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PHASE TRANSITION AND FRAGMENT PRODUCTION IN THE LATTICE GAS MODEL

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The critical behavior of fragment production is studied within a Lattice Gas Model in the canonical ensemble. Finite size effects on the liquid-gas phase transition are analyzed by a direct calculation of the partition function, and it is shown that phase coexistence and phase transition are relevant concepts even for systems of a few tens of particles. Critical exponents are extracted from the behavior of the fragment production yield as a function of temperature by means of a finite size scaling. The result is that in a finite system well defined critical signals can be found at supercritical (Kertész line) as well as subcritical densities inside the coexistence zone.

I. INTRODUCTION

It is generally believed that heavy ion collisions may provide an experimental way to explore the properties of nuclear matter under different thermodynamical conditions. Then, an important experimental issue is to extract information on the nuclear equation of state (EOS) from reaction data. In particular, considering the analogy between the nucleon-nucleon force and a Van der Waals interaction it is expected that the EOS presents the characteristics of a liquid-gas phase transition. In the recent years, different indications of such a transition have been accumulated. On one side, studying the decay of hot nuclear system it was observed a sudden opening of the multifragmentation [1,2] and vaporization [3] channels associated with the disappearance of a large residual nucleus. These observations were interpreted as signatures of the transition from the survival of a liquid phase at low temperature towards the massive production of a dilute gas system at high excitation energy through the apparition of a phase mixture in the intermediate energy domain [4,5]. Moreover, this direct observation of various phases has been completed by the extraction of thermodynamical signals of a first order phase transition. Indeed, it has been reported an anomaly of the evolution of the observed temperature as a function of the excitation energy (the so-called caloric curve) [6] which shows a structure similar to a first order phase transition in the framework of statistical equilibrium models [5,7,4]. Moreover, statistical equilibrium models, extremely successful in reproducing multifragmentation patterns, systematically suggest low freeze out densities [8,5] which are in complete agreement with the idea that the transition occurs in the middle of the coexistence region.

On the other hand, the observation of critical behaviors like power laws in the charge distribution of the multifragmenting system [9] have been interpreted as an evidence of a second order phase transition as expected in a single specific thermodynamical point, the critical point. Campi and Krivine have pointed out [10] that a critical behavior in the clustering properties of a multifragmenting system can be observed also at high densities (supercritical) along the Kertész line [11] thus suggesting the picture of an "early" equilibrated multifragmentation when the system is dense. This idea is supported by molecular dynamics simulations where however thermodynamical equilibrium is apparently not reached [12].

The presence at the same time of first and second order transition signals is still a puzzle and the density at which the partitioning of the system occurs is still an open question. The main result of this paper is that a critical behavior in fragment observables can be consistent with the thermodynamics of phase coexistence and the occurrence of a low freeze out density due to finite size effects. In order to reach this conclusion we will study an exactly solvable model for second and first order phase transition, the Lattice Gas Model of Lee and Yang [13]. Of course this is a very simplified model which can be interpreted as a model for a classical fluid with a Van der Waals type of equation of state. Therefore, it should not be interpreted as a reasonable parametrization of the nuclear EOS but as a model case to investigate phase transitions and critical properties. The pertinence of the reached conclusions for the nuclear physics problematics relies on the fact that critical behaviors correspond to universal properties which do not depend on the details of the model considered. A shorter version of this work was already published in ref. [14].

II. THERMODYNAMICS OF THE LATTICE GAS MODEL

The Lattice Gas Model, where the grandcanonical partition function of a gas with one type of atoms is mapped into the canonical ensemble of an Ising model for spin 1/2 particles in presence of an external magnetic field, has

successfully described the liquid-gas phase transition for atomic systems. This same model has already been applied to nuclear physics in refs. [15,10,16–19].

In our implementation the N sites of a lattice are characterized by an occupation number τ which is defined as $\tau = 0$ for a vacancy, and $\tau = 1$ for a nucleon. Particles occupying nearest neighboring sites interact with an energy ϵ . The Hamiltonian is given by

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} \tau_i + \sum_{i \neq j} \epsilon \tau_i \tau_j \quad (1)$$

where the sum runs only on closest neighbours. The coupling constant $\epsilon = 5.5$ MeV is fixed such as to reproduce the saturation properties of nuclear matter. In all the calculations shown below the numerical realization of the model is a three-dimensional cubic lattice with periodic boundary conditions characterized by a linear size L , a number of particles A_0 (or equivalently a density $\rho/\rho_0 = A_0/L^3$) and a temperature T . Statistical averages are taken over events obtained with a standard Metropolis sