Boltzmann temperature in out-of-equilibrium lattice gas

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Abstract

We investigate the quench of Ising and Potts models via Monte Carlo dynamics, and find that the distribution of the site-site interaction energy has the same form as in the equilibrium case. This form directly derives from the Boltzmann statistics and allows to measure the instantaneous temperature during the systems relaxation. We find that, after an undercritical quench, the system equilibrates in a finite time at the heatbath temperature, while the energy still decreases 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 proportional to the Boltzmann probability density at the chosen temperature, i.e.:

$$P(E) \propto \exp[-\beta E],$$

where $E$ is the system energy and $\beta$ is the inverse heatbath temperature in Boltzmann’s constant units. Temperature is usually a parameter with an imposed value, the fluctuating quantity being the energy, and this corresponds to simulate a canonical ensemble. It has been recently shown [1] 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.

Our work aims to investigate the possibility of associating an instantaneous temperature to a system even when this is out of the equilibrium. Therefore we have employed the method developed in Ref. [1] 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 [2, 3, 4] 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. [1] 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

$$H = - \sum_{\langle i<j \rangle} \sigma_i \sigma_j,$$

where the sum $\langle \ldots \rangle$ is over nearest neighbors sites and $\sigma_k = \pm 1$, the temperature is obtained from the distribution of the quantity:

$$\gamma = - \sum_{[v]} \sigma_0 \sigma_v,$$

that represents the interaction energy of a generic site $k = 0$ with its neighbors $[v]$. The Hamiltonian, Eq. (1), can be separated into $H = \gamma + H_r$, where

$$H_r = - \sum_{\langle l<m \rangle} \sigma_l \sigma_m,$$

with the the sum extended to all pairs not including the site 0. Say $P(\{\sigma\})$ the (Boltzmann) probability for the system of $N+1$ sites to stay in the configuration $\{\sigma\} = \{\sigma_0, \sigma_1, \ldots, \sigma_N\}$, this is given by

$$P(\{\sigma\}) = \frac{1}{Z} e^{-\beta \gamma} e^{-\beta H_r},$$

where $\beta$ is the inverse temperature (in Boltzmann’s constant units) and $Z$ the partition function. The probability $P(\epsilon)$ of a configuration with $\gamma = \epsilon$, ($\epsilon = -4, -2, 0, 2, 4$) can be obtained as

$$P(\gamma = \epsilon) = \sum_{\{\sigma\}} \delta(\epsilon, \gamma) P(\{\sigma\}) = \sum_{\{\sigma\}} \delta(\epsilon, \gamma) \exp[-\beta \gamma] \exp[-\beta H_r] = \exp[-\beta \epsilon] \sum_{\sigma_0} \sum_{\{\sigma_r\}} \delta(\epsilon, \gamma) \exp[-\beta H_r],$$

where $\delta(\alpha, \beta) = 1$ if $\alpha = \beta$ and $= 0$ otherwise, and $\{\sigma_r\}$ is the set of all possible configurations of the system with $\sigma_0$ fixed. All and only those configurations yielding $\gamma = \epsilon$ contribute to the sums in the last term, so they add to a number which only may depend on the temperature and $\epsilon$, thus:

$$P(\gamma = \epsilon) = e^{-\beta \epsilon} a(\beta, \epsilon).$$
In order to avoid the explicit computation of \(a(\beta, \epsilon)\), which is as difficult as that of the partition function, let us consider:

\[
P(\gamma = -\epsilon) = \sum_{\{\sigma\}} \delta(-\epsilon, \gamma) P(\{\sigma\}) = \sum_{\{\sigma\}} \delta(-\epsilon, \gamma) \exp[-\beta \gamma] \exp[-\beta \mathcal{H}_r] = \exp[\beta \epsilon] \sum_{\sigma_0} \sum_{\{\sigma_r\}} \delta(-\epsilon, \gamma) \exp[-\beta \mathcal{H}_r].
\]

By letting \(\sigma_0 \rightarrow \sigma_0' = -\sigma_0\), thus \(\gamma \rightarrow -\gamma\), and the last expression yields

\[
P(\gamma = -\epsilon) = \exp[\beta \epsilon] \exp[-\beta \mathcal{H}_r],
\]

that is, since \(\delta(-\epsilon, -\gamma) = \delta(\epsilon, \gamma)\),

\[
P(\gamma = -\epsilon) = e^{\beta \epsilon} a(\beta, \epsilon).
\]

Thence the ratio

\[
\frac{P(\gamma = \epsilon)}{P(\gamma = -\epsilon)} = e^{-2\beta \epsilon},
\]

does not depend on \(a(\epsilon, \beta)\).

