Temperature of nonequilibrium lattice systems

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Abstract

We investigate the thermal quench of Ising and Potts models via Monte Carlo dynamics. We find that the local distribution of the site-site interaction energy has the same form as in the equilibrium case, a result that allows us to measure the instantaneous temperature during the systems relaxation. We also find that, after an undercritical quench, the system equilibrates at the heatbath temperature in a finite time, while the total energy is still decreasing due to the coarsening process.
I. INTRODUCTION

A key quantity in Monte Carlo simulation of equilibrium systems is the heatbath temperature $T$. Monte Carlo dynamics follows a Markovian process whose stationary state is the Gibbs canonical probability distribution

$$P(\sigma) = \frac{1}{Z} \exp\{-\beta \mathcal{H}(\sigma)\}, \quad (1)$$

where $\mathcal{H}(\sigma)$ is the energy of the state $\sigma$, $Z$ is the partition function and $\beta$ is the inverse heatbath temperature in Boltzmann’s constant units. Temperature is a parameter with a given fixed value, the fluctuating quantity being the energy, and this corresponds to simulate a canonical ensemble. Our work aims to investigate the possibility of associating an instantaneous temperature to a system when it is out of the equilibrium as it happens, for instance, in a transient regime that follows a quenching. This possibility has been rigorously proved in some cases. Van Enter et al. [1] have shown that this can be done through the Gibbs measure, that is preserved in Ising spin systems at any time for overcritical quenching with spin-flip dynamics and the same result has then been extended to Kawasaki dynamics [3]. It has also been proved that the Gibbs measure is preserved for indefinite time in systems with weak site-site coupling [2] under a variety of conditions. On the contrary, when heating from an ordered, low temperature state to an overcritical temperature the Gibbs measure is preserved only for a finite time [1, 3]. There is however a convergence to the equilibrium measure and it is not clear whether or not a temperature can be identify. In this work we address the problem from a computational point of view for the case of a quench from high temperature.

It has been recently shown [4] that also a microcanonical formulation can be constructed, in which the system energy is constrained whereas the temperature is computed as a dependent quantity. In this formulation the temperature is found to assume the correct value at equilibrium, thus establishing the equivalence of simulating the microcanonical and the canonical ensemble. We have employed the method developed in Ref. [4] in a non equilibrium case, by computing the temperature of the Ising model along a quench from high temperature. We have then extended the method to the Potts model with $q$ states. With similar aims different approaches for off-lattice systems (molecular dynamics) have been recently introduced [5–7] that however are not suitable for lattice models.
In the method adopted here computation bases on the statistical distribution of the site-site interaction energies. The most interesting finding is that the shape of the distribution computed along the quench is very similar to the one which characterizes the system at equilibrium, but corresponds to a different value of the temperature. Thence it is possible to associate an instantaneous temperature to the non equilibrium states of the system.

In Section II we recall how temperature can be determined in the Ising system at equilibrium; in Sec. III the method is applied to the same system in non equilibrium and in Sec. IV it is extended to the Potts model with \( q \) states. Main results are summarized in Sec. V.

II. THE ISING MODEL

In Ref. [4] the equilibrium temperature is computed on the base of the statistical properties of the site-site interaction energies for a generic lattice gas model. In the case of the Ising model, with Hamiltonian

\[
\mathcal{H} = - \sum_{\langle ij \rangle} \sigma_i \sigma_j,
\]

where the sum is over the nearest neighbors sites and \( \sigma_i = \pm 1 \), it is convenient to write down the Hamiltonian as a sum of two terms

\[
\mathcal{H} = \gamma + \mathcal{H}_r,
\]

where the first represents the interaction energy between a generic site, which is labeled site 0, and the other sites

\[
\gamma = - \sum_i \sigma_0 \sigma_i,
\]

where the summation is over the nearest neighbors of site 0. The second term \( \mathcal{H}_r \) represents the interaction energy among other sites, excluding the site 0. The canonical probability distribution \( \mathcal{P}(\sigma) \) of the state \( \sigma = (\sigma_0, \sigma_1, \ldots, \sigma_N) \) is then written as

\[
\mathcal{P}(\sigma) = \frac{1}{Z} e^{-\beta \gamma e^{-\beta \mathcal{H}_r}},
\]

where \( \beta = 1/T \), and \( T \) is the heatbath temperature.

The temperature can be obtained from the distribution of the energies assumed by \( \gamma \). In the present case, the possible values of the energy are \( \varepsilon = -4, -2, 0, 2, 4 \). If we denote by \( P(\varepsilon) \) the probability of one of the possible values assumed by \( \gamma \), that is,

\[
P(\varepsilon) = \sum_{\sigma} \delta(\varepsilon, \gamma) \mathcal{P}(\sigma),
\]
then, it is possible to write $P(\epsilon)$ in the following form

$$P(\epsilon) = e^{-\beta \epsilon} A(\epsilon),$$

(7)

which follows from (5), where the quantity $A$ is given by

$$A(\epsilon) = \frac{1}{Z} \sum \delta(\epsilon, \gamma) e^{-\beta \mathcal{H}_t},$$

(8)

where $\delta(\gamma, \epsilon)$ is the Kronecker delta.

