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Reply to Chakrabarty et al.: Particles move even in ideal glasses

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In their letter, Chakrabarty et al. [1], point out that their data on the relaxation dynamics are inconsistent with the thermodynamic data presented in our paper [2]. They argue that from their results and the predictions of the random first-order transition theory [3] one must conclude that our configurational entropy s_c is quantitatively not accurate. In the following we will show that this conclusion is not necessarily valid.

The main argument of Chakrabarty et al. [1] (figure 1, Left, of Ref. [1]) is that the self part of the intermediate scattering function $F_s(k, t)$ decays to zero even in the glass phase (defined by $s_c = 0$) and that hence this phase cannot be nonergodic. Although this observation is interesting, it does not imply the mentioned conclusion. This can be seen by considering the case of a simple crystal. In a crystal the diffusion constant of a tagged particle is nonzero (because a crystal at nonzero temperatures will have a finite concentration of defects) and hence $F_s(k, t)$ decays to zero at long times. From this one can, however, not conclude that a crystal is an ergodic system because its structure is obviously independent of time (i.e., the collective correlation functions do not decay to zero).

Thus, also in the case of the ideal glass transition in the pinned system one has to study not only the time dependence of the self functions, but also the one of the collective functions. This is done in FIG. 1, where we compare the time dependence of these two functions for different values of c at the temperature at which Chakrabarty et al. [1] have presented their data. The arrows indicate the static overlap function from Fig. 2C of our article [2], that is, the expected long time limit of the collective function, showing the consistency of statics and dynamics. These data also show that with increasing c the self and collective functions decouple from each other and that the relaxation time of the latter increases rapidly, and thus shows a behavior that is qualitatively consistent with the presence of a nonergodic transition.

Regarding the accuracy of our configurational entropy, we point out that in our paper [2] we obtained the entropy by using a thermodynamic integration of the potential energy from the high temperature limit to temperatures inside the ideal glass state. In a completely independent calculation, we have estimated the vibrational entropy

for the glass state via a harmonic approximation that should give accurate results at lower temperatures. Because inside the glass state the two approaches give the same result, we feel confident that the configurational entropy has been obtained with good accuracy.

Finally, we mention that the concentration for which Chakrabarty et al. [1] present their results is close to or beyond the endpoint of the glass transition line (Fig. 4 in our paper [2]). Thus, unusual dynamics can be expected, and it will be interesting to study this dynamics in more detail.

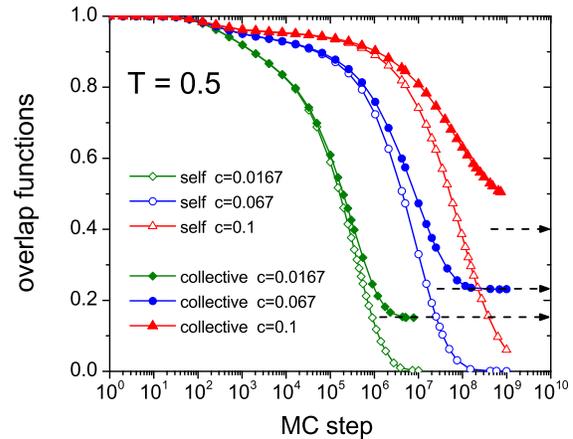


FIG. 1: Time dependence of the self and collective overlap correlation functions (open and filled symbols, respectively) for pinning concentrations c approaching the ideal glass transition of a pinned system at $T = 0.5$. The horizontal arrows indicate the value of the static overlap function from Fig. 2C of our paper [2] and show that the static data are consistent with the dynamic data at long times.

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