arXiv:1004.2389v1 [cond-mat.dis-nn] 14 Apr 2010

Non-equilibrium Relations for Spin Glasses with Gauge Symmetry

Masayuki Ohzeki and Hidetoshi Nishimori

Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551,

Japan

We study the applications of non-equilibrium relations such as the Jarzynski equality and fluctuation theorem to spin glasses with gauge symmetry. It is shown that the exponentiated free-energy difference appearing in the Jarzynski equality reduces to a simple analytic function written explicitly in terms of the initial and final temperatures if the temperature satisfies a certain condition related to gauge symmetry. This result is used to derive a lower bound on the work done during the non-equilibrium process of temperature change. We also prove identities relating equilibrium and non-equilibrium quantities. These identities suggest a method to evaluate equilibrium quantities from non-equilibrium computations, which may be useful to avoid the problem of slow relaxation in spin glasses.

1. Introduction

Equilibrium and non-equilibrium properties of spin glasses have been studied for many years by experimental, numerical and analytical methods.[1–3] Although most of the theoretical problems have been solved fairly satisfactorily at the mean-field level,[4] it is still difficult to establish analytical results for finite-dimensional systems. Numerical approaches are powerful tools in finite dimensions but are often hampered by slow relaxation if one wishes to evaluate equilibrium quantities at low temperatures, and ingenious methods have been proposed to circumvent this difficulty.[5–10] In particular, Neal[7] proposed annealed importance sampling, in which one changes the temperature and measures physical quantities in a spirit similar to the Jarzynski equality.[11,12] Hukushima and Iba[8,9] improved Neal's method by incorporating a branching process for the stability of the algorithm. Their method, which they called population annealing, showed outstanding performance comparable to the exchange Monte Carlo.

Non-equilibrium relations such as the Jarzynski equality and fluctuation theorem[13–15] represent important developments in non-equilibrium statistical physics because they directly relate non-equilibrium and equilibrium quantities (Jarzynski equality) or the probability of a non-equilibrium process and its inverse process (fluctuation theorem). It is the purpose of the present paper to apply the non-equilibrium relations to the context of spin glasses and show that non-trivial simplifications are observed under certain conditions on the system parameters. Several additional non-equilibrium relations are also derived that connect equilibrium

and non-equilibrium quantities. These results are not only interesting in their own right but may be useful to extract information from non-equilibrium numerical simulations following the idea of Neal and Hukushima and Iba.

This paper is organized as follows. In the next section, we recall the basic formulation in order to fix the notation and set the stage for further developments in the following sections. In §3, we establish several non-equilibrium relations by using gauge symmetry. In the last section, we give a summary of the results obtained in the present study.

2. Formulation

Let us consider the $\pm J$ Ising model of spin glasses on an arbitrary lattice,

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j, \tag{1}$$

where the distribution function of quenched randomness is specified as

$$P(\tau_{ij}) = p\delta(\tau_{ij} - 1) + (1 - p)\delta(\tau_{ij} + 1) = \frac{e^{K_p \tau_{ij}}}{2\cosh K_p} \tag{2}$$

with τ_{ij} being the sign of J_{ij} ($J_{ij} = \tau_{ij} J$). The parameter K_p has been defined as $e^{-2K_p} = (1 - p)/p$. The product βJ will be written as K. The following analyses can readily be applied to other distribution functions of J_{ij} as long as they satisfy a certain type of gauge symmetry.[16,17]

Suppose that the system evolves following a stochastic dynamics governed by the master equation. For simplicity, we will formulate our theory for discrete time steps although the continuous case can be treated similarly. We change the value of the coupling K from K_0 at $t = t_0$ to K_T at $t = t_n$ in n steps of time evolution, $(K_0, K_1, \cdots, K_n = K_T)$. Correspondingly, the spin configuration changes as $\mathbf{S}_0$ (at $t = t_0$), $\mathbf{S}_1$ (at $t = t_1$), $\cdots$, $\mathbf{S}_n$ (at $t = t_n$). These configurations will be collectively denoted as $\{\mathbf{S}\}$. Notice that each $\mathbf{S}_i$ stands for a configuration of N spins at time $t = t_i$. The system is assumed to be in equilibrium at $t = t_0$.