In order to avoid the explicit computation of $A(\epsilon)$, which is as difficult as the computation of the partition function, we use the following important property $A(-\epsilon) = A(\epsilon)$ which follows by performing the transformation $\sigma_0 \rightarrow -\sigma_0$ in the summation of equation (8) and using the property $\delta(-\gamma, \epsilon) = \delta(\gamma, -\epsilon)$, and finally remembering that $\mathcal{H}_t$ does not contain $\sigma_0$. Hence the ratio

$$\frac{P(\epsilon)}{P(-\epsilon)} = e^{-2\beta \epsilon},$$

(9)

does not depend on $A(\epsilon)$.

If we denote by $n(\epsilon)$ the number of lattice sites such that the interaction energy $\gamma$ is $\epsilon$ then it follows that the left-hand side of (9) can be estimated by the ratio $R(\epsilon) = n(\epsilon)/n(-\epsilon)$. Therefore, from (9) it follows that this ratio is distributed in energy according to

$$R(\epsilon) = e^{-2\beta \epsilon}$$

(10)

so that the quantity $\ln R$ is linear in the energy $\epsilon$ and its slope gives an estimate of the inverse of the temperature.

This equation, which was derived from the canonical distribution, can be used to define temperature in systems described by a microcanonical probability distribution. In Ref. [4] it has been checked that Eq. (10) is well satisfied when simulating the canonical ensemble, and has been used to compute temperature in a microcanonical Monte Carlo simulation with the Kawasaki [8] dynamics. Most important for our purpose, the Eq. (10) can be used to define temperature in nonequilibrium systems as long as the local distribution of energies follows the exponential law given by the right-hand side of this equation. The temperature obtained in this manner we call local or instantaneous temperature $\theta$ to distinguish it from the heatbath temperature $T$. In the regime in which the system is in equilibrium with the heatbath both temperature should be the same.
III. QUENCHING OF THE ISING MODEL

Monte Carlo simulations are extensively employed even for studying non equilibrium properties of systems [8]. Among the others, the properties of systems prepared far from equilibrium and then allowed to relax towards their equilibrium state. If for instance the system is initially at high temperature and is put then in contact with a finite temperature heat bath, it starts to cool down and eventually approaches the heat bath temperature. Despite the intrinsic artificial nature of Monte Carlo dynamics, physical relevance is generally attributed to results obtained via single site dynamics [8]. It is therefore tempting to use Eq. (10) for probing the system temperature during the cooling. One wishes, in particular, to answer the following two questions:

(1) Is the system in a sort of equilibrium on very short scales, i. e. does Eq. (10), which was derived by assuming the equilibrium statistics, hold during the system cooling?

(2) If yes, how does the instantaneous temperature decrease in time during the cooling?

In order to answers the above questions we have performed Monte Carlo simulations in a square lattice Ising model which was quenched from infinite to a finite temperature. We have found that the answer to question (1) is affirmative. The quench was accomplished by (a) starting the simulation with a random configuration, which, according to Eq. (10), corresponds to an infinite instantaneous temperature, and (b) using the Metropolis algorithm with the temperature of the heatbath. For later convenience we adopted the following Hamiltonian:

\[ \mathcal{H} = \frac{1}{2} \sum_{\langle ij \rangle} (1 - \sigma_i \sigma_j), \]

which is obtained from (2) by a linear transformation. For the Ising model so defined the possible site energy level are 0, 1, 2, 3, 4 and Eq. (10) turns into

\[ R(\epsilon) = e^{-2\beta(\epsilon^2 - 1)} \]

and (Eq. (9))

\[ R(\epsilon) = \frac{P(\epsilon)}{P(4 - \epsilon)}. \]

We performed quenchings for a final temperature above and below the critical temperature \( T_c = 1.123092 \ldots \). In Fig. 1, the quantity \( \ln R \) as a function of \( \epsilon \) is shown for a quench
from infinite temperature to a final temperature $T = 1.5$ at some different instants of time. In this case the quench temperature is above the critical temperature $T_c$, and a few Monte Carlo steps are sufficient for driving the system to thermal equilibrium. However, before this happens the system already displays a linear relation between $\ln R$ and $\epsilon$, from which, in agreement with [1], an instantaneous temperature $\theta$ can be derived as seen also in the inset of Fig. 1 where $\ln R/\epsilon$ is plotted as a function of $\epsilon$. A linear regression obtained at the equilibrium regime yields $\theta = 1.500096$, with correlation coefficient 1.

