Finite size effects and the order of a phase transition in fragmenting nuclear systems

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We discuss the implications of finite size effects on the determination of the order of a phase transition which may occur in infinite systems. We introduce a specific model to which we apply different tests. They are aimed to characterise the smoothed transition observed in a finite system. We show that the microcanonical ensemble may be a useful framework for the determination of the nature of such transitions.

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Since the first attempt to use fragmentation experiments on nuclei \cite{1–4} in order to construct the caloric curve which links the temperature to the excitation energy, many efforts have been made by different groups in order to put the experimental results on firm grounds. Further work is certainly necessary in order to eliminate as much as possible the remaining uncertainties which are present and difficult to get under control. At the present stage it is not possible to see a clear-cut sign for the existence of a phase transition and hence even more difficult to get information about its order.

The approximate plateau observed in the first experimental measurements was interpreted as a sign for the presence of a first order liquid-gas phase transition \cite{1}. This was in agreement with the theoretical expectation that the equation of state should present the characteristics of a liquid-gas transition \cite{2}. However, the latest analyses obtained by means of peripheral collisions show a monotonously increasing curve and the onset of a steep rise on the high energy side of the caloric curve \cite{3}.

This last result \cite{3,4,5} may be interpreted as a sign for a second order phase transition. It cannot be explained with the most commonly used theoretical models showing a liquid-gas transition (Fisher droplet model \cite{6}, lattice gas model (LGM) \cite{7}), which present a single critical point in the phase diagram. This raises the question of the adequacy of the LGM which is the simplest model describing a short-ranged interaction between classical particles inside a fixed volume. A possible explanation of this fact has been proposed recently by the authors of Ref. \cite{8}. They observed that finite size effects could produce a scaling behaviour in fragment observables inside the coexistence region. These signals appear to be suppressed in the thermodynamic limit. If this scaling behaviour is related to the thermodynamic transition it shows that a finite system can present misleading indications concerning the order of the transition in the infinite system. However, these indications are physical when one deals with small systems like fragmenting nuclei. In this sense one can speak about “phase transitions in finite systems” or “crossovers” (smoothed transitions). In the following we shall elaborate on this subject.

The LGM is usually formulated in the framework of the grand canonical ensemble. The basic variables of this model are the temperature $T$ and the density $\rho$ of particles. In the grand canonical formulation, the number of particles is not strictly fixed, but it is conserved only in the mean. This model presents a first order transition for all values of $\rho$ except for $\rho = 0.5$, for which the phase transition is second order. In Ref. \cite{9} we considered a canonical framework for this model, the Ising model with fixed magnetization (IMFM). This constraint is important because it allows a direct exploration of the coexistence region, which is forbidden in the grand canonical formalism, but physically relevant because the system seen as an ensemble of interacting particles can take values of $(T, \rho)$ in this region. Since we are interested in finite crossovers, the ensemble in which the theoretical model is formulated is important when we try to match it with experimental results.

In the IMFM the number $A$ of particles which are located on a lattice is strictly fixed in a fixed finite volume $V = L^3$. The Hamiltonian reads

$$H_{\text{IMFM}} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + V_0 \sum_{\langle ij \rangle} \sigma_i \sigma_j, \quad (1)$$

where $V_0$ is a constant potential strength and $\{\sigma_i = \pm 1\}$. The interaction acts between nearest neighbours.

The Hamiltonian can be rewritten in terms of $s_i = (\sigma_i + 1)/2$, the total number of particles is $\sum_i s_i = A$, and the density $\rho = A/V$ is fixed as a constraint so that the partition function in the canonical ensemble reads
$$Z = \sum_{\{\sigma\}} e^{-\beta H_{\text{IMFM}}} \delta_{\sum_i \sigma_i, A},$$

where $\beta = T^{-1}$ is the inverse temperature.

In Ref. [13] we worked out this model in 3$d$ for finite systems with linear dimensions ranging from $L = 10$ to $L = 48$. The energy sampling of simulation events and the determination of critical exponents relying on finite size scaling (FSS) assumptions lead to the conclusion that the system experiences a second order transition at every value of the density $\rho$.

This result was in contrast with the common understanding that the LGM has a first order transition line except for a single point located at $\rho = 0.5$. The main argument to explain this difference was the following. If one looks at the phase diagram and lowers the temperature for fixed density from above the transition line in the canonical description of this model it is possible to cross this line and enter into the 'coexistence' zone. In the grand canonical formulation (LGM) [13], the states of this zone are not accessible as equilibrium states. Indeed, in the IMFM the magnetisation $m = \sum_i \sigma_i$ which is equivalent to the density $\rho$ is not discontinuous at the separation line as it should be in a first order transition. However, we could not firmly establish the nature of the transition in the thermodynamic limit because of limitations imposed by numerics on the size of the largest system which could be generated. This is the reason for which we discuss different tests aimed to characterise the smoothed crossover.

The observed behaviour of the caloric curve and the specific heat cannot exclude a possible non-homogeneity in the 'coexistence' zone and the importance of surface effects. Hence our first test concerns the topology of the finite system in the vicinity of the line which separates the two phases. Fig. 1 shows two configurations generated in the framework of the IMFM for a 2$d$ system with linear size $L = 400$. They correspond to two values of the density, just below the transition line (low temperature side). In the ordinary Ising model, the case $\rho = 0.5$ corresponds to a second order phase transition, and $\rho = 0.3$ to a first order transition. In the second case, the non-homogeneous configurations are those which dominate in the thermodynamic limit below the transition. One expects the system to be divided in two well-defined phases separated by a transition domain of linear dimension $\xi$, where $\xi$ is the correlation length. However, as one can see in Fig. 1, in the IMFM the system looks rather homogeneous in both cases and one expects a self-similar pattern at different scales which is a qualitative indication of a continuous behaviour. At very low temperatures, the system is made up of large and compact clusters and hence gets non-homogeneous, but we checked that this happens for $\rho = 0.5$ as well as for any other value of $\rho$.

