Comment on "Partial equivalence of statistical ensembles in a simple spin model with discontinuous phase transitions"

Ji-Xuan Hou *

School of Physics, Southeast University, Nanjing 211189, China

(Received 10 May 2020; accepted 21 August 2020; published 15 September 2020)

In a recent paper by Fronczak *et al.* [Phys. Rev. E **101**, 022111 (2020)], a simple spin model has been studied in full detail via microcanonical approaches. The authors stress that the range of microcanonical temperature $\beta_m > 1$ is unattainable in this model and the system undergoes a phase transition when the external parameter $a = 1$ in the microcanonical ensemble. The purpose of this comment is to state that the treatment of the microcanonical entropy in the commented paper is inappropriate since the fact that ergodicity is broken in the microcanonical dynamics is ignored by the authors. The phase transition in the microcanonical ensemble, considered in the commented paper, could occur only with a nonlocal dynamics which is often difficult to justify physically.

DOI: 10.1103/PhysRevE.102.036101

In a recent paper [1], Fronczak *et al.* calculated the thermodynamic quantities, including the microcanonical entropy and the microcanonical temperature, of a simple spin model using the microcanonical approach. This model was built up via a local-spin-flipping procedure [2]. The authors show that the range of the microcanonical temperature $\beta_m > 1$ is unattainable in this model since all macrostates with $\beta_m > 1$ are unavailable. The authors also conclude that the microcanonical transition arises as a result of singularity in entropy that appears at the external parameter $a = 1$.

All the symbols here are the same as the commented paper. Using the microcanonical ensemble, the energy per spin of the system u is conserved. u is determined by the positive rate of spins n_+ and the external parameter a. For a given a, n_+ is not a single-valued function of u. Thus, two different macroscopic realizations of the system, $n_+^{(1)}$ and $n_+^{(2)}$, can be found under a certain value of u. The authors simply add up the numbers of the microstates of these two macroscopic realizations to obtain the microcanonical entropy of the system [see Eq. (5) in the commented paper]. One can even compare these two numbers of the microstates to determine which macroscopic realization corresponds to the metastable state and which macroscopic realization corresponds to the equilibrium state.

However, the treatment of the microcanonical entropy above is inappropriate. The dynamics of the system is strongly affected by the feature of disconnected accessible magnetization values. As pointed out by Mukamel *et al.* [3], starting from an initial macroscopic realization, the system is not able to move to the other macroscopic realization via local dynamics. In other words, the ergodicity is broken in the microcanonical dynamics. The system will be trapped permanently in the metastable state as far as the energy is conserved. Therefore, it is better not to distinguish the metastable state and the equilibrium state and one has to admit that both macroscopic realizations are stable thermodynamically. Thus, the entropy of the system no longer is a univalent function of u,

$$s^{(1)} = \frac{1}{N} \ln \binom{N}{Nn_+^{(1)}}, \quad s^{(2)} = \frac{1}{N} \ln \binom{N}{Nn_+^{(2)}}. \tag{1}$$

Which value of entropy should the system take depends on how the system is initially prepared. For example, the system stays in state (1) if the initial condition lies within macroscopic realization (1), and the value of entropy takes $s^{(1)}$.

Due to the breakdown of ergodicity, the discontinuous jump in n_+ discussed in the commented paper is infeasible dynamically, and states (1) and (2) cannot interconvert by slowly adjusting the external parameter a. Therefore, no phase transition can be observed at $a = 1$ in the microcanonical ensemble.

By the usual thermodynamic relation $\beta_m = \partial s/\partial u$, both $\beta_m^{(1)}$ and $\beta_m^{(2)}$ of these two macroscopic realizations can be obtained. The microcanonical temperature is also not a univalent function of u, and both the ranges of $\beta_m > 1$ and $\beta_m < 1$ become available.

In summary, by looking at the most probable state as determined by the maximum of the entropy, the phase transition considered in the commented paper could occur only with a nonlocal dynamics. However, nonlocal dynamics is often difficult to justify physically, even more so if one considers systems with continuous dynamical variables instead of spin systems. On the other hand, if the phase transition is defined by the jump shown by the system subject to its local dynamics, the phase transition cannot be observed in the presence of ergodicity breaking. These two definitions coincide in the absence of ergodicity breaking.

*jxhou@seu.edu.cn

[1] A. Fronczak, P. Fronczak, and G. Siudem, Phys. Rev. E **101**, 022111 (2020).

[2] A. Fronczak, P. Fronczak, and A. Krawiecki, Phys. Rev. E **93**, 012124 (2016).

[3] D. Mukamel, S. Ruffo, and N. Schreiber, Phys. Rev. Lett. **95**, 240604 (2005).