A subcritical quench at heatbath temperature $T = 0.5$ is shown in Fig. 2. In this case the system takes a long time to reach thermal equilibrium, but Eq. (10) is quite well satisfied. It can be seen from the inset that deviations from the linear dependence exist but they are however small. Quasi-equilibrium is satisfied at any instant and in this case a linear regression on the last curve gives $\theta = 0.5026449$ with a correlation coefficient 0.9999925.

The existence of such an equilibrium-like distribution for the system allows for extracting a local temperature $\theta$ during the system cooling. Fig. 3 shows the behavior of the energy as function of this temperature for a quench at a temperature $T = 0.5$ which is below the critical temperature. It is seen that a first regime exists in which the energy is linear with $\theta$. Then, a second regime follows where a remarkable property can be noticed: while the local temperature $\theta$ has already attained the heatbath temperature, the total energy, on the contrary, is still decreasing. In fact this kind of systems is characterized by a coarsening process and takes an infinite time to reach equilibrium, the energy decaying as $1/\sqrt{t}$, but it is seen that the local temperature is already at equilibrium during the coarsening. This behaviour is better appreciated by looking at the inset of Fig. 3 where it is seen that energy decreases algebraically while the local temperature is constant.

When the system is quenched at a temperature above $T_c$, energy relaxes exponentially to equilibrium and the second regime does not appear. This is shown in Fig. 4 and in the related inset. For comparison, the equilibrium curve is also reported in the figures, showing that it still lies below the non-equilibrium one.
IV. THE POTTS MODEL

In order to test the above conclusions on a wider class of systems, we have derived Eq. (10) for the case of the $q$ states Potts model, with Hamiltonian:

$$\mathcal{H}(\eta) = \sum_{(ij)} \{1 - \delta(\eta_i, \eta_j)\}, \quad (11)$$

where again the sum is over the nearest neighbors and and $\eta_i$ is the state of site $i$. Each variable $\eta_i$ can assume one out of $q$ different states, which we identify as an integer, that is, $\eta_i = 1, 2, \ldots, q$. When $q = 2$ the Hamiltonian (11) reduces to the Ising Hamiltonian (2). Again the system energy, given by Eq. (11), is written as a sum of two terms

$$\mathcal{H}(\eta) = \gamma + \mathcal{H}_r, \quad (12)$$

where the first term

$$\gamma = \sum_i \{1 - \delta(\eta_0, \eta_i)\}, \quad (13)$$

where the summation is over the nearest neighbors of site 0, is the interaction energy of the site 0 with its neighbors. The second term $\mathcal{H}_r$ represents the energy of interaction of the rest of the system. In the present case of the Potts model the possible values of $\gamma$ are also $\epsilon = 0, 1, 2, 3, 4$.

Let us denote by $P(\epsilon)$ the probability that $\gamma$ assumes the value $\epsilon$, that is,

$$P(\epsilon) = \sum_\eta \delta(\gamma, \epsilon) \mathcal{P}(\eta) \quad (14)$$

where $\mathcal{P}(\eta)$ is the canonical probability distribution given by

$$\mathcal{P}(\eta) = \frac{1}{Z} e^{-\beta \mathcal{H}(\eta)} = \frac{1}{Z} e^{-\beta \gamma} e^{-\beta \mathcal{H}_r} \quad (15)$$

In analogy with the Ising model, this quantity can be written as

$$P(\epsilon) = e^{-\beta \epsilon} A(\epsilon) \quad (16)$$

where the quantity $A(\epsilon)$ has the following property. Let $\epsilon$ be the value assumed by $\gamma$ and let $\epsilon'$ be the value assumed by $\gamma$ when $\eta_0$ is transformed to $\eta_0'$. It is straightforward to show that $A(\epsilon) = A(\epsilon')$, which is the desired property. It follows then that

$$\frac{P(\epsilon)}{P(\epsilon')} = e^{-\beta (\epsilon - \epsilon')} \quad (17)$$
To estimate the left-hand side of this equation, we determine the number of sites \( n(\epsilon) \) whose interaction energy equals \( \epsilon \) and the number of sites \( n(\epsilon') \) whose interaction energy equals \( \epsilon' \). The ratio \( R(\epsilon, \epsilon') = n(\epsilon)/n(\epsilon') \) is an estimate of the left-hand side of (17) so that we may write

\[
R(\epsilon, \epsilon') = e^{-\beta(\epsilon - \epsilon')}
\]  

(18)

Thence even for the Potts model a local temperature can be defined from the site-site energy statistics.