This equation derives from the canonical distribution and can be used to estimate the lattice temperature \(T_B\) in numerical simulations of the Ising model since, by the law of the large numbers, one can approximate

\[
\frac{P(\gamma = \epsilon)}{P(\gamma = -\epsilon)} \approx \frac{n(\gamma = \epsilon)}{n(\gamma = -\epsilon)} = R,
\]

being \(n(\gamma = \epsilon)\) the number of lattice sites with \(\gamma = \epsilon\), and thence

\[
r = T_B \cdot \epsilon
\]

with

\[
r = -2 (\ln R)^{-1}.
\]

If necessary, better estimates can be obtained by computing averages of \(n(\epsilon, \beta)\) over time, since the system is at equilibrium. In Ref. it has been checked that Eq. (3) is well satisfied when simulating the canonical ensemble, and has been used to compute temperature in a microcanonical Monte Carlo simulation with the Kawasaki dynamics.
III. NON EQUILIBRIUM ISING MODEL

Monte Carlo simulations are extensively employed even for studying non equilibrium properties of systems [5]. 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 [5]. It is therefore tempting to use Eq. (2) for probing the system temperature during the cooling. One wishes, in particular, to answer the following two questions:

1) is the system at equilibrium on very short time scales? i.e. does Eq. (3), which was derived by assuming the Boltzmann (equilibrium) statistics, hold during the system cooling?

2) if yes, how does temperature decrease in time during the cooling?

In order to answers the above questions we have performed Monte Carlo simulations in which the 2d Ising model was quenched from infinite to finite temperature. We have found that the answer to question 1) is affirmative.

In Fig. 1, $r(\epsilon)$ is shown for a quench from $T = \infty$ to $T = 3.0$ at some different times. In this case the quench temperature is above $T_c$, 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 $\epsilon$ and $r$, from which an instantaneous temperature can be derived, as seen also in the inset where $r/\epsilon$ is shown. A linear regression of $r$ vs $\epsilon$ at equilibrium yields $T = 2.996$, with correlation coefficient = 1.

A subcritical quench is shown in Fig 2. Here $T = 2.0$. In this case the system takes a long time to reach thermal equilibrium, but Eq. (3) is quite well satisfied. It can be seen from the inset that deviations from the linear dependence exist. They are however small for any $\epsilon$, and their average is zero. Quasi-equilibrium is satisfied at any instant and in this case a linear regression on the last curve gives $T_B = 2.058$ with a correlation coefficient = 0.9998.

The existence of such an equilibrium-like distribution for the system allows for extracting a Boltzmann temperature $T_B$ during the system cooling. Figure 3 shows the behavior of
the energy as function of this temperature for a quench at $T = 2.0$, i.e. below the critical temperature $T_c \simeq 2.26$. It is seen that a first regime exists in which the two quantities are proportional. Then, a second regime is entered where a remarkable property can be noticed: the Boltzmann temperature attained that of the heatbath but, on the contrary, the energy is still relaxing. In fact this kind of systems is characterized by a coarsening process and takes an infinite time to go to equilibrium, the energy decaying as $1/\sqrt{t}$, but it is seen that temperature is already at equilibrium during the coarsening. This behaviour is better pointed out in the inset, where it is seen that energy decreases algebraically while $T_B$ 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. (3) for the case of the $q$ states Potts model, with Hamiltonian:

$$H = \sum_{\langle i<j \rangle} (1 - \delta_{\eta_i\eta_j})$$

where again the sum is over the nearest neighbors, $\delta_{\alpha\beta}$ is the Kronecker’s function, and $\eta_k$ is the state of site $k$. Each site can assume one out of $q$ different states, so that one can identify the state with an integer: $\eta_k = 1, 2, \ldots, q$ and the system energy Eq. (4) can be written as

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

where

$$\gamma = \sum_v (1 - \delta_{\eta_0\eta_v})$$

is the interaction energy of the site in 0 with its neighbors, and

$$\mathcal{H}_r = \sum_{\langle i<j \rangle} \xi(\eta_i, \eta_j)$$

is the energy interaction of the rest of the system.
Let us now define $\gamma_\rho$ the energy Eq. (5) when $\eta_0 = \rho$ and similarly $\gamma_\omega$ the same quantity when $\eta_0 = \omega$. In analogy with the case of the Ising model:

$$\frac{P(\rho, \eta_1, \ldots, \eta_N)}{P(\omega, \eta_1, \ldots, \eta_N)} = \exp[-\beta(\gamma_\rho - \gamma_\omega)] = \exp[-\beta\gamma_\rho].$$

(6)

Thus the probability for $\gamma_\rho\omega$ to assume the value $\epsilon$ is given by

$$\sum_{\eta_1, \ldots, \eta_N} \delta(\epsilon, \gamma_\rho\omega) P(\rho, \eta_1, \ldots, \eta_N) = \sum_{\eta_1, \ldots, \eta_N} \delta(\epsilon, \gamma_\rho) \exp[-\beta\gamma_\rho\omega] P(\omega, \eta_1, \ldots, \eta_N) = \exp[-\beta\epsilon] \sum_{\eta_1, \ldots, \eta_N} \delta(\epsilon, \gamma_\rho\omega) P(\omega, \eta_1, \ldots, \eta_N).$$

