic solver of classical optimization problems that makes full use of quantum fluctuations. We consider work statistics given by a repetition of quantum annealing processes by employing the Jarzynski equality proposed in nonequilibrium statistical physics. In particular, we analyze a nonequilibrium average of the exponentiated work performed by a transverse field. A special symmetry, gauge symmetry, leads to a non-trivial relationship between quantum annealing toward different targets in the theory of spin glasses. We believe that our results will be a step toward an alternative realization of efficient quantum computation as well as our better understanding of nonequilibrium behavior of systems under quantum control.

1. Introduction

We should often solve difficult problems in a reasonable time, which is closely related to the efficiency in cost and time in industry and distribution systems. A well-known instance is to find the minimum path for a person to visit all the cities, called the traveling salesman problem, which is a typical optimization problem [1, 2]. The goal of quantum computation is to solve problems hard to solve quickly on classical computer in a moderate time by use of superpositions, tunneling effects, and entanglement of quantum nature. Quantum annealing is a method to realize quantum computation [3, 4, 5, 6]. Conventional quantum computation uses successive, discrete unitary operations to enhance the probability of the desired state representing the answer of a hard optimization problem. In contrast, quantum annealing uses continuous dynamics represented by a time-dependent Schrödinger equation. Dynamical behavior of quantum systems during such processes is still poorly understood, and an adiabatic control of quantum dynamics is often employed, called the quantum adiabatic computation [7]. Such a quantum adiabatic computation, however, has a bottleneck for a certain type of the optimization problems [8, 9].

A recent study of quantum annealing indicates a possible deviation from adiabatic controls [10]. In the present paper, we proceed along this line and analyze the work performed by quantum fluctuations in a non-adiabatic control of system parameter. The analysis makes use of several remarkable properties found in statistical physics. One is an exact relationship between nonequilibrium processes and equilibrium states at the beginning and end, the Jarzynski equality [11, 12]. Another is a special symmetry, called the gauge symmetry, found in spin glasses

[13, 14]. As detailed below, a combination of these theories enables us to obtain exact relations between equilibrium and nonequilibrium quantities and to evaluate several quantities related to dynamical processes in quantum systems [15].

After an introduction of the Jarzynski equality, we develop our analyses by use of gauge symmetry to show the derivation of an exact identity related with the performed work during quantum annealing.

2. Quantum annealing and spin glasses

We consider the following time-dependent Hamiltonian in quantum annealing

$$H(t) = -f(t)J \sum_{\langle ij \rangle} \tau_{ij} \sigma_i^z \sigma_j^z - \Gamma(1-f(t)) \sum_i \sigma_i^x, \quad (1)$$

where $f(t) = t/T$, and t runs continuously from 0 to T . The initial Hamiltonian $H(0)$ is composed only of the transverse-field term $-\Gamma \sum_i \sigma_i^x$. The final Hamiltonian $H(T)$ is chosen to describe the optimization problem to be solved. We take a simple spin glass Hamiltonian as $H(T)$, the $\pm J$ Ising model, on an arbitrary lattice throughout this paper for convenience. The sign of the interaction τ_{ij} follows the distribution function

$$P(\tau_{ij}) = p\delta(1 - \tau_{ij}) + (1-p)\delta(1 + \tau_{ij}) = \frac{e^{\beta_p J \tau_{ij}}}{2 \cosh \beta_p J}, \quad (2)$$

where p is the concentration of the ferromagnetic interaction $J > 0$, and $\exp(-2\beta_p J) = (1-p)/p$. A sufficiently slow decrease of the strength of the transverse field changes the trivial initial state to the nontrivial ground state of the target Hamiltonian $H(T)$. This is the idea of quantum adiabatic computation realized in $T \rightarrow \infty$. Instead of the adiabatic control, in the present study, let us consider the repetition of fast quantum annealing (T small) starting from an equilibrium ensemble. We may not be able to always reach the desired state since the system does not trace the instantaneous ground state when the adiabatic condition is not satisfied. Therefore we need to repeat the process to hit the correct ground state in such a non-adiabatic realization of quantum annealing.

We next point out that a class of models of spin glasses has a special symmetry known as the gauge symmetry. We define the gauge transformation as the following local unitary operator for Pauli spin matrices, and the change of the sign of the interaction [16]:

$$\sigma_i^\alpha \rightarrow G \sigma_i^\alpha G^{-1}, G = \prod_i G_i, \quad G_i = \begin{cases} 1 & (\xi_i = +1) \\ \exp(i\pi \sigma_i^x / 2) & (\xi_i = -1) \end{cases} \quad (3)$$

where $\alpha = x, y, z$ and $\tau_{ij} = \tau_{ij} \xi_i \xi_j$, where ξ is a classical gauge variable taking only ± 1 . After the above gauge transformation, the time-dependent Hamiltonian (1) is invariant, but the distribution function (2) is modified into $P(\tau_{ij}) = \exp(\beta_p J \tau_{ij} \xi_i \xi_j) / 2 \cosh \beta_p J$. This property helps us to derive the following results.

