Comment on "Glassiness in a Model without Energy Barriers"

Recently, Ritort [1] proposed a simple microscopic model without energy barriers, which allows for analytical treatment [2, 3] and displays essential dynamical features of real glasses [1], thus manifesting the role of entropy barriers in glassiness. In statistics, however, the model exhibits a pathological feature: negative entropy at low temperatures. In this Comment we point out that such a pathological feature has its origin in Maxwell-Boltzmann (MB) statistics and does not appear when the more natural Bose-Einstein (BE) statistics are used. We also investigate the dynamics of the model with BE statistics via the Monte Carlo (MC) method, which again reveals the glassy behavior, although they are less pronounced.

We use the grand-canonical ensemble with BE statistics and obtain the thermodynamic quantities per particle as functions of the temperature T: the free energy $f(T) = -2T\log(1 + e^{1/T})$, the internal energy $u(T) = -2/(1 + e^{-1/T})$, and the entropy $s(T) = [u(T) - f(T)]/T$ in the limit $N \to \infty$. Figure 1 shows the behavior of the entropy for the two statistics. It should be noted that the number of ground-state configurations in BE statistics is equal to N, yielding zero entropy per particle at $T = 0$, as expected. On the other hand, in MB statistics with the correct Gibbs factor taken into account, the number of configurations is given by the unphysical value $N/N!$. It is thus obvious that such *incorrect counting* is the origin of the negative entropy at low temperatures.

To investigate the glassy behavior of the model with BE statistics, we have performed MC simulations. Figure 2 demonstrates that the glassy behavior such as slow relaxation and hysteresis persists. The relaxation time τ at $T = 0$ has also been measured for N ranging from 10 to 100 to obtain the result $\tau \sim N^{2.03}$, which may be understood in the following way: The average time required for the configuration with n occupied states to relax to that with $n - 1$ occupied states is expected to be proportional to $\Omega(n)/\Omega(n-1)$, where $\Omega(n)$ is the number of configurations with n occupied states. In the model with BE statistics, $\Omega(n)$ is given by $({}_N C_n)({}_{N-1}C_{N-n})$, where ${}_N C_n \equiv N!/n!(N-n)!$. Thus τ can be estimated via

$$\tau \sim \sum_{n=2}^{N} \frac{\Omega(n)}{\Omega(n-1)} \approx N^2 + \mathcal{O}(N\log N) \qquad (1)$$

for large N, which agrees well with the MC result. The same argument can also be applied to the model with MB statistics, yielding $\tau \sim 2^N \approx e^{0.69N}$, again in good agreement with the numerical result $\tau \sim e^{0.67N}$ in Ref. [1]. The faster relaxation in the model with BE statistics, which is consistent with the results in Ref. [3], reflects the smaller effects of entropy barriers.

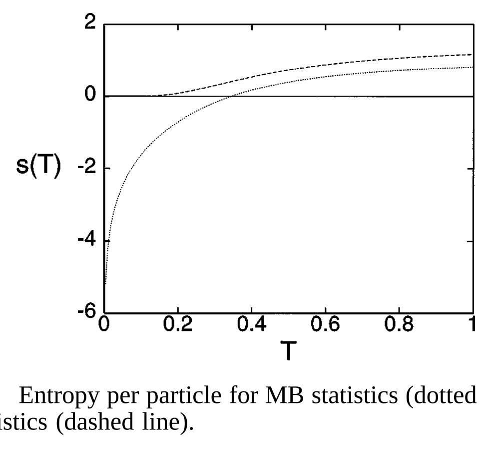

FIG. 1. Entropy per particle for MB statistics (dotted line) and BE statistics (dashed line).

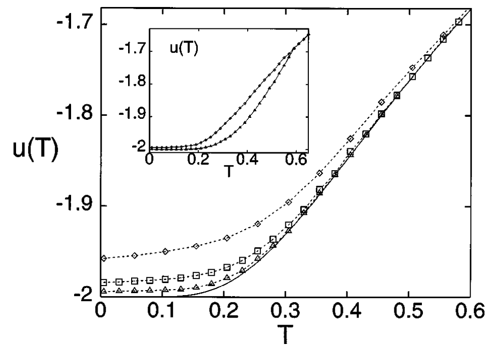

FIG. 2. Energy $u(T)$ vs temperature T for cooling processes in the system of $N = 10^4$, with the number of MC sweeps per temperature step ($\Delta T = 0.005$) given by 10 ($\diamond$), 100 ($\square$), and 1000 ($\triangle$). The solid line denotes the analytic result. Inset: $u(T)$ vs T upon cooling (the upper curve) and heating (the lower curve).

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