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In this paper we present canonical lattice gas calculations with various surface conditions. We discuss the inclusion of a finite volume constraint through the use of a pressure as an associated Lagrange multiplier. We show that even in small systems the critical fragment size distributions are not much affected by the surface conditions. Critical signals are therefore shown to be a robust indicator of phase transitions in finite systems.

The determination of the nuclear equation of state is one of the longstanding problems in physics. Since the intranuclear potential resembles to a Van der Waals force which is attractive except for a hard repulsive core at short distance, it is expected that nuclear matter should present an equation of state including a liquid - gas phase transition [1]. Some first evidences of a possible signal of a phase transition in heavy ions collisions have been reported. In particular, finite size scaling [2] has been experimentally observed in the charge partitions of finite multifragmenting nuclei [3] and has been tentatively related to the occurrence of a phase transition.

Phase transitions are well understood in infinite systems for which non analytical behaviors in the relevant thermodynamical potential are expected. It has been recently discussed that these behaviors are signaled by anomalies in the partition function of the corresponding finite system [4] [5] [6]. It has been also shown that fragment size distributions exhibit a critical behavior with the critical exponents of the liquid - gas universality class if fragmentation occurs in the coexistence region [6]. However the theoretical study of ref. [6] concerns finite systems within periodic boundary conditions, *i.e.* with no surface. In the realistic case, because of the finite ratio between surface and volume energies, surfaces conditions can have non negligible effects on the equation of state of finite systems as well as on the associated partition observables. This is in particular the case of atomic nuclei which are finite systems with a very small number of constituents. In this letter we focus on the effects of surface conditions on the critical partitions of a finite system undergoing a liquid-gas phase transition in the framework of the canonical lattice gas model. Using different boundary conditions as well as a direct constraint of a finite radius in the partition function we will show that in all cases a critical fragmentation should be expected in the phase transition region.

Our implementation of the lattice gas model [7] consists of N sites in a three dimensional cubic geometry with an elementary mesh side r_0 . Each site i is characterized by an occupation number $n_i = 1$ for a particle and $n_i = 0$ for a vacancy. Particles interact only with nearest neighbors with a coupling energy ϵ . Then the lattice-gas Hamiltonian reads

$$H = \sum_{i=1}^N \left(\frac{\vec{p}_i^2}{2m} - \frac{\epsilon}{2} \sum_j n_j \right) n_i \quad (1)$$

where the second sum $\sum_j$ runs over the z nearest neighbors of the i -th site and $\vec{p}_i$ represents the particle momentum. The number of occupied sites is fixed to be equal to the nucleon number A_0 , while we set the energy $\epsilon = 5.5$ MeV in order to get the typical scale for the binding energy of nuclear matter. The canonical statistical ensemble can be sampled by giving to each individual partition the canonical probability

$$P^{(n)} = \frac{1}{Z(\beta)} \exp(-\beta E^{(n)}) \quad (2)$$

where $E^{(n)}$ is the actual energy of the (n) -th partition while $\beta = 1/T$ is the Lagrange multiplier associated to the total average energy constraint, $\langle E \rangle$.

A density can be imposed at each site by defining a N -dimensional Lagrange multiplier $\vec{\lambda}$ so that the partition probability reads

$$P^{(n)} = \frac{1}{Z(\beta, \vec{\lambda})} \exp[-\beta E^{(n)} - \sum_{i=1}^N \lambda_i n_i^{(n)}] \quad (3)$$

where $n_i^{(n)}$ is the actual occupation of the site i . This probability is equivalent to the canonical distribution obtained with a constrained Hamiltonian H'

$$H' = H + \sum_{i=1}^N \frac{\lambda_i}{\beta} n_i \quad (4)$$

so that λ_i can be seen as a one body external field defined at each position i .

A more global constraint can be introduced by imposing an averaged volume for the ensemble of the events. For example, noting r_i the distance to the center of the lattice, one can introduce the observable

$$V = \sum_{i=1}^N \frac{4\pi}{3} r_i^3 n_i \quad (5)$$

and an associated global Lagrange multiplier λ_v so that the partition function reads

$$Z = \sum_{(n)} \exp \left[-\beta E^{(n)} - \lambda_v V^{(n)} \right] \quad (6)$$

Equations (4),(6) show that constraining an average spherical volume is equivalent to impose an external potential $\lambda(r) = 4\pi\lambda_v r^3/3\beta$. The thermodynamical potential can be written as

$$-T \ln Z = \langle E \rangle - TS + T\lambda_v \langle V \rangle \quad (7)$$

where S is the entropy. By identifying $T \ln Z$ with the Gibbs free energy we can recognize that the Lagrange multiplier λ_v acts as an external pressure $P = \lambda_v T$.

