Comment on "Partial energies fluctuations and negative heat capacities" by X. Campi et al.

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Studying the energy partitioning published by [1] we show that the presented results do not fulfill the sum rule due to energy conservation. The observed fluctuations of the energy conservation test point to a numerical problem. Moreover, analysis of the binding energies show that the fragment recognition algorithm adopted by Campi et al. leads with a sizeable probability to fragments containing up to the total mass even for excitation energies as large as 3/4 of the total binding. This surprising result points to another problem since the published inter-fragment energy is not zero while a unique fragment is present. This problem may be due to either the fragment recognition algorithm or to the definition of the inter and intra-fragment energy. These numerical inconsistencies should be settled before any conclusion on the physics can be drawn.

In a recent article[1] X. Campi et al. present results from numerical experiments on the liquid gas phase transition of a Van der Valls fluid using a molecular dynamics simulations. They acknowledge the fact that in a microcanonical ensemble the kinetic energy fluctuation ($\sigma_K^2/T^2$) can be used to reconstruct the heat capacities in the context of phase transitions as proposed in ref.[2], but they criticize the experimental evaluation of such a quantity from the observed partitions as used in ref. [3].

Before discussing the actual criticisms of Campi et al. to our work, we would like to point out that the numerical results presented in ref. [1] are inconsistent.

Campi et al. present 4 quantities,

- the exact kinetic energy $K = E - V$, where $E$ is the total energy and $V$ the total interaction energy,
- the quantity supposed to be the approximation to the kinetic energy introduced in ref. [3], $K' = E - \sum_i B_i$ where the sum runs over the fragments and where $B_i$ are the fragment ground state energy [4],
- the inter-fragment interaction $V_{\text{inter}} = \sum_{i<j} V_{ij}$
- and the intra-fragment energy $V_{\text{intra}} = \sum_i V_i$ which they show as a configurational excitation energy $\Delta V = \sum_i V_i - B_i$

Since $V = V_{\text{inter}} + V_{\text{intra}}$ the above quantities should at any time fulfill the exact sum rule

$$S = K - K' + V_{\text{inter}} + \Delta V = 0$$ (1)

The right side of figure 1 shows the sum rule [1] as obtained from the data of ref. [1], which are shown in the left part of the same figure.

Fig 1 shows that in the Campi et al. calculations the sum rule $S$ is not zero, suggesting a possible numerical mistake. If the error on the average $< S > = -8.871$ is of the order of a few percent, the more worrying, considering that the aim of the Campi et al. paper is to discuss fluctuations, are the enormous fluctuations presented by this quantity which should be exactly conserved in time. Indeed the observed variance of $S$ is 3819 while the one of $K'$ criticized by Campi et al. to be too large is only 784. The problem can be more easily understood looking at figure 2 which is the same as figure 3 of ref.[1] on an enlarged time scale. In this figure we can see that the fluctuations of $\Delta V$ and $V_{\text{inter}}$ are approximately in phase. If we consider that the fluctuations of $K$ are very small as shown in figure 1, for the sum rule to be exactly fulfilled, $K'$ should be positively correlated with $\Delta V$ and $V_{\text{inter}}$ which is clearly not the case in the calculation of Campi et al.

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Therefore, before entering into any discussions about the physical meaning of Campi et al. findings, one should be sure that the numerics is under control.

In order to understand better what might be going on, we have used $K$, $V_{\text{inter}}$ and $\Delta V$ combined with the Lennard Jones mass table\textsuperscript{4} and the excitation energy reported in \textsuperscript{1} to disentangle the various components entering in the calculation and in particular the total binding energy of the partitioned system, $B = \sum_i B_i$. We have thus used for the total energy $E = E^* + B_{64} = -73.62$ since $E^*/N = 4$ according to \textsuperscript{1} and since $B_{64} = -329.62$ according to the mass table\textsuperscript{4}. Then we can get $V$ from $K = E - V$ and thus $V_{\text{intra}}$ from $V = V_{\text{inter}} + V_{\text{intra}}$ and finally $B$ from...
\[ \Delta V = V_{\text{intra}} - B. \] The results are shown in figure 3. Before discussing the fact that \(B\) is a very poor approximation of \(V_{\text{intra}}\) in the calculations performed by Campi et al., one is surprised by the fact that \(B\) is reaching exactly \(B_{64} = -329.62\) at time step 711 in the figure 3 of ref. [1]. This means that there is a non negligible probability that the system is composed by a unique fragment containing exactly all the particles (for comparison \(B_{63} = -323.49\)). For this peculiar single-fragment event Campi et al. report a non zero inter-fragment energy (\(V_{\text{inter}} = -29\)), which again points to a numerical problem. This might be related to the sum rule problem discussed above but it is likely to be a different one, since the first problem is related to \(K'\) while in the second one the information about \(K'\) is not used. One of the problems may lie in the fragment definition algorithm employed by Campi et al. In this respect it may be worthwhile to notice that, even if the classical Lennard Jones molecular dynamics is in itself an exact well controlled model, on the other hand the definition of physical clusters in these kind of models and their relationship with measured fragments is subject to many controversies [5].

In conclusion, our study of the results published by Campi et al. clearly show two numerical problems:

- the sum rule taking care of the energy conservation in the energy partition is violated and presents fluctuations,
- the analysis of the total binding energy of the partitioned system shows that even at excitation energies above the critical point, the fragment recognition algorithm used in ref [1] predicts the existence of residues of very large masses, containing up to the 64 particles of the considered system, and pointing to a problem in the definition of the inter-fragment energy since in the case of a unique fragment this latter is not zero.

These numerical inconsistencies should be settled before any conclusion on the physics can be drawn.

To progress on this issue, we have repeated the Campi et al analysis of the independent fragment approximation for the evaluation of the interaction energy on another well controlled exact model. We show in a forthcoming paper that this approximation is accurate provided that the required consistency tests are taken into account.

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