Generalized Metropolis dynamics with a generalized master equation

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Abstract

The extension of Boltzmann-Gibbs thermostatistics, proposed by Tsallis, introduces an additional parameter q to the inverse temperature β. Here, we show that a previously introduced generalized Metropolis dynamics to evolve spin models is not local and does not obey the detailed energy balance. In this dynamics, locality is only retrieved for $q = 1$, which corresponds to the standard Metropolis algorithm. We propose a generalized master equation, which gives rise to a local generalized Metropolis dynamics that obeys the detailed energy balance.

Generalized Metropolois Algorithm

The system equilibrium is described by the generalized Boltzmann-Gibbs distribution

$$P_{1-q}(E_i) = \frac{[e_{1-q}(-\beta' E_i)]^q}{\sum_{i=1}^{\Omega}[e_{1-q}(-\beta' E_i)]^q} , \quad (1)$$

where Ω is the number of accessible states of the system and $\beta' = \beta / \sum_{i=1}^{\Omega}\{[e_{1-q}(-\beta E_i)]^q + (1-q)\beta\langle E\rangle_{1-q}\}$, where $\langle E\rangle_{1-q} = \sum_{i=1}^{\Omega} E_i P_{1-q}(E_i)$. The function

$$e_\alpha(x) = \begin{cases} (1+\alpha x)^{1/\alpha} & \text{for } \alpha x > -1 \\ 0 & \text{otherwise} , \end{cases} \quad (2)$$

is the generalized exponential [2, 3].

To recover the additive property of the argument, when multiplying two generalized exponential functions: $e_\alpha(a)e_\alpha(b) = e_\alpha(a \oplus_\alpha b)$ $[e_\alpha(a)/e_\alpha(b) = e_\alpha(a \ominus_\alpha b)]$ and $e_\alpha(a) \otimes_\alpha e_\alpha(b) = e_\alpha(a+b)$ $[e_\alpha(a) \oslash_\alpha e_\alpha(b) = e_\alpha(a-b)]$ consider the following algebraic operators [4, 5]:

$$a \oplus_\alpha b = a + b + \alpha ab \quad (3)$$

$$a \ominus_\alpha b = \frac{a-b}{1+\alpha b} \quad (4)$$

$$a \otimes_\alpha b = (a^\alpha + b^\alpha - 1)^{1/\alpha} \quad (5)$$

$$a \oslash_\alpha b = (a^\alpha - b^\alpha + 1)^{1/\alpha} . \quad (6)$$

However, in equilibrium, the Ising model prescribes an adapted Metropolis dynamics that considers a generalized version of exponential function [6, 7]:

$$w[\sigma_i^{(b)} \to \sigma_i^{(a)}] = \frac{P_{1-q}[E^{(a)}]}{P_{1-q}[E^{(b)}]} = \left\{\frac{e_{1-q}[-\beta' E^{(a)}]}{e_{1-q}[-\beta' E^{(b)}]}\right\}^q . \quad (7)$$

More precisely, consider the Ising model in a square lattice, one can show that:

$$\frac{e_{1-q}[-\beta' E^{(a)}]}{e_{1-q}[-\beta' E^{(b)}]} = e_{1-q}\{-\beta'[E^{(a)} \ominus_{1-q} E^{(b)}]\} \quad (8)$$

or:

$$\frac{e_{1-q}[-\beta' E^{(a)}]}{e_{1-q}[-\beta' E^{(b)}]} \neq e_{1-q}\{-\beta'[E^{(a)} - E^{(b)}]\} , \quad (9)$$

where $E^{(a)} - E^{(b)}$ is the energy difference, which depends only the spins that directly interact with the flipped spin, violating the detailed energy balance.

In Refs [6, 7], the authors consider (with no explanations) the equality in Eq. 9, instead of considering Eq. 8. Thus, the detailed energy balance is violated, since the system is updated following a local calculation of the generalized Metropolis algorithm of Eq. 7.

Recovering locality in the generalized Metropolis algorithm

Based on the operators of Eq. 3 to Eq. 6, we propose the following generalized master equation:

$$\frac{dP_{1-q}[E^{(a)}]}{dt} = \sum_{\sigma_i^{(b)}} w[\sigma_i^{(b)} \to \sigma_i^{(a)}] \otimes_{\tilde{q}/q} P_q[E^{(b)}] \ominus_{\tilde{q}/q} w[\sigma_i^{(a)} \to \sigma_i^{(b)}] \otimes_{\tilde{q}/q} P_q[E^{(a)}] . \quad (10)$$

where $P_q(E)$ is given by Eq. 1. Here, it is suitable to call $\tilde{q} = 1-q$ and write the generalized exponentials as a function of $\tilde{q}$. In equilibrium, $dP_{1-q}/dt = 0$ and a dynamics governed by Eq 1.