The constrained lattice gas model can be easily treated in a mean field approach. The mean field Hamiltonian including the $\bar{\lambda}$ field reads

$$H_{MF} = \sum_{i=1}^N \left[\frac{\bar{p}_i^2}{2m} - Jz \langle n_i \rangle + \frac{\lambda_i}{\beta} \right] n_i \equiv \sum_{i=1}^N h_i n_i \quad (8)$$

In the grand canonical case it is easy to get the partition function

$$Z_{MF} = \prod_{i=1}^N (1 + e^{-\beta h_i + \mu}) \quad (9)$$

where μ is the chemical potential. Using the equation of state $\langle n_i \rangle = \partial_{\lambda_i} \ln Z_{MF}$ we get a self consistent equation for the average occupation

$$\langle n_i \rangle = \frac{1}{1 + e^{-(\lambda_i + \mu) - \beta Jz \langle n_i \rangle}} \quad (10)$$

which allows to compute the associated volume. The mean field approximation has been already widely employed in the lattice gas context [8,9]. However, because of the complete lack of correlations and fluctuations, this approximation is expected to badly fail in the phase transition region [6].

FIG. 1. Upper part: isotherms in the pressure versus average volume plane of the constrained Lattice Gas model for a system of $A_0 = 108$ particles. Lower part: density profiles at a temperature $T = 3$ (left) and $T = 15$ MeV (right). Symbols: Metropolis calculation at $T = 3$ (dots), $T = 5$ (circles) and $T = 15$ MeV (squares). Lines: mean field approximation.

In order to have an exact calculation of the equation of state and of the density profiles we use a standard mass conserving Metropolis method to sample events according to the canonical probability with or without the volume constraint. The occupation of two randomly selected sites are exchanged according to the probabilities of the associated partitions. For each couple of Lagrange multipliers β, λ_v a large ensemble of events (typically 10^6) is generated and the associated average volume $\langle V \rangle$ is calculated. Then the relation between P, V and T can be inverted in order to get the desired volume. The associated equation of state $P = P(T, \langle V \rangle)$ is compared to the mean field approximation in figure 1 for a system of $A_0 = 108$ particles. Both calculations trivially agree in the infinite pressure limit corresponding to a closely packed lattice configuration, and in the zero pressure, high temperature limit where the particles randomly occupy all the available volume (1728 sites in this calculation). We can also see that at temperatures higher than about 10 MeV the mean field and the exact calculation are very similar for all pressure values, while in the phase transition region ($T \leq 6 \text{ MeV}$) large discrepancies are apparent.

FIG. 2. Density profiles for a system of 108 particles at two temperatures $T = 3$ MeV (left) and $T = 15$ MeV (right). Symbols: Metropolis sampling with a Lagrange pressure such that $\langle V \rangle = 108$ (upper part) and $\langle V \rangle = 216$ (lower part). Full lines: sharp boundary conditions in spherical symmetry for the same values of $T, \langle V \rangle$ as the symbols.

The use of the Lagrange multipliers λ_i associated to each lattice site i allows to explore any arbitrary shape for the system in a self consistent way. In particular the constrained calculation $\lambda_i \propto r_i^3$ introduced above leads to a diffuse spherical density distribution shown in figure 2 for two different temperatures and average volumes. In order to study the role of the surface conditions on fragment distributions, we can compare the constrained calculation with a sharp boundary condition imposed on a spherical surface. The lines in figure 2 represent the respective density profiles for a boundary condition ad-

justed such a way that the two calculations lead to identical mean volumes. In the upper part of figure 2 the volume of the sharp sphere is defined to be twice the mass considered so that at high temperature the value of the density corresponds to the critical density in the thermodynamical limit $\rho = \rho_c = \rho_0/2$. In the lower part of the figure the volume is doubled to consider a more realistic freeze out condition for nuclear fragmentation. At $T = 3$ MeV the densities are surprisingly close. This demonstrates the preeminence of the interaction on the boundary conditions. Indeed, the fluid forms a drop of liquid which develops a self consistent density profile independently of the surface conditions. At higher temperature, $T = 15$ MeV, the boundary conditions start to be important. The system with an imposed sharp boundary finally becomes uniform.

FIG. 3. Finite size scaling analysis for a spherical system with $A_0 = 108$ with a diffuse surface. Part a): maximum fragment production yield displayed as a function of the fragment mass (black dots) and mass distribution at $T = 6.1$ MeV (squares) compared to a power law fit (line). Part b): distance to the critical point of the mass dependent maximum production temperature (dots) compared to a power law fit (line). Part c): scaling function f (see text) for temperatures $3 \leq T \leq 10$ MeV and fragment masses $4 \leq A \leq 20$.

Besides the thermodynamical observables, one may wonder about the effects of the surface on the cluster partitions. In order to define clusters we have used the algorithm defined in ref. [8]. A. Coniglio and W. Klein have demonstrated that nearest neighbors have to be connected with a bond breaking probability in the form of a Boltzmann factor [10] to insure the fragment distribution to become critical at the critical point. X. Campi and H. Krivine [11] have reinterpreted this algorithm by discussing it in terms of monomer evaporation. If the kinetic energy is distributed according to a Boltzmann law, the Coniglio-Klein algorithm [10] is equivalent to the requirement that the binding energy of each monomer (nucleon) is negative. A way to implement this requirement is to compare for each pair of neighboring particles their

relative kinetic energy with the potential energy of each bond [8]. If the kinetic energy is greater than the interaction energy, the link is broken. If not, the link is kept. The fragments so formed are referred in the literature as Coniglio-Klein fragments [11].