By multiplying the left hand side by $1 = \sum_{\eta_0} \delta(\eta_0, \rho)$ and the right hand side by $1 = \sum_{\eta_0} \delta(\eta_0, \omega)$ one gets

$$\sum_{\{\eta\}} \delta(\eta_0, \rho) \delta(\epsilon, \gamma_\rho\omega) P(\{\eta\}) = e^{-\beta\epsilon} \sum_{\{\eta\}} \delta(\eta_0, \omega) \delta(\epsilon, \gamma_\rho\omega) P(\{\eta\}),$$

where $\{\eta\}$ is the system configuration, and thus finally

$$\exp[-\beta\epsilon] = \frac{\langle \delta(\eta_0, \rho) \delta(\epsilon, \gamma_\rho\omega) \rangle}{\langle \delta(\eta_0, \omega) \delta(\epsilon, \gamma_\rho\omega) \rangle}. \quad (7)$$

Thence even for the Potts model the temperature can be derived from the site-site energy statistics. The same argument as above holds for any pair of different states $\eta_0^{(\alpha)}, \eta_0^{(\beta)}$, so that one can also write

$$\exp[-\beta\epsilon] = \frac{1}{q(q-1)} \sum_{\eta_0^{(\alpha)}, \eta_0^{(\beta)}} \frac{\langle \delta(\eta_0, \eta_0^{(\alpha)}) \delta(\epsilon, \gamma_{\eta_0^{(\alpha)}\eta_0^{(\beta)}}) \rangle}{\langle \delta(\eta_0, \eta_0^{(\beta)}) \delta(\epsilon, \gamma_{\eta_0^{(\alpha)}\eta_0^{(\beta)}}) \rangle}. \quad (8)$$

This can be helpful for improving statistics in out of equilibrium simulations where the thermal average cannot be obtained by averaging over time like in equilibrium cases. One thus replaces thermal averages with system averages in Eq. (8).

It is found that the Potts model obeys Eq. (refpottstemperature) even in the non-equilibrium regime, allowing to extract an instantaneous temperature $T_B$ like done for the Ising model. Figure 5 shows the Boltzmann temperature $T_B$ vs time for a quench of a seven state Potts model at $T = 0.5$, i.e. below the critical temperature $T_c \simeq 0.77$. 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 the second regime is entered in which $T_B$ 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 $T_B = T$ after a certain time, as for the Ising model.

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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 by shifting energies by adding 2 and compressing them by a factor \( 1/2 \) \( (T - c \simeq 1.13) \). A common feature is that as \( T \) is decreased below a given value, the system seems unable to reach the equilibrium temperature.

Figure 7 shows \( T_B \) vs time for the Ising model with linear lattice size \( L = 1000 \). The Boltzmann temperature attains the value of \( T \) if this is above \( T_i > 0.3 \) but if \( T \) is equal or below this value it doesn’t. We expect that this is a finite size effect and that the system eventually relaxes to the ground state with \( T_B = 0 \). The case of the Potts model shown in Fig. 8. In this case \( T_i \simeq 0.3 \). It can be observed that \( T_i \approx 0.42T_c \) for Potts whereas \( T_i \approx 0.15T_c \) for Ising. Moreover the limit energy is clearly larger for Potts than for Ising. Figure 9 displays the behaviour of \( T_B \) after a quench at \( T = 0 \). An increase of \( T_i \) 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 \( T_B \) via Eq. (2) 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 \( T_B \) 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 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 obeyed by the system while cooling after a quench, allowing to associate a Boltzmann-like temperature to its non equilibrium states. While cooling, the Boltzmann temperature decreases until the value of the heat 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 heat bath temperature is not too low and the statistical sampling is effective for the considered system size.

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FIG. 1: The distribution of $r(\epsilon)$, Eq. (3), for the Ising model after a supercritical quench at different times. In the inset the quantity $r(\epsilon)/\epsilon$ is shown (see text). The time interval between curves is of 5 mcs.

FIG. 2: The distribution of $r(\epsilon)$, Eq. (3), for the Ising model out of equilibrium. In the inset the quantity $r/\epsilon$ is shown. The time interval between curves is of 5 mcs.
FIG. 3: Energy vs Temperature during a quench of the Ising model at $T < T_c$ (black curve). The red dashed curve is the equilibrium curve. Inset: energy and $T_B$ vs time.

FIG. 4: Energy vs Temperature during a quench of the Ising model at $T > T_c$ (black curve). The red dashed curve is the equilibrium curve. Inset: energy and $T_B$ vs time.
FIG. 5:  Energy vs Temperature during a quench of the 7 state Potts model at $T < T_c$ (black curve). The red curve is the equilibrium curve. The inset shows $T_B$ and energy behavior in time.

FIG. 6:  Energy vs Temperature during a quench of the 7 state Potts model at $T > T_c$ (black curve). Red curve is the equilibrium curve. In the inset, $T_B$ and energy vs time.
FIG. 7: $T_B$ 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: $T_B$ vs time in the 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 Boltzmann temperature for a quench of the Ising and Potts models at $T = 0$ in lattices of different size.