Comment on ”Negative heat capacities and first order phase transitions in nuclei” by L.G. Moretto et al

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In a recent paper L.G. Moretto et al. \cite{1} claim that the negative heat capacities presented in our previously published paper \cite{2} are “artifacts” coming from the use of periodic boundary conditions in the Lattice-Gas calculations. We stress in this comment that this claim is wrong: in ref. \cite{2} we did not use periodic boundary conditions and anyhow the boundary conditions are irrelevant for the statistical ensemble used in \cite{2}. The second claim of \cite{1} is that, because of the Coulomb repulsion, systems “with $A > 60$ should present no anomalous negative heat capacities”. We show that this conclusion is contradicted by exact Lattice-gas simulations including Coulomb forces which present negative heat capacities even for $A > 200$.

Let us start with the discussion about the boundary conditions. It is clearly stated in ref. \cite{2} that $L^3$ [the lattice size] is large enough (typically greater than $20^3$ lattice sites) so that the boundary conditions do not affect the calculations with a constraining $\lambda$. This means that the results of ref. \cite{2} do not depend upon the conditions used at the boundary, and in fact the calculations were made without periodic boundary conditions. At that time we checked the independence of the boundaries comparing $N = 8000$ and $N = 27000$ lattices. To see a sizeable effect of the boundary, we have decreased the size of the lattice. A fast calculation of 50000 events for 216 particles in a $N = 5832$ lattice at an energy $E = 0.4 \epsilon$ confined by a Lagrange multiplier log $\lambda = -8 \epsilon$, gives a temperature $T = (0.687 \pm 0.004) \epsilon$, a heat capacity $C = -16.3 \pm 0.2$, and a kinetic energy fluctuation $\sigma^2_k / T^2 = 1.64 \pm 0.03$. If periodic boundary conditions are imposed, the temperature becomes $T = (0.682 \pm 0.004) \epsilon$, the heat capacity $C = -16.9 \pm 0.4$ and the fluctuation $\sigma^2_k / T^2 = 1.63 \pm 0.07$. The temperature decrease in the phase transition region is $\Delta T = (7.6 \pm 0.4) \times 10^{-3} \epsilon$ ($\Delta T = (6.7 \pm 0.6) \times 10^{-3} \epsilon$) with (without) periodic boundary conditions. This shows that the boundary conditions do not affect the thermodynamics. Indeed, in ref. \cite{2} we have analyzed an ensemble of particles in the vacuum for which only the average spatial extension of the system is defined (isobar ensemble). Then, provided that the lattice in which the system has still to be discretized for technical reasons is big enough, boundary conditions are irrelevant since the particles never explore the outer region.

In a previous paper \cite{3} we have considered a canonical Lattice Gas model in a box of constant volume (isochore ensemble), and there we have used periodic boundary conditions. In these calculations negative compressibilities are reported but the heat capacity is always positive. In fact, in the canonical ensemble the heat capacity is proportional to the energy variance and can never be negative \cite{4}.

Concerning the isochore microcanonical ensemble, the published results \cite{5} show that the heat capacity at constant volume $C_V$ is always positive. Therefore, contrary to what is claimed in ref. \cite{1}, published results dealing with Lattice Gas calculations with typical nuclear size systems and periodic boundary conditions \cite{2-3} do not show any negative heat capacity.

We may incidentally note that recently a debate has started in the statistical physics community after the observation of a negative heat capacity branch for very large systems in the the constant-magnetization microcanonical Ising model \cite{7} (equivalent to the microcanonical isochore Lattice Gas model). In these cases however, the densities involved are so low that once again boundary conditions are irrelevant. Moreover, the sizes discussed are orders of magnitude larger than the nuclear ones.

Finally we would like to stress that we have recently demonstrated that negative heat capacities in finite systems are the origin of first order phase transitions with a finite latent heat: to present an energy discontinuity at the thermodynamic limit, finite systems must present a negative microcanonical heat capacity if the number of particles is large enough \cite{6}.

Let us now comment about the effect of Coulomb. The conclusion of ref. \cite{1} is based on a simple model of a unique cluster in equilibrium with a gas. However, this configuration is not the most probable one both in statistical models \cite{8,9} and in nuclear physics experiments at high excitation energy \cite{10}. In particular, the negative heat capacity region is characterized by a large ($m \geq 3$) multiplicity of fragments \cite{11}. Therefore any conclusion drawn considering only the specific channel of multiplicity 1 is not valid. If we would follow the simple model of ref. \cite{1} and consider partitions with $m = 3 - 5$ fragments of similar mass \cite{10}, this would lead to a figure analogous to figure 5 of ref. \cite{1} but with an abscissa approximately multiplied by $m$ (or more, since all the light particles have to be included), because the inter-fragment coulomb interaction can be neglected if the volume is large. One would then find $A \approx 200$ as the limit of negative heat capacities.

Of course fragments do not have the same size and
to get a quantitative result one needs to compute the relative weight of all the possible channels; this is indeed what is done in nuclear statistical models [9, 12, 13] which show that the intermediate state between the compound nucleus and the vaporized system is multifragmentation: the presence of many drops in equilibrium.

In the case of the Lattice Gas model the different partitions and their relative weight can be calculated without any approximation. In the negative heat capacity energy regime there are in average three fragments of size greater than 4.2. The sudden opening of this multifragment channel causes a convex intruder in the entropy that is responsible of the negative heat capacity. The effect of the Coulomb interaction in the Lattice Gas model can be appreciated from Figure 1 which shows a caloric curve at constant $\lambda = 3p$ for a system of $A = 207$ particles and charge $Z = 82$ [14]. A clear backbending is visible. In the charged Lattice-gas model, the energy interval corresponding to the backbending decreases with increasing charge [14], showing that the idea that Coulomb tends to suppress the negative heat capacity is qualitatively correct. However, when all the available channels are correctly weighted, the quantitative effect is very different then the one reported in ref. [1]. Only a slight effect of the Coulomb interaction has also been reported in the isochore framework [12].

Obviously the result of Figure 1 is model dependent. Different macroscopic models show a higher [13] or lower [12] sensitivity to the Coulomb depending on the detailed implementation of the Coulomb and nuclear interactions. On the other hand molecular dynamics (which can be solved exactly as the Lattice Gas model) leads to caloric curves which are almost independent of Coulomb [16]. Whether this can be interpreted as an evidence of metastable long time tails, the relaxation time of long range interactions being excessively long, is a subject of debate [17]. In any case these examples and the results of Figure 1 show that a definitive understanding of the effect of a non saturating long range interaction on a first order phase transition cannot certainly be achieved through the oversimplified model of ref. [1].

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