Heat fluctuations in Ising models coupled with two different heat baths

2008 J. Phys. A: Math. Theor. 41 332003

(http://iopscience.iop.org/1751-8121/41/33/332003)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **41** (2008) 332003 (7pp) doi:10.1088/1751-8113/41/33/332003

FAST TRACK COMMUNICATION

Heat fluctuations in Ising models coupled with two different heat baths

A Piscitelli[1], **F Corberi**[2] **and G Gonnella**[1]

[1] Dipartimento di Fisica, Università di Bari and Istituto Nazionale di Fisica Nucleare, Sezione di Bari, via Amendola 173, 70126 Bari, Italy
[2] Dipartimento di Matematica ed Informatica, via Ponte don Melillo, Università di Salerno, 84084 Fisciano (SA), Italy

E-mail: antonio.piscitelli@ba.infn.it, federico.corberi@sa.infn.it and giuseppe.gonnella@ba.infn.it

Received 17 June 2008, in final form 1 July 2008
Published 17 July 2008
Online at stacks.iop.org/JPhysA/41/332003

Abstract
Monte Carlo simulations of Ising models coupled to heat baths at two different temperatures are used to study a fluctuation relation for the heat exchanged between the two thermostats in a time τ. Different kinetics (single-spin-flip or spin-exchange Kawasaki dynamics), transition rates (Glauber or Metropolis), and couplings between the system and the thermostats have been considered. In every case the fluctuation relation is verified in the large τ limit, both in the disordered and in the low temperature phase. Finite-τ corrections are shown to obey a scaling behavior.

PACS numbers: 05.70.Ln, 05.40.−a, 75.40.Gb

(Some figures in this article are in colour only in the electronic version)

In equilibrium statistical mechanics expressions for the probability of different microstates, such as the Gibbs weight in the canonical ensemble, are the starting point of a successful theory which allows the description of a broad class of systems. A key point of this approach is its generality. Specific aspects, such as, for instance, the kinetic rules or the details of the interactions with the external reservoirs, are irrelevant for the properties of the equilibrium state.

In non-equilibrium systems general expressions for probability distributions are not available; however, the recent proposal [1–3] of relations governing the fluctuations is of great interest. They were formalized, for a class of dynamical systems, as a theorem for the entropy production in stationary states [3]. Fluctuation relations (FRs) have been established successively for a broad class of stochastic and deterministic systems [4–11] (see [12] for recent reviews). They are expected to be relevant in nano and biological sciences [13] at scales where typical thermal fluctuations are of the same magnitude as the external drivings. Testing the generality of FRs and the mechanisms of their occurrence in experiments [14, 15] or numerical simulations, particularly for interacting systems, is therefore an important issue in basic statistical mechanics and applications.

In this work, we consider the case of non-equilibrium steady states of systems in contact with two different heat baths at temperatures $T_n (n = 1, 2)$. In this case the FR, also known as the Gallavotti–Cohen relation [3], connects the probability $\mathcal{P}(\mathcal{Q}^{(n)}(\tau))$ to exchange the heat $Q^{(n)}(\tau)$ with the nth reservoir in a time interval τ, to that of exchanging the opposite quantity $-Q^{(n)}(\tau)$, according to

$$\ln \frac{\mathcal{P}(\mathcal{Q}^{(n)}(\tau))}{\mathcal{P}(-\mathcal{Q}^{(n)}(\tau))} = \mathcal{Q}^{(n)}(\tau)\Delta\beta^{(n)}, \qquad (1)$$

where $\Delta\beta^{(1)} = \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$ and $\Delta\beta^{(2)} = -\Delta\beta^{(1)}$. This relation is expected to hold in the large τ limit; in particular τ must be much larger than the relaxation times in the system. An explicit derivation of (1) for stochastic systems can be found in [16]. In specific systems, the validity of (1) was shown for a chain of oscillators [17] coupled at the extremities to two thermostats while the case of a Brownian particle in contact with two reservoirs has been studied in [18]. A relation similar to (1) has also been proved for the heat exchanged between two systems initially prepared in equilibrium at different temperatures and later put in contact [19].