The fluctuation theorem[13–15] relates the probability $P_{K_0 \to K_T}(\{\mathbf{S}\})$ that such a sequence is realized with the probability $P_{K_T \to K_0}(\{\mathbf{S}\})$ of the inverse process as

$$\frac{P_{K_0 \to K_T}(\{\mathbf{S}\})}{P_{K_T \to K_0}(\{\mathbf{S}\})} e^{-\beta W} = \frac{Z(K_T; \{\tau_{ij}\})}{Z(K_0; \{\tau_{ij}\})}. \tag{3}$$

Here W is the work done to the system during the non-equilibrium process. More precisely, the work for a single time step δW is defined as

$$\beta \cdot \delta W = (K_{i+1} - K_i) E(\mathbf{S}_i). \tag{4}$$

where $E(\mathbf{S}_i)$ is the instantaneous energy for the spin configurations $\mathbf{S}_i$ given by the Hamiltonian (1) divided by J. The right-hand side of eq. (3) is the ratio of equilibrium partition functions at two different couplings with a fixed configuration of quenched randomness.

Equation (3) immediately leads to, for an observable $O(\{\mathbf{S}\})$,

$$\left\langle O(\{\mathbf{S}\})\mathrm{e}^{-\beta W}\right\rangle_{K_0\to K_T} = \langle O_{\mathrm{r}}(\{\mathbf{S}\})\rangle_{K_T\to K_0}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}, \tag{5}$$

where O_{r} denotes the observable which depends on the backward process $K_T \to K_0$. The brackets with subscript $K_0 \to K_T$ denote the average with the weight $P_{K_0\to K_T}(\{\mathbf{S}\})$ over possible non-equilibrium processes. For $O = O_{\mathrm{r}} = 1$, eq. (5) reduces to the Jarzynski equality.[11, 12]

If we choose an observable depending only on the final state, which we denote by O_T, instead of $O(\{\mathbf{S}\})$, O_{r} becomes an observable at the initial state in the backward process. Then $\langle O_{\mathrm{r}}\rangle_{K_T\to K_0}$ equals to the ordinary thermal average at the initial equilibrium state with the coupling constant K_T, to be denoted by $\langle\cdots\rangle_{K_T}$, and eq. (5) reads

$$\left\langle O_T\mathrm{e}^{-\beta W}\right\rangle_{K_0\to K_T} = \langle O\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}. \tag{6}$$

3. Non-equilibrium relations on the Nishimori Line

We now consider the application of the relations (5) and (6) to the context of spin glasses.

3.1 Gauge-invariant quantities

We apply the non-equilibrium relation (6) to a gauge-invariant quantity $G(\{\tau_{ij}\})$. After the configurational average (to be expressed as $[\cdots]_{K_p}$), we have

$$\left[\left\langle G_T(\{\tau_{ij}\})\mathrm{e}^{-\beta W}\right\rangle_{K_0\to K_T}\right]_{K_p} = \left[\langle G(\{\tau_{ij}\})\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_p}. \tag{7}$$

The quantity on the left-hand side is the configurational as well as non-equilibrium averages of the observable $G(\{\tau_{ij}\})$ at final time T, that is after the protocol $K_0 \to K_T$ with the factor $e^{-\beta W}$. On the other hand, $\langle G(\{\tau_{ij}\})\rangle_{K_T}$ on the right-hand side means the configurational and thermal average of the equilibrium state for the final Hamiltonian.