The next point concerns the caloric curve for the IMFM in 3$d$. In the thermodynamic limit the caloric curve of a system which undergoes a first order transition shows a plateau which signals the generation of latent heat. This is why the first experimental caloric curves [1], apparently showing a plateau, were considered as a reminiscence of a liquid-gas phase transition present in nuclear matter. In the framework of the IMFM, we constructed the caloric curve for different sizes of 3$d$ systems. Fig. 2 shows these curves for $L = 10, 24$ and $48$ and a density $\rho = 0.3$. All three curves exhibit an inflection point and the slope of the curve in the interval of energy where it increases rapidly gets steeper with increasing $L$. However, one observes only a very small change between $L = 24$ and $L = 48$ which seems to indicate that the asymptotic limit is close. It is nevertheless clear that for $L = 48$ there is no sign for the appearance of a real plateau. Thus for this system one observes a behaviour of the caloric curve which indicates a continuous transition between two homogeneous phases in the asymptotic limit. Such a behaviour is in qualitative agreement with recent data analyses [1]. Similarly to the FSS analysis, it again does not allow to establish what happens in the infinite system.

As a third test we introduce the microcanonical approach in order to compare the caloric curve with the same curve obtained in the framework of the canonical ensemble. It is well established that a closed thermalised system with fixed energy and number of particles, which is a finite microcanonical ensemble shows a caloric curve which is multivalued in energy for fixed temperature, i.e. shows an oscillation (“S” curve behaviour). As a consequence the specific heat gets negative for fixed volume over certain intervals of energy [16,17]. This effect is due to the non-homogeneity of the system which characterizes a first order transition. The surface energy of the clusters in the coexistence phase can be read from the area of the domains obtained by means of a Maxwell construction in the region of energy where the two phases coexist [16]. The canonical caloric curve does not show this effect.
In order to test the existence or absence of this phenomenon in our model we introduce a Metropolis Monte Carlo microcanonical algorithm [18]. We apply it to the \( q \)-state Potts model [19] in two dimensions, which presents a second order transition for \( q \leq 4 \) and a first order transition for \( q \geq 5 \) and is used here as a test model. As expected, the system shows the two types of caloric curves, i.e. the characteristic “S” behaviour of the caloric curve when the transition is first order (\( q = 5 \)), and a monotonous rise when the transition is second order (\( q = 4 \)), see Fig. 3. This can be compared to a canonical simulation of the Potts model which is also shown in the figure. The backbending is absent for \( q = 5 \).

In the case of the 3d IMFM, precise canonical and microcanonical simulations lead to the results shown in Fig. 4. The figures correspond to densities of \( \rho = 0.3 \) and \( \rho = 0.5 \). There exists no sign for the existence of multivaluedness of the energy for fixed temperature which would indicate a first order transition. We also observe from these figures that microcanonical and canonical results are already the same for a still relatively small lattice volume (\( L = 10 \)). This result supports the previous indications of a continuous transition in the thermodynamic limit.

These results raise the general question of the role played by constraints on the order of the transition. In order to investigate this point further we consider the Potts model for \( q \geq 5 \) and introduce different constraints. In practice we fix the number \( N(p) \) of spins in a given direction (\( p = 0, \ldots , q - 1 \)) to a given value and generate the caloric curve for the systems in the framework of the microcanonical ensemble. Some results are shown in Fig. 5. One sees that the curves no longer correspond to a multivalued temperature \( T \) as a function of energy but show a smooth increase, with the presence of an inflection point as expected for a second order transition when one goes to the thermodynamic limit. This result goes the same direction as the result obtained from the IMFM and confirms indeed the fact that constraints may have drastic effects on the order of the transition.

In summary, different tests show that the IMFM, in its microcanonical or canonical formulation, exhibits the characteristic features of an homogeneous system which will undergo a smooth transition from one phase to the other in the thermodynamic limit. It may be surprising to find such a behaviour in the framework of the LGM, but the constraints imposed on the model seem to produce this effect. The strongest argument pointing towards this conclusion concerns the microcanonical test which indicates that the expected effect characterizing a discontinuous transition on the caloric curve is not seen. This is also in agreement with the finite size scaling analysis carried out in Ref. [13]. It shows that microcanonical calculations may be of help in the characterization of the phase crossover in finite systems. As already stated above, we however cannot conclude that the phase transition is indeed necessarily of second order in the thermodynamic limit. Hence it may also be difficult to decide about the order of a phase transition in infinite nuclear matter from experimental results extracted from finite nuclei collisions.

The sharpest experimental test would correspond to measurements in which energy and number of particles are strictly fixed and hence the fragmenting system could be assimilated to a microcanonical ensemble. Its caloric curve would then be able to reveal not only the characteristics of the crossover in the finite system but also the nature of the thermodynamic transition. Very recently it was claimed that the analysis of fragmentation events
show negative values for the specific heat. The confirmation of these results would be a proof for the presence of a first order phase transition and confirm the predictions of models which were proposed in the near past.

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