The purpose of this communication is to study the relation (1), and the pre-asymptotic corrections at finite τ, in Ising models in contact with two reservoirs, as a paradigmatic example of statistical systems with phase transitions. This issue was considered analytically in a mean field approximation in [20] where the distributions $\mathcal{P}(\mathcal{Q}^{(n)}(\tau))$ have been explicitly computed in the large τ limit. Here, we numerically study the model with short-range interactions. This allows us to analyze the generality of the FR (1) with respect to details of the kinetics and of the interactions with the reservoirs, and to study the effects of finite τ. We also investigate the interplay between the ergodicity breaking and the FRs.

We consider a two-dimensional Ising model defined by the Hamiltonian $H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j$, where $\sigma_i = \pm 1$ is a spin variable on a site i of a rectangular lattice with $N = M \times L$ sites, and the sum is over all pairs $\langle ij\rangle$ of nearest neighbors. A generic evolution of the system is given by the sequence of configurations $\{\sigma_1(t), \ldots, \sigma_N(t)\}$ where $\sigma_i(t)$ is the value of the spin variable at time t. We will study the behavior of the system in the stationary state. In order to see the effects of different kinetics, Monte Carlo single-spin-flip and spin-exchange (Kawasaki) dynamics have been considered, corresponding to systems with non-conserved or conserved magnetization, respectively. Metropolis transition rates have been used; for single-spin-flip dynamics we also used Glauber transition rates.

Regarding the interactions with the reservoirs we have considered two different implementations. In the first, the system is *statically* divided into two halves. The left part (the first $M/2$ vertical lines) of the system interacts with the heat bath at temperature T_1 while the right part is in contact with the reservoir at $T_2 > T_1$. We have used both open or periodic boundary conditions. In the second implementation (for single-spin-flip only) each spin σ_i, at a given time t, is put *dynamically* in contact with one or the other reservoir depending on the (time dependent) value of $h_i = (1/2)\left|\sum_{\langle j\rangle_i}\sigma_j\right|$, where the sum runs over the nearest neighbor spins σ_j of σ_i. Notice that h_i is one half of the (absolute value) of the local field. In two dimensions, with periodic boundary conditions, the possible values of h_i are $h_i = 0, 1, 2$. At each time, spins with $h_i = 1$ are connected to the bath at $T = T_1$ and those with $h_i = 2$ with the reservoir at $T = T_2$. Namely, when a particular spin σ_i is updated, the temperature T_1 or T_2 is entered into the transition rate according to the value of h_i. Loose spins with $h_i = 0$ can flip back and forth regardless of temperature because these moves do not change the energy of the system. Then, as in the usual Ising model, they are associated with temperature-independent transition rate (equal to 1/2 or 1 for Glauber or Metropolis transition rates). This model was introduced in [21] and further studied in [22]. It is characterized by a line of critical points in the plane T_1, T_2, separating a ferromagnetic from a paramagnetic phase analogously to the equilibrium Ising model.

Denoting with $t_k^{(n)}$ the times at which an elementary move is attempted by coupling the system to the nth reservoir, the heat released by the bath in a time window $t \subset [s, s+\tau]$ is defined as

$$\mathcal{Q}^{(n)}(\tau) = \sum_{\{t_k^{(n)}\}\subset[s,s+\tau]} \left[H\left(\sigma\left(t_k^{(n)}\right)\right) - H\left(\sigma\left(t_k^{(n)} - 1\right)\right)\right]. \tag{2}$$

In the stationary state, the properties of $\mathcal{Q}^{(n)}(\tau)$ will be computed by collecting the statistics over different sub-trajectories obtained by dividing a long history of length t_F into many (t_F/τ) time windows of length τ, starting from different s.

$T_1, T_2 > T_c$. We begin our analysis with the study of the relation (1) in the case with both temperatures well above the critical value $T_c \simeq 2.269$ of the equilibrium Ising model. In the following, we will measure times in Monte Carlo steps (MCS) (1 MCS = N elementary moves).