Let us apply the gauge transformation $S_i \to S_i\sigma_i,\ J_{ij} \to J_{ij}\sigma_i\sigma_j\ (\forall i,j)$.[16,17] The right-hand side of eq. (7) is then rewritten explicitly as,

$$\left[\langle G(\{\tau_{ij}\})\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_p} = \sum_{\{\tau_{ij}\}}\frac{\langle G(\{\tau_{ij}\})\rangle_{K_T}\prod_{\langle ij\rangle}\mathrm{e}^{K_p\tau_{ij}\sigma_i\sigma_j}}{(2\cosh K_p)^{N_B}}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}, \tag{8}$$

where N_B is the number of bonds on the lattice. All the quantities in this equation are invariant under the gauge transformation. After the summation over $\{\sigma_i\}$ and division by 2^N, we obtain[16,17]

$$\left[\langle G(\{\tau_{ij}\})\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_p} = \sum_{\{\tau_{ij}\}}\frac{\langle G(\{\tau_{ij}\})\rangle_{K_T}Z(K_p;\{\tau_{ij}\})}{2^N(2\cosh K_p)^{N_B}}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}. \tag{9}$$

It is useful to analyze here the quantity $[\langle G(\{\tau_{ij}\})\rangle_{K_T}]_{K_p}$. Similarly to the above calculation,

the following identity can be derived by the gauge transformation,

$$[\langle G(\{\tau_{ij}\})\rangle_{K_T}]_{K_p} = \sum_{\{\tau_{ij}\}} \frac{\langle G(\{\tau_{ij}\})\rangle_{K_T} Z(K_p; \{\tau_{ij}\})}{2^N (2\cosh K_p)^{N_B}}. \tag{10}$$

Setting $K_p = K_0$ in eq. (9) and $K_p = K_T$ in eq. (10), we reach the following non-equilibrium relation,

$$\left[\langle G_T(\{\tau_{ij}\}) e^{-\beta W}\rangle_{K_0 \to K_T}\right]_{K_0} = [\langle G(\{\tau_{ij}\})\rangle_{K_T}]_{K_T} \left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{11}$$

If we set $G_T(\{\tau_{ij}\}) = 1$ in eq. (11), the Jarzynski equality for spin glass is obtained,

$$\left[\left\langle e^{-\beta W}\right\rangle_{K_0 \to K_T}\right]_{K_0} = \left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{12}$$

Equation (12) leads to, using Jensen's inequality for the average of $e^{-\beta W}$,

$$[\langle W\rangle_{K_0 \to K_T}]_{K_0} \geq -\frac{N_B}{\beta} \log\left(\frac{2\cosh K_T}{2\cosh K_0}\right). \tag{13}$$

The right-hand side corresponds to ΔF in the Jarzynski equality in the usual representation.

By substituting $G_T(\{\tau_{ij}\}) = H$ into eq. (11), we obtain

$$\left[\left\langle H e^{-\beta W}\right\rangle_{K_0 \to K_T}\right]_{K_0} = [\langle H\rangle_{K_T}]_{K_T} \left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{14}$$

This equation shows that the internal energy after the cooling or heating process starting from a temperature on the Nishimori line (NL),[16,17] defined by $K = K_p$ which is in the present case $K = K_p = K_0$, is proportional to the internal energy in the equilibrium state on the NL corresponding to the final temperature.

It is straightforward to obtain a non-equilibrium relation for gauge-invariant quantities depending on the intermediate spin configurations,

$$\left[\left\langle G(\{\mathbf{S}\}) e^{-\beta W}\right\rangle_{K_0 \to K_T}\right]_{K_0} = [\langle G_r(\{\mathbf{S}\})\rangle_{K_T \to K_0}]_{K_T} \left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{15}$$

For instance, the autocorrelation function satisfies

$$\left[\left\langle S_i(0) S_i(T) e^{-\beta W}\right\rangle_{K_0 \to K_T}\right]_{K_0} = [\langle S_i(0) S_i(T)\rangle_{K_T \to K_0}]_{K_T} \left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{16}$$