It is found that the Potts model obeys Eq. (18) even in the nonequilibrium regime, allowing to extract a local temperature \( \theta \) at a given instant of time like for the Ising model. Figure 5 shows the local temperature \( \theta \) versus time for a quench of a seven state Potts model at \( T = 0.5 \), i.e. below the transition temperature \( T_c = 0.773058 \ldots \). It is seen that like for the Ising model a first regime exists in which the two quantities are proportional. Then even in this case a second regime follows in which \( \theta \) is that of the heatbath but the energy is still relaxing due to the coarsening process. The supercritical case reported in Fig. 6 shows that the local and the heatbath temperature are the same after a certain time, as for the Ising model.

V. LOW TEMPERATURE BEHAVIOUR

We have performed many quenches at different final temperature \( T \) for the the Potts model with \( q = 7 \) and \( q = 2 \). The latter is equivalent to the Ising model. A common feature is that if the heatbath temperature \( T \) is smaller than a given value \( T^* \), the system seems unable to reach the equilibrium temperature, that is, the local temperature \( \theta \) does not attain the heatbath temperature.

Fig. 7 shows the local temperature \( \theta \) vs time for the square Ising model with linear lattice size \( L = 1000 \). The local temperature \( \theta \) attains the heatbath temperature \( T \) if this temperature is larger than \( T^* \approx 0.34 \) but if \( T \) is equal or below this value it does not. We expect that this is a finite size effect and that the system eventually relaxes to the equilibrium state with local temperature \( \theta = T \). The case of the Potts model is shown in Fig. 8. In this case \( T^* \approx 0.33 \). It can be observed that \( T^* \approx 0.42T_c \) for Potts whereas \( T^* \approx 0.3T_c \) for Ising. Moreover the limit energy is clearly larger for Potts model than it is for the Ising model. Fig. 9 displays the behaviour of the local temperature after a quench at \( T = 0 \). An increase
of $T^*$ with increasing size for both Ising and Potts model is seen. Although extrapolation to $L = \infty$ appears to give a still finite temperature, it must be point out that the evaluation of the local temperature $\theta$ via Eq. (10) becomes difficult for quenches at very low temperature, since almost all sites are in the same state and statistical sampling for $\epsilon \neq 0$ becomes very poor. Reliable estimates of the local temperatures can be obtained only for finite values of the quench temperature above a bound which depends on system size and kind.

VI. SUMMARY

In this work a method for associating an instantaneous temperature to non equilibrium lattice models has been presented which is based on the the probability distribution of the site-site interaction energies and which is derived from the equilibrium Boltzmann statistics. It is found that the same form of distribution is obeyd by the system while cooling after a quench, allowing to associate a temperature to its non equilibrium states. While cooling, the local temperature decreases until the value of the heath bath is attained, both for supercritical and undercritical quenches. The latter case is particularly worth of notice, since there the system undergoes a coarsening process and equilibrium is never attained from the energetical point of view. The method proofs valid for generic Potts model with $q$ states, provided the heath bath temperature is not to low and the statistical sampling is effective for the considered system size.

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FIG. 1: The distribution of $\ln R$ as a function of $\epsilon$ for the Ising model after a quench to a temperature $T = 1.5$, above the critical temperature. The quantity $\ln R/\epsilon$ is shown in the inset. The time interval between curves is of 5 mcs.

FIG. 2: The distribution of $\ln R$ as a function of $\epsilon$ for the Ising model after a quench to a temperature $T = 0.5$, below the critical temperature. The quantity $\ln R/\epsilon$ is shown in the inset. The time interval between curves is of 5 mcs.
FIG. 3: Energy vs temperature $\theta$ during a quench of the Ising model at $T < T_c$. The dashed curve is the equilibrium curve. The inset shows the energy and $\theta$ (continuous line) vs time.

FIG. 4: Energy vs temperature $\theta$ during a quench of the Ising model at $T > T_c$. The dashed curve is the equilibrium curve. The inset shows the energy (dashed line) and $\theta$ vs time.
FIG. 5: Energy vs temperature $\theta$ during a quench of the 7-state Potts model at $T < T_c$. The dashed curve is the equilibrium curve. The inset shows $\theta$ and energy (dashed line) behavior in time.

FIG. 6: Energy vs temperature $\theta$ during a quench of the 7-state Potts model at $T > T_c$. The dashed curve is the equilibrium curve. In the inset, $\theta$ (continuous line) and energy vs time.
FIG. 7: Temperature $\theta$ vs time for the Ising model for different quench temperatures $T$; the behaviour at very low temperatures is magnified in the inset. Data are averages over 10 realisations.

FIG. 8: Temperature $\theta$ vs time for the 7-state Potts model for different quench temperatures $T$; in the inset the behaviour at very low temperatures. Data are averages over 10 realisations.
FIG. 9: Energy vs temperature $\theta$ for a quench of the Ising and Potts models at $T = 0$ in lattices of different size.