The typical behavior of the heat probability distribution (PD) is reported in the upper panel of figure 1 for the case with static coupling to the baths, single-spin-flip with Metropolis transition rates, $T_1 = 2.9, T_2 = 3$, and a square geometry with $L = M = 10$ (much larger sizes are not suitable because trajectories with a heat of opposite sign with respect to the average value would be too rare). As expected, $\mathcal{Q}^{(1)}(\tau)$ $(\mathcal{Q}^{(2)}(\tau))$ is on average negative (positive) and the relation $\langle Q^{(1)}(\tau)\rangle + \langle Q^{(2)}(\tau)\rangle = 0$ is verified. Regarding the shape of the PD, due to the central limit theorem, one expects a Gaussian behavior for τ greater than the (microscopic) relaxation time (in this case it is of few MCS ($\sim$5)), namely $\mathcal{P}(\mathcal{Q}^{(n)}(\tau)) = (2\pi)^{-1/2}\left(\sigma_\tau^{(n)}\right)^{-1} \exp\left[-\frac{(\mathcal{Q}^{(n)}(\tau)-\langle\mathcal{Q}^{(n)}(\tau)\rangle)^2}{2(\sigma_\tau^{(n)})^2}\right]$, with $\langle\mathcal{Q}^{(n)}(\tau)\rangle \sim \tau$ and $\sigma_\tau^{(n)} \sim \sqrt{\tau}$. This form is found with good accuracy, as shown in the inset of figure 1, where data collapse of the curves with different τ is observed by plotting $\left(\sigma_\tau^{(1)}\right)^{1/2}\mathcal{P}(\mathcal{Q}^{(1)}(\tau))$ against $(\mathcal{Q}^{(1)}(\tau) - \langle\mathcal{Q}^{(1)}(\tau)\rangle)/\sigma_\tau^{(1)}$.

In order to study the FR (1), we plot the logarithm of the ratio $\mathcal{P}(\mathcal{Q}^{(n)}(\tau))/\mathcal{P}(-\mathcal{Q}^{(n)}(\tau))$ as a function of $\Delta\beta^{(n)}\mathcal{Q}^{(n)}(\tau)$, see figure 2 (inset). For every value of τ the data are well consistent with a linear relationship (however, for large values of the heat the statistics becomes poor), in agreement with the Gaussian form of the PDs. To verify the FR (1), the slopes of the plot

$$D^{(n)}(\tau) = \frac{\ln\frac{\mathcal{P}(\mathcal{Q}^{(n)}(\tau))}{\mathcal{P}(-\mathcal{Q}^{(n)}(\tau))}}{\mathcal{Q}^{(n)}(\tau)\Delta\beta^{(n)}} \tag{3}$$

must tend to 1 when $\tau \to \infty$. We show in figure 2 the behavior of the *distance* $\epsilon^{(n)} = 1 - D^{(n)}(\tau)$ from the asymptotic behavior, for the case with static coupling to the baths. This quantity indeed goes to zero for large τ (the same is found for dynamic couplings). $\epsilon^{(n)}$ depends in general on the temperatures, the geometry of the system and on τ. Its behavior can be estimated on the basis of the following argument.

In systems as those considered in this communication, where generalized detail balance [16] holds, the ratio between the probability of a trajectory in configuration space, given a certain intial condition, and its time reversed reads

$$\frac{\mathcal{P}(\text{traj})}{\mathcal{P}(-\text{traj})} = \mathrm{e}^{\mathcal{Q}^{(n)}(\tau)\Delta\beta^{(n)} - \frac{\Delta E}{T_{n'}}}, \tag{4}$$

where $\Delta E = \mathcal{Q}^{(1)}(\tau) + \mathcal{Q}^{(2)}(\tau)$ is the difference between the energies of the final and initial states, and $n' \neq n$. For systems with bounded energy, equation (4) is the starting point [16] for obtaining the FR (1) in the large-τ limit. Since $\mathcal{Q}^{(n)}(\tau)$ increases with τ while ΔE is limited,