This gives a non-trivial relation between the cooling and heating processes but with different amount of quenched randomness characterized by K_0 and K_T. Let us consider the cooling process from a temperature on the NL given by $(1/K_0, 1/K_0)$ to a point away from the NL $(1/K_0, 1/K_T)$ as depicted by the downward arrow in Fig. 1. The above equation relates this process with the inverse process from a temperature on the NL $(1/K_T, 1/K_T)$ to a point away from the NL $(1/K_T, 1/K_0)$ drawn as the upward arrow in Fig. 1. The process of the upward arrow passes through the ferromagnetic and paramagnetic phases, whereas the cooling process goes through the spin glass phase. These apparently very different processes are related by eq. (16), which is a non-trivial observation.
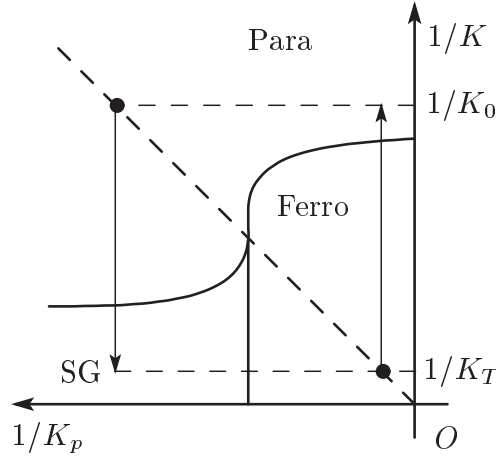
Fig. 1.   The processes of eq. (16) drawn as two arrows on the phase diagram. The solid curves are the phase boundaries and the dashed line of 45° represents the NL.

We can establish another type of non-equilibrium relation following Ozeki.[18] We consider a non-equilibrium relaxation of the local magnetization $\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T}$, where F means that the initial state is $\mathbf{S}_0 = (+1, +1, \cdots, +1)$. We evaluate the time evolution of the local magnetization as

$$\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T} = \sum_{\{\mathbf{S}\}} S_i(T) e^{\Delta t M(\mathbf{S}_n | \mathbf{S}_{n-1}; t_n)} \cdots e^{\Delta t M(\mathbf{S}_1 | \text{F}; t_1)}, \tag{17}$$

where $\Delta t (\ll 1)$ is the unit time interval and $M(\mathbf{S} | \mathbf{S}'; t_n)$ is the transition rate from state $\mathbf{S}'$ to state $\mathbf{S}$ following the master equation. The initial condition F is different from the case of non-equilibrium relations, where the equilibrium distribution is assumed initially.

Let us apply the gauge transformation to $\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T}$,[18]

$$\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T} = \sum_{\{\mathbf{S}\}} S_i \sigma_i(T) e^{\Delta t M(\mathbf{S}_n | \mathbf{S}_{n-1}; t_n)} \cdots e^{\Delta t M(\mathbf{S}_1 | \sigma; t_1)}. \tag{18}$$

The configurational average for $\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T}$ is thus

$$\left[\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T} \right]_{K_p}$$

$$= \sum_{\{\tau_{ij}\}} \sum_{\{\mathbf{S}\}} S_i(T) \sigma_i \frac{1}{(2 \cosh K_p)^{N_B}} \prod_{\langle ij \rangle} e^{K_p \tau_{ij} \sigma_i \sigma_j} e^{\Delta t M(\mathbf{S}_n | \mathbf{S}_{n-1}; t_n)} \cdots e^{\Delta t M(\mathbf{S}_1 | \sigma; t_1)}. \tag{19}$$

If we set $K_p = K_0$ and take the summation over all configurations of σ, we obtain

$$\left[\langle S_i(T) \rangle^{\text{F}}_{K_0 \to K_T} \right]_{K_0} = \sum_{\{\tau_{ij}\}} \frac{Z(K_0; \{\tau_{ij}\})}{2^N (2 \cosh K_0)^{N_B}} \langle S_i(T) S_i(0) \rangle_{K_0 \to K_T}. \tag{20}$$