The detailed balance (a sufficient condition to equilibrium) for the generalized master equation is

$$w[\sigma_i^{(b)} \to \sigma_i^{(a)}] \oslash_{\tilde{q}/q} w[\sigma_i^{(a)} \to \sigma_i^{(b)}] = P_q[E^{(a)}] \oslash_{\tilde{q}/q} P_q[E^{(b)}] , \quad (11)$$

which leads to a new generalized Metropolis algorithm:

$$\begin{aligned} w(\sigma_i^{(b)} \to \sigma_i^{(a)}) &= \min\left\{1, \left[e_{\tilde{q}}(-\beta' E^{(a)})\right]^q \oslash_{\tilde{q}/q} \left[e_{\tilde{q}}(-\beta' E^{(b)})\right]^q\right\} = \min\left\{1, \left[e_{\tilde{q}}(-\beta'(E^{(a)} - E^{(b)}))\right]^q\right\} \\ &= \min\left\{1, \left[e_{\tilde{q}}(\beta' J\left[\sigma_{i_x,i_y}^{(a)} - \sigma_{i_x,i_y}^{(b)}\right] S_{i_x,i_y})\right]^q\right\} \end{aligned} \quad (12)$$

and now the transition probability depends only on energy between the read site and its neighbors, i.e., locality is retrieved.

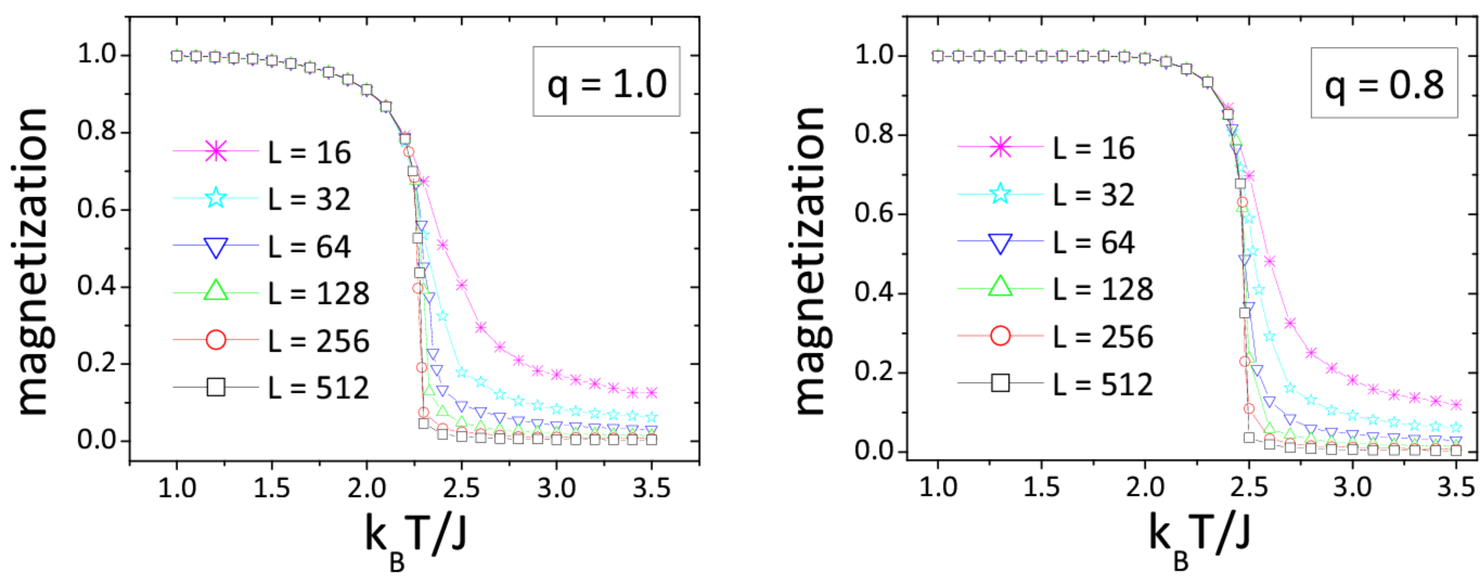

Figure : System magnetization versus temperature for $q = 1.0$, 0.8 and 0.6. Using the dynamics based on Metropolis II, we observe phase transitions for critical values upper to $\log(1+\sqrt{2})/2$ as $q < 1$ differently from previous studies, which are based on Metropolis I.

Conclusion

We have proposed a generalized master equation leading to a generalized Metropolis algorithm. This algorithm is local and satisfies the detailed energy balance to calculate the time evolution of spins systems. We calculate the critical temperatures using the generalized Metropolis dynamics. The critical parameters have been obtained using Monte Carlo simulations in two different ways. Firstly, we show the phase transitions from curves $\langle M\rangle$ versus $k_B T/J$, considering the magnetization averaging, in equilibrium, under different MC steps. We have also studied the Metropolis algorithm of Refs. [6, 7]. We show that it does not preserve locality neither the detailed energy balance in equilibrium. When the extensive case is considered, both methods lead to the same expected values.

For a more complete elucidation about existence of phase transitions for $q \neq 1$, we have performed simulations for small systems MC simulations, recalculating the whole lattice energy in each simple spin flip, according to Metropolis I algorithm only to check the variations on the critical behavior of the model. Notice that this does not apply to Metropolis II algorithm, since it has been designed to work as the standard Metropolis one. Our numerical results show discontinuities in the magnetization, but no finite size scaling, corroborating the results of Ref. [8], which used the broad histogram technics to show that no phase transition occurs for $q \neq 1$ using Metropolis I algorithm.

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