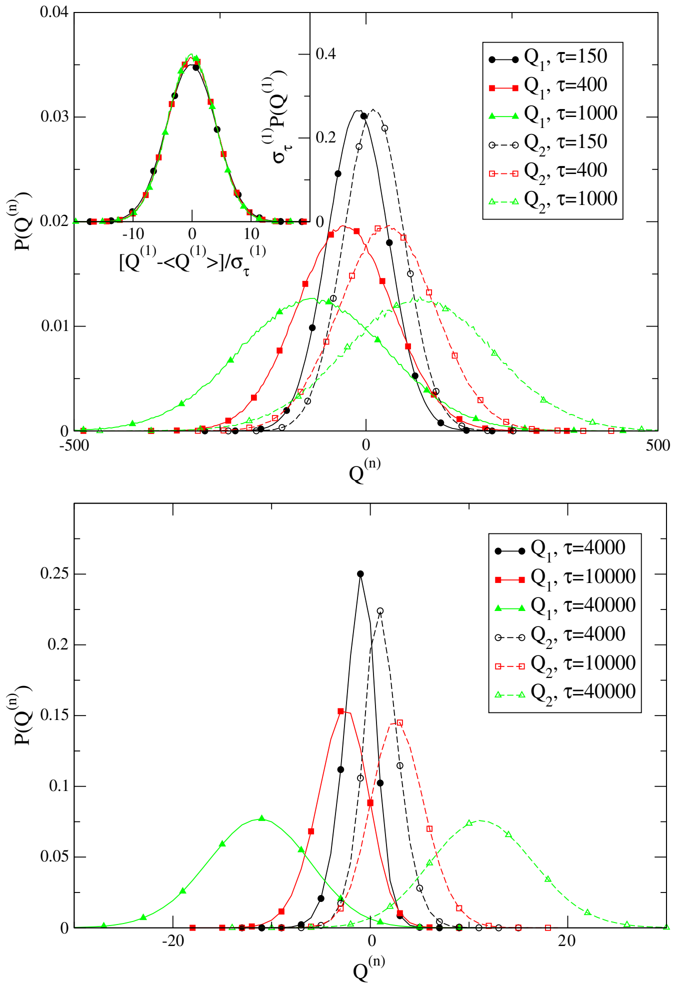

Figure 1. Upper panel ($T_1, T_2 > T_c$): heat PDs for $\mathcal{Q}^{(1)}$ (on the left) and $\mathcal{Q}^{(2)}$ (on the right) for a system with $T_1 = 2.9$, $T_2 = 3$, size 10×10 and $t_F = 6 \times 10^8$ MCS. In the inset, $\sigma_\tau^{(1)}\mathcal{P}(\mathcal{Q}^{(1)}(\tau))$ is plotted against $(\mathcal{Q}^{(1)}(\tau) - \langle\mathcal{Q}^{(1)}(\tau)\rangle)/\sigma_\tau^{(1)}$. Curves for different τ collapse on a Gaussian mastercurve. Lower panel ($T_1, T_2 < T_c$): same kind of plot for $T_1 = 1$, $T_2 = 1.3$, size 10×10 and $t_F = 10^9$ MCS. The skewness of the distributions (see the text) is equal to 2.35, 0.589, 0.11 for the cases $\tau = 4000, 10000, 40000$, respectively.

in fact, the latter can be asymptotically neglected and, after averaging over the trajectories, the FR (1) is recovered. Keeping τ finite, instead, from equations (3) and (4) one has that for the considered trajectory the *distance* of the slope from the asymptotic value is

$$\epsilon^{(n)}(\text{traj}) \simeq \frac{\Delta E}{T_{n'}\mathcal{Q}^{(n)}(\tau)\Delta\beta^{(n)}}. \tag{5}$$

We now assume that the behavior of $\epsilon^{(n)}$ can be inferred by replacing ΔE and $\mathcal{Q}^{(n)}(\tau)$ with their average values whose behavior can be estimated by scaling arguments. Starting with the average of $\mathcal{Q}^{(n)}(\tau)$, we argue that this quantity is proportional to $N_{\text{flux}}\tau$, with N_{flux} being the number of couples of nearest neighbor spins interacting with baths at different temperatures.