Since the autocorrelation function is gauge-invariant, the right-hand side can be shown to be

the configurational average using the same method as in eq. (10),[18)]

$$\left[\langle S_i(T)\rangle^{\mathrm{F}}_{K_0\to K_T}\right]_{K_0} = \left[\langle S_i(0)S_i(T)\rangle_{K_0\to K_T}\right]_{K_0}. \tag{21}$$

Similarly we can prove that the autocorrelation function with the exponentiated work satisfies

$$\left[\langle S_i(T)\mathrm{e}^{-\beta W}\rangle^{\mathrm{F}}_{K_T\to K_0}\right]_{K_T} = \left[\langle S_i(0)S_i(T)\mathrm{e}^{-\beta W}\rangle_{K_T\to K_0}\right]_{K_T}. \tag{22}$$

Comparison of eqs. (16) (with K_T and K_0 exchanged), (21) and (22) reveals

$$\left[\langle S_i(T)\rangle^{\mathrm{F}}_{K_0\to K_T}\right]_{K_0} = \left[\langle S_i(T)\mathrm{e}^{-\beta W}\rangle^{\mathrm{F}}_{K_T\to K_0}\right]_{K_T}\left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{23}$$

3.2 Gauge-non-invariant quantities

As a typical gauge-non-invariant quantity, we choose $S_i(T)$ for O in eq. (5). After the configurational average, we have

$$\left[\left\langle S_i(T)\mathrm{e}^{-\beta W}\right\rangle_{K_0\to K_T}\right]_{K_p} = \left[\langle S_i\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_p}. \tag{24}$$

Gauge transformation for the right-hand side in this equation yields

$$\left[\langle S_i\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_p} = \sum_{\{\tau_{ij}\}}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\langle S_i\rangle_{K_T}\sigma_i\prod_{\langle ij\rangle}\frac{\mathrm{e}^{K_p\tau_{ij}\sigma_i\sigma_j}}{2\cosh K_p}. \tag{25}$$

As usual, we sum both sides of this equation over all the possible configurations of σ and divide the obtained quantity by 2^N to find

$$\left[\langle S_i\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_p} = \sum_{\{\tau_{ij}\}}\frac{Z(K_p;\{\tau_{ij}\})}{2^N(2\cosh K_p)^{N_B}}\langle S_i\rangle_{K_T}\langle\sigma_i\rangle_{K_p}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}. \tag{26}$$

The following relation can also be derived in a similar manner,

$$[\langle S_i\rangle_{K_0}]_{K_p} = \sum_{\{\tau_{ij}\}}\frac{Z(K_p;\{\tau_{ij}\})}{2^N(2\cosh K_p)^{N_B}}\langle S_i\rangle_{K_0}\langle\sigma_i\rangle_{K_p}. \tag{27}$$

Setting $K_p = K_0$ in eq. (26) and $K_p = K_T$ in eq. (27), we find a relation

$$\left[\langle S_i\rangle_{K_T}\frac{Z(K_T;\{\tau_{ij}\})}{Z(K_0;\{\tau_{ij}\})}\right]_{K_0} = [\langle S_i\rangle_{K_0}]_{K_T}\left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{28}$$

Thus a non-equilibrium relation results,

$$\left[\langle S_i(T)\mathrm{e}^{-\beta W}\rangle_{K_0\to K_T}\right]_{K_0} = [\langle S_i\rangle_{K_0}]_{K_T}\left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{29}$$

The same method yields

$$\left[\langle S_0(T)S_r(T)\mathrm{e}^{-\beta W}\rangle_{K_0\to K_T}\right]_{K_0} = [\langle S_0 S_r\rangle_{K_0}]_{K_T}\left(\frac{2\cosh K_T}{2\cosh K_0}\right)^{N_B}. \tag{30}$$