3. Analysis

3.1. Jarzynski equality

Let us introduce another piece of theoretical tool, the Jarzynski equality, which is a generalization of the second law of thermodynamics. We here use the quantum version of the Jarzynski equality for the $\pm J$ Ising model, not the original version for the classical case [11, 12], with a specific configuration $\{\tau_{ij}\}$ as follows [17, 18],

$$\langle e^{-\beta W} \rangle_{0 \rightarrow T} = \frac{Z_\beta(T; \{\tau_{ij}\})}{Z_\beta(0; \{\tau_{ij}\})}, \quad (4)$$

where $Z_\beta(t; \{\tau_{ij}\})$ is the partition function for the instantaneous Hamiltonian, and β is the inverse temperature. The performed work during a nonequilibrium process is given by the difference between the outputs of the measurements of the initial and final energies as $W = E_m(T) - E_n(0)$, where m and n denote the indices of the eigenstates as $H(T)|m(T)\rangle = E_m(T)|m(T)\rangle$ and $H(0)|n(0)\rangle = E_n(0)|n(0)\rangle$. The left-hand side of equation (4) expresses the average of the exponentiated work over all the realizations of nonequilibrium processes starting from the equilibrium ensemble, and is evaluated as

$$\begin{aligned} \langle e^{-\beta W} \rangle_{0 \rightarrow T} &= \sum_{m,n} e^{-\beta(E_m(T) - E_n(0))} P(m|n) \frac{e^{-\beta E_n(0)}}{Z_\beta(0; \{\tau_{ij}\})} \\ &= \frac{1}{Z_\beta(0; \{\tau_{ij}\})} \sum_{m,n} e^{-\beta E_m(T)} P(m|n) = \frac{Z_\beta(T; \{\tau_{ij}\})}{Z_\beta(0; \{\tau_{ij}\})}, \end{aligned} \quad (5)$$

where we use the path probability for a nonequilibrium process as, $P(m|n) = |\langle m(T) | U_{0 \rightarrow T} | n(0) \rangle|^2$. Here $U_{0 \rightarrow T}$ is the time evolution operator.

3.2. Jarzynski equality for quantum annealing : Symmetric distribution

The partition function for the initial Hamiltonian $H(0)$ does not depend on the configuration $\{\tau_{ij}\}$ since it is given only by the transverse field, $Z_\beta(0; \{\tau_{ij}\}) = (2 \cosh \beta \Gamma)^N$. Here N is the number of spins. Let us now consider the configurational average of the Jarzynski equality for quantum annealing by summation over all the possible configurations $\{\tau_{ij}\}$ as

$$\left[\langle e^{-\beta W} \rangle_{0 \rightarrow T} \right]_{\beta_p} = \frac{[Z_\beta(T; \{\tau_{ij}\})]_{\beta_p}}{(2 \cosh \beta \Gamma)^N}. \quad (6)$$

The explicit expression of the quantity on the right-hand side is

$$\frac{[Z_\beta(T; \{\tau_{ij}\})]_{\beta_p}}{(2 \cosh \beta \Gamma)^N} = \frac{1}{(2 \cosh \beta \Gamma)^N (2 \cosh \beta_p J)^{N_B}} \sum_{\tau_{ij}} \prod_{\langle ij \rangle} e^{\beta_p J \tau_{ij}} Z_\beta(T; \{\tau_{ij}\}), \quad (7)$$

where N_B is the number of interactions. If we set $\beta_p = 0$, which corresponds to the case with the symmetric distribution of the interaction ($p = 1/2$), the above quantity can be evaluated as

$$\left[\langle e^{-\beta W} \rangle_{0 \rightarrow T} \right]_{\beta_p=0} = \frac{2^N (2 \cosh \beta J)^{N_B}}{2^{N_B} (2 \cosh \beta \Gamma)^N}. \quad (8)$$

3.3. Inverse statistics on special subspace

Let us show that the gauge transformation reveals a non-trivial property of the nonequilibrium average of the exponentiated work during quantum annealing. We take the configurational average of the inverse of the nonequilibrium-averaged exponentiated work as

$$\left[\frac{1}{\langle e^{-\beta W} \rangle_{0 \rightarrow T}} \right]_{\beta_p} = \frac{(2 \cosh \beta \Gamma)^N}{(2 \cosh \beta_p J)^{N_B}} \sum_{\tau_{ij}} \frac{\prod_{\langle ij \rangle} e^{\beta_p J \tau_{ij}}}{Z_\beta(T; \{\tau_{ij}\})}. \quad (9)$$