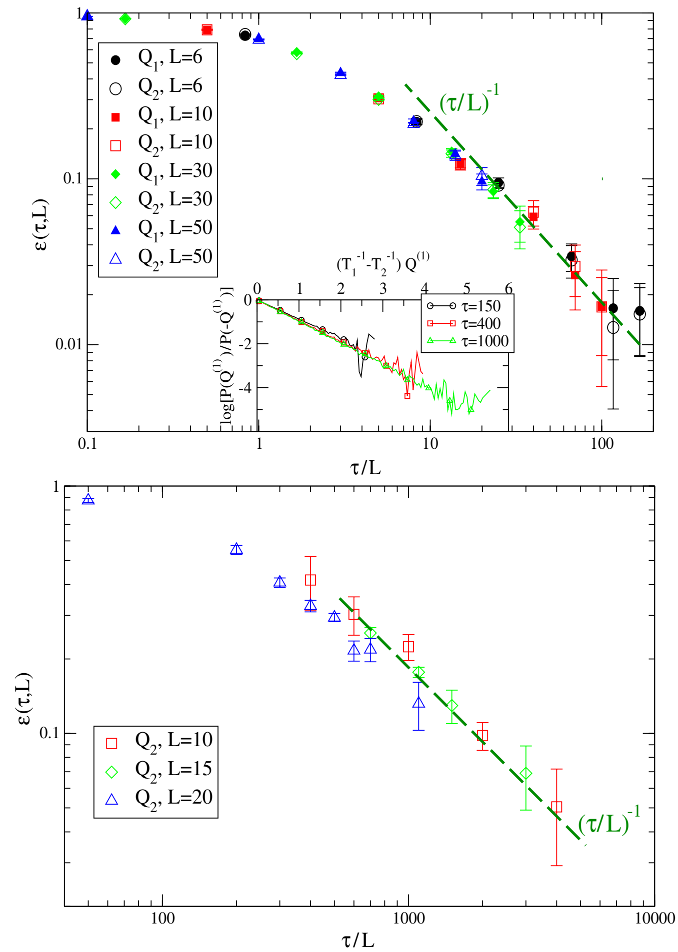

Figure 2. Same parameters of figure 1 (different sizes). Upper panel ($T_1, T_2 > T_c$): $\epsilon(\tau, L)$ is plotted against τ/L for different L. Inset: $\log[\mathcal{P}(\mathcal{Q}^{(1)}(\tau))/\mathcal{P}(-\mathcal{Q}^{(1)}(\tau))]$ is plotted against $(1/T_1 - 1/T_2)\mathcal{Q}^{(1)}(\tau)$. Lower panel ($T_1, T_2 < T_c$): $\epsilon^{(2)}$ is plotted against τ/L for different L.

This is because between these spins a neat heat flux occurs. In the model with static coupling to the baths one has $N_{\text{flux}} \propto L$. With dynamic coupling, instead, since every spin in the system can feel one or the other temperature, one has $N_{\text{flux}} \propto N$. Concerning the average of ΔE, this is an extensive quantity proportional to the number N of spins. We then arrive at

$$\epsilon^{(n)} \simeq (T_{n'} \Delta\beta^{(n)})^{-1} \begin{cases} L\tau^{-1} & \text{static coupling to baths} \\ \tau^{-1} & \text{dynamic coupling to baths.} \end{cases} \tag{6}$$

This result is expected to apply for sufficiently large τ when our scaling approach holds.

We recall that finite-τ corrections have been shown to be of order $1/\tau$ for the classes of dynamical systems considered in [3, 23]. The same is found in [24] for models based on a Langevin equation[3], in cases corresponding to the experimental setup of a resistor in parallel

[3] In the system studied in [24], $1/\tau$ corrections have been predicted for any range of work fluctuations and only for some range of heat fluctuations. Moreover, differently than in our case, the slope 1 in work fluctuations is reached from above, i.e., ϵ is negative.

with a capacitor [15]. Faster decays ($\sim 1/\tau^2$) have been predicted for other topologies of circuits [24]. On the other hand, FRs in transient regimes, which are not considered in this communication, are exact at any τ ($\epsilon = 0, \forall\tau$) [25].

In our model with static couplings the data of figure 2 confirm the prediction of the argument above: curves with different L collapse when plotted against $x = \tau/L$ and $\epsilon^{(n)} \propto x^{-1}$ for sufficiently large τ. Similar behaviors have been found by varying the geometry (we also considered rectangular lattices with $L > M$), transition rate and dynamics. The scaling prediction (6) has been verified for the Ising model with Kawasaki dynamics and squared geometry with $L = 10, 20, 40$, and in the case of the system dynamically coupled to the heat baths for sizes between $L = 6$ and $L = 60$.