In order to study the influence of the surface conditions on critical behaviors we have compared the following different systems with the same number of particles :

1. a finite cubic system with periodic boundary conditions at half normal density corresponding to the critical density ;
2. a finite cubic system without periodic boundary conditions with the same volume as in (1) ;
3. a finite sphere with the same volume as in (1) and sharp edges ;
4. a finite sphere with a diffuse surface obtained using a constraint on the average volume, the volume being fixed to be the same as the average one of case (3).

A critical point is characterized by a fragment size distribution which follows a finite size scaling [2]

$$\frac{dN}{dA}(A) = A^{-\tau} f(A^\sigma (T - T_c)) \quad (11)$$

where τ and σ are critical exponents, T_c the critical temperature and f is an universal scaling function.

A precise way to determine τ consists in performing a power law fit of the distribution of the maximum production yield of each fragment size. Indeed, at the maximum f_{max} of the scaling function, each fragment A is produced with a maximum yield

$$\frac{dN}{dA}(A) |_{max} = A^{-\tau} f_{max} \quad (12)$$

at a given temperature $T_{max}(A)$. For the diffuse sphere case (4) the associated maximum production is displayed in figure 3a. One can see that the distribution of maximum production yield indeed exhibits a power law behavior with a critical exponent τ around 2, close to the expected value of the liquid-gas universality class.

The critical temperature T_c can be determined using the fact that the fragment size distribution is a power law at T_c with the same exponent τ

$$\frac{dN}{dA}(A) |_{T_c} = A^{-\tau} f(0) \quad (13)$$

The mass distribution at the critical temperature $T = 6.1$ MeV is also shown in figure 3a. It is interesting to remark that, at variance with what is frequently assumed [8], this temperature does not coincide with the temperature giving a minimum value for the fitted τ , due to finite size effects [12].

The last exponent σ appearing in the scaling function can be obtained using the value extracted for T_c and the fact that the maximum of f occurs for an argument x_{max} fulfilling the relation

$$x_{max} = A^\sigma (T_{max} - T_c) \quad (14)$$

for each size A . A power law fit of $(T_{max} - T_c)$ as a function of A thus gives the value of σ . This analysis is presented for the constrained volume calculation in figure 3b. Finally we can reconstruct the universal function f by plotting $dN/dA \cdot A^\tau$ as a function of $A^\sigma \cdot (T - T_c)$. The universality of the critical behavior is tested for the diffuse sphere calculation in figure 3c. One can see that all the different data points collapse on a single curve demonstrating the validity of the universal scaling. In fact using the requirement that around the critical point fragment production should exhibit a finite size scaling allows to define unambiguously the critical temperature within less than 0.5 MeV even for a finite system of a typical nuclear size.

The quality of the critical exponents fit is comparable for all the surface conditions examined and the resulting critical parameters are presented in table 1. The slight variation of the critical temperature can be related to the variations of the density profiles inside the system. If the volume of the system is varied the critical exponents remain unchanged as well as the agreement between the different surface conditions; only the critical temperature extracted from finite size scaling is seen to decrease monotonically with increasing volume in agreement with our previous findings [6,12]. In other words, it is apparent that the change of the surface shape only slightly affects the detailed structure of the scaling function and does not change qualitatively the critical behavior.

In this paper we have discussed the various ways to fix the volume of a finite system. We have shown that if the system is not contained in a box, *i.e.* if the volume is at best known only in average, the maximum entropy argument naturally leads to introduce a Lagrange multiplier for the volume constraint which should be interpreted as a pressure.

System	τ	$T_c(\text{MeV})$	σ
Cubic periodic	2.0	6.5	0.8
Cubic non periodic	2.0	6.0	0.7
Sharp sphere	1.9	6.2	0.7
Diffuse sphere	2.1	6.1	0.6

TABLE I. Critical parameters for the different surface conditions of a system of 108 particles at the critical density (see text)

Comparing the exact calculation with the mean field approximation we have shown that this approximation cannot be used in the vicinity of the phase transition.

From the thermodynamical point of view, surface conditions are expected to influence the properties of the system since isochoric or isobar constraints correspond to different statistical ensembles [14]. However, comparing different types of surface conditions we have shown that the critical behavior of mass partitions are not affected much by the different surface shapes and boundary conditions. Finite size scaling seems to be valid irrespective of the surface shape even for a system as small as the one under study $A_0 = 108$. The critical exponents τ , σ and the critical temperature are almost independent of the density profile. Only the scaling function appears to slightly change from one case to another but the accuracy of finite size scaling is almost as good for all the studied cases. We have checked that this conclusion remains valid for a wide range of total masses, from few tens to few hundreds.

For a realistic application to fragmentation data however other physical ingredients have to be added to the model. In particular the possible influence on the results of the chosen thermodynamical ensemble (microcanonical versus canonical) has to be checked [13] and the persistence of signals must be verified respect to the long range Coulomb interaction [14]. The fact that minor violations to the scaling in the size of the largest cluster are observed in the macroscopic microcanonical statistical model MMMC [15] which includes the Coulomb field is in this sense very encouraging.

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