Equations (29) and (30) relate the equilibrium physical quantities evaluated away from the NL (the right-hand sides) with other quantities measured by non-equilibrium processes from a point on the NL to another point away from the NL (the left-hand sides) as depicted in Fig. 2.
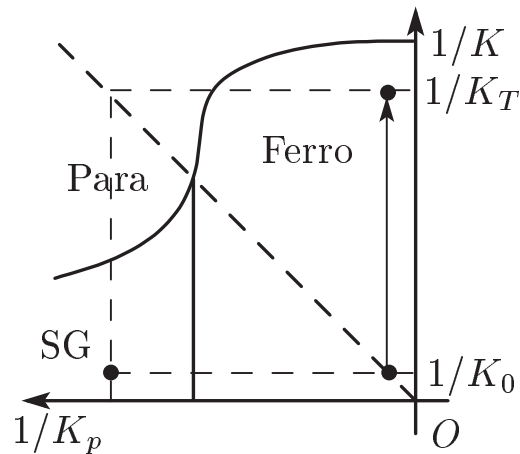
Fig. 2. Equations (29) and (30) relate equilibrium physical quantities evaluated at a point $(1/K_0, 1/K_T)$ (the lower-left dot in each panel) with other physical quantities evaluated by non-equilibrium processes shown in an arrow. The lower-left dot is in the spin glass phase whereas the corresponding arrow is in the ferromagnetic phase.

4. Summary

We have studied applications of non-equilibrium relations, typically the Jarzynski equality, to the context of spin glasses with gauge symmetry. It has been shown that the configurational average greatly simplifies a number of expressions appearing in non-equilibrium relations. In particular, the right-hand side of the Jarzynski equality, usually written as $e^{-\beta \Delta F}$, reduces to a trivial analytic function of the initial and final temperatures, which has been used to prove a simple lower bound on the work. Many identities have also been derived for gauge-invariant and gauge-non-invariant quantities, which relate physical quantities measured at quite different environments. Most notably, the equilibrium values of the single-site magnetization and correlation function have been proved to be proportional to the non-equilibrium values of the corresponding quantities measured at different parts of the phase diagram. This result may possibly be useful to numerically evaluate equilibrium physical quantities in the spin glass phase from non-equilibrium calculations away from the spin glass phase with the aid of annealed importance sampling or population annealing method.[7–9]

References

1) K. Binder, and A. P. Young: Rev. Mod. Phys. **58** (1986) 801.
2) A. P. Young (ed.): *Spin Glasses and Random Fields* (World Scientific, Singapore, 1997).
3) N. Kawashima, and H. Rieger: in *Frustrated Spin Systems*, ed. T. H. Diep (World Scientific, Singapore, 2004).
4) M. Mézard, G. Parisi and M. A. Virasoro: *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).
5) R. H. Swendsen, and J. S. Wang: Phys. Rev. Lett. **58** (1987) 56.
6) K. Hukushima, and K. Nemoto: J. Phys. Soc. Jpn. **65** (1996) 1604.
7) R. M. Neal: Statistics and Computing, **11** (2001) 125.
8) Y. Iba: Trans. Jpn. Soc. Artif. Intel. **16** (2001) 279.
9) K. Hukushima, and Y. Iba: AIP. Conf. Proc. **690** (2003) 200.
10) Y. Ozeki and N. Ito: J. Phys. A: Math. Theor. **40** (2007) R149.
11) C. Jarzynski: Phys. Rev. Lett. **78** (1997) 2690.
12) C. Jarzynski: Phys. Rev. E **56** (1997) 5018.
13) G. E. Crooks: J. Stat. Phys. **90** (1998) 1481.
14) G. E. Crooks: Phys. Rev. E **60** (1999) 2721.
15) G. E. Crooks: Phys. Rev. E **61** (2000) 2361.
16) H. Nishimori: Prog. Theor. Phys. **66** (1981) 1169.
17) H. Nishimori: *Statistical Physics of Spin Glasses and Information Processing: An Introduction* (Oxford Univ. Press, Oxford, 2001).
18) Y. Ozeki: J. Phys. A: Math. Gen. **28** (1995) 3645.