$T_1, T_2 < T_c$. Let us first recall the behavior of the Ising model in contact with a single bath at a temperature $T < T_c$. When $N = \infty$ the system is confined into one of the two pure states which can be distinguished by the sign of the magnetization $m(T) = (1/N)\sum_{i=1}^{N}\sigma_i$. This state is characterized by a microscopic relaxation time $\tau_{\rm eq}(T)$ which is related to the fast flip of correlated spins into thermal islands with the typical size of the coherence length. At finite N, instead, genuine ergodicity breaking does not occur. The system still remains trapped into the basin of attraction of the pure states but only for a finite ergodic time $\tau_{\rm erg}(N, T)$, which diverges when $N \to \infty$ or $T \to 0$. Then, as compared to the case $T > T_c$, there is the additional timescale $\tau_{\rm erg}(N, T)$, beside $\tau_{\rm eq}(T)$, which can become macroscopic. This whole phenomenology is reflected by the behavior of the autocorrelation function $C(t-t') = \left\langle \sum_i \sigma_i(t')\sigma_i(t)\right\rangle$. When, for large N, the two timescales $\tau_{\rm eq}(T)$, $\tau_{\rm erg}(N, T)$ are well separated, it first decays from $C(0) = 1$ to a plateau $C(t - t') = m(T)^2$ on times $t - t' \simeq \tau_{\rm eq}(T)$, due to the fast decorrelation of spins in thermal islands. The later decay from the plateau to zero, observed on a much larger timescale $t - t' \simeq \tau_{erg}(N, T)$, signals the recovery of ergodicity. Note also that, from the behavior of $C(t - t')$, both the characteristic timescales can be extracted.

The same picture applies qualitatively to the case of two subsystems in contact with two thermal baths, where each system is trapped in states with broken symmetry for a time $\tau_{\rm erg}(N, T_n)$ ($\tau_{\rm erg}(N, T_1) > \tau_{\rm erg}(N, T_2)$ since $T_1 < T_2$), which can be evaluated from the autocorrelation functions $C^{(n)}(t - t') = \left\langle \sum_i \sigma_i^{(n)}(t)\sigma_i^{(n)}(t')\right\rangle$, where $\sigma_i^{(n)}$ denote spins in contact with the bath at $T = T_n$. Since the FR is expected for τ larger than the typical timescales of the system, it is interesting to study the role of the additional timescales $\tau_{\rm erg}(N, T_n)$ on the FR. By varying T_1, T_2 and N appropriately one can realize the limit of large τ in the two cases with (i) $\tau \ll \tau_{\rm erg}(N, T_2)$ or (ii) $\tau \gg \tau_{\rm erg}(N, T_1)$. In case (i), in the observation time-window τ, the system is practically confined into broken symmetry states while in case (ii) *ergodicity* is restored. Not surprisingly, in the latter case, we have observed a behavior very similar to that with $T_1, T_2 > T_c$. The PDs for case (i) are shown in the lower panel of figure 1. The distributions are more narrow and non-Gaussian. We calculated the skewness of the distributions defined as $\langle(\mathcal{Q}(\tau) - \langle\mathcal{Q}(\tau) >)^3\rangle/\langle(\mathcal{Q}(\tau) - \langle\mathcal{Q}(\tau)\rangle)^2\rangle^{3/2}$. This quantity is zero for Gaussian distributions while for the case of the lower panel of figure 1 we found values different from zero which have been reported in the caption of the figure. These data show that the PDs slowly approach a Gaussian form increasing τ. Moreover, differently than in the high temperature case, an asymmetry between the distributions of $\mathcal{Q}^{(1)}(\tau)$ and $\mathcal{Q}^{(2)}(\tau)$ can be observed.