Here we apply the gauge transformation to the above equality. The quantity on the left-hand side does not change, since the Hamiltonian and the time-evolution operator are invariant. On the other hand, the quantity on the right-hand side becomes

$$\left[\frac{1}{\langle e^{-\beta W} \rangle_{0 \rightarrow T}} \right]_{\beta_p} = \frac{(2 \cosh \beta \Gamma)^N}{(2 \cosh \beta_p J)^{N_B}} \sum_{\tau_{ij}} \frac{\prod_{\langle ij \rangle} e^{\beta_p J \tau_{ij} \xi_i \xi_j}}{Z_\beta(T; \{\tau_{ij}\})}. \quad (10)$$

Setting $\beta = \beta_p$ and taking the summation over all configurations of ξ_i leads us to

$$\left[\frac{1}{\langle e^{-\beta W} \rangle_{0 \rightarrow T}} \right]_{\beta} = \frac{2^{N_B} (2 \cosh \beta \Gamma)^N}{2^N (2 \cosh \beta J)^{N_B}}, \quad (11)$$

which implies that

$$\left[\langle e^{-\beta W} \rangle_{0 \rightarrow T} \right]_{\beta_p=0} = \left(\left[\frac{1}{\langle e^{-\beta W} \rangle_{0 \rightarrow T}} \right]_{\beta_p=\beta} \right)^{-1}. \quad (12)$$

This equality represents a non-trivial relationship in quantum annealing driven toward two different states in spin glasses $\beta_p = 0$ and $\beta_p = \beta$. It is important to remark that we do not use any approximations in the above calculation, and we deal with the nonequilibrium average during quantum annealing, which does not assume to be quasi-static, unlike quantum adiabatic computation.

4. Summary

We can obtain several further exact equalities for the repetition of non-adiabatic quantum annealing and establish non-trivial relations that hold between quantum annealing toward different spin glasses, as will be announced shortly in a separate paper. Exactness of our results would be useful as a benchmark to check experimental conditions of nonequilibrium process in quantum spin dynamics. Notice that our results are scalable, which means independence of the system size, since the Jarzynski equality holds for any size if we take all fluctuations into account in estimation of the expectation value on the left-hand side of equation (4). Finite errors on the ratio of the partition functions may be attributed to the rare event on nonequilibrium processes. The present study will help us to understand and manipulate quantum dynamics efficiently.

References

- [1] Garey M R and Johnson D S 1979 *Computers and Intractability: A Guide to the Theory of NP-Completeness* (San Francisco: Freeman)
- [2] Hartmann A K and Weigt M 2005 *Phase Transitions in Combinatorial Optimization Problems: Basics, Algorithms and Statistical Mechanics* (Wiley-VCH, Weinheim)
- [3] Kadowaki T and Nishimori H 1998 *Phys. Rev. E* **58** 5355
- [4] Das A and Chakrabarti B K 2008 *Rev. Mod. Phys.* **80** 1061
- [5] Morita S and Nishimori H 2008 *J. Math. Phys.* **49** 125210
- [6] Ohzeki M and Nishimori H 2011 to appear in *J. Comp. Theor. Nanoscience*
- [7] Farhi E, Goldstone J, Gutmann S and Sipser M, arXiv:0001106
- [8] Jörg T, Krzakala F, Kurchan J and Maggs A C 2008 *Phys. Rev. Lett.* **101** 147204
- [9] Young A P, Knysh S and Smelyanskiy V N 2010 *Phys. Rev. Lett.* **104** 020502
- [10] Ohzeki M 2010 *Phys. Rev. Lett.* **105** 050401
- [11] Jarzynski C 1997 *Phys. Rev. Lett.* **78** 2690
- [12] Jarzynski C 1997 *Phys. Rev. E* **56** 5018
- [13] Nishimori H 1981 *Prog. Theor. Phys.* **66** 1169
- [14] Nishimori H *Statistical Physics of Spin Glasses and Information Processing: An Introduction* (Oxford Univ. Press, Oxford, 2001)
- [15] Ohzeki M and Nishimori H 2010 *J. Phys. Soc. Jpn.* **79** 084003
- [16] Morita S, Nishimori H and Ozeki Y 2006 *J. Phys. Soc. Jpn.* **75** 014001
- [17] Tasaki H arXiv:0009244
- [18] Campisi M, Talkner P and Hänggi P 2009 *Phys. Rev. Lett.* **102** 210401