Regarding the slopes $D^{(n)}(\tau)$, they converge to 1 also in this case even if the times required to reach the asymptotic behavior are much longer than in the high temperature case (but always smaller than $\tau_{\rm erg}(N, T_2)$). This suggests that the FR (1) holds even in states where ergodicity is broken and that the presence of the macroscopic timescales $\tau_{\rm erg}(N, T_n)$ does not affect the validity of the FR in this system. Regarding the scaling of $\epsilon^{(n)}$, the data are much more noisy than in the case $T_1, T_2 > T_c$, particularly for $\epsilon^{(1)}$. Despite this, the data presented in the lower panel of figure 2 for $\epsilon^{(2)}$ are consistent with the scaling (6) suggesting that it is also correct in this situation.

In this communication we have considered different realizations of Ising models coupled to two heat baths at different temperatures. We studied the fluctuation behavior of the heat exchanged with the thermostats and found that the FR (1) is asymptotically verified in all the cases considered. We also analyzed the effects of finite-time corrections and their scaling behavior. The picture is qualitatively similar in the high and low temperature phases, although very different timescales are required to observe the asymptotic FR.

Acknowledgments

The authors are grateful to A Pelizzola and L Rondoni for useful discussions.

References

[1] Evans D J, Cohen E G D and Morriss G P 1993 *Phys. Rev. Lett.* **71** 2401
[2] Evans D J and Searles D J 1994 *Phys. Rev.* E **50** 1645
[3] Gallavotti G and Cohen E G D 1995 *J. Stat. Phys.* **80** 931
Gallavotti G and Cohen E G D 1995 *Phys. Rev. Lett.* **74** 2694
[4] Jarzynski C 1997 *Phys. Rev. Lett.* **78** 2690
[5] Kurchan J 1998 *J. Phys. A: Math. Gen.* **31** 3719
[6] Lebowitz J L and Spohn H 1999 *J. Stat. Phys.* **95** 333
[7] Maes C 1999 *J. Stat. Phys.* **95** 367
[8] Crooks G E 1999 *PhD Thesis* University of California at Berkeley
Crooks G E 1999 *Phys. Rev.* E **60** 2721
[9] Hatano T and Sasa S 2001 *Phys. Rev. Lett.* **86** 3463
[10] van Zon R and Cohen E G D 2003 *Phys. Rev. Lett.* **91** 110601
[11] Seifert U 2005 *Phys. Rev. Lett.* **95** 040602
[12] For recent reviews see e.g. Harris R J and Schütz G M 2007 *J. Stat. Mech.* P07020
Gallavotti G 2007 *Preprint* arXiv:0711.2755
Ritort F 2008 *Adv. Chem. Phys.* **137** 31
Rondoni L and Mejia-Monasterio C 2007 *Nonlinearity* **20** R1
Chetrite R and Gawedzki K 2007 *Preprint* arXiv:0707.2725
[13] Bustamante C, Liphardt J and Ritort F 2005 *Phys. Today* **58** 43
[14] Wang G M, Sevick E M, Mittag E, Searles D J and Evans D J 2002 *Phys. Rev. Lett.* **89** 050601
[15] Garnier N and Ciliberto S 2005 *Phys. Rev.* E **71** 060101
[16] Bodineau T and Derrida B 2007 *C. R. Phys.* **8** 540
[17] Lepri S, Livi R and Politi A 1998 *Physica* D **119** 140
[18] Visco P 2006 *J. Stat. Mech.* P06006
[19] Jarzynski C and Wojcik D K 2004 *Phys. Rev. Lett.* **92** 230602
[20] Lecomte V, Racz Z and van Wijland F 2005 *J. Stat. Mech.* P02008
[21] de Oliveira M J, Mendes J F F and Santos M A 1993 *J. Phys. A: Math. Gen.* **26** 2317
[22] Drouffe J M and Godrèche C 1999 *J. Phys. A: Math. Gen.* **32** 249
Sastre F, Dornic I and Chatè H 2003 *Phys. Rev. Lett.* **91** 267205
Andrenacci N, Corberi F and Lippiello E 2006 *Phys. Rev.* E **73** 046124
[23] Rondoni L and Morriss G P 2003 *Open Sist. Inf. Dyn.* **10** 105
[24] van Zon R, Ciliberto S and Cohen E G D 2004 *Phys. Rev. Lett.* **92** 130601
[25] See e.g. Jarzynski C 2000 *J. Stat. Phys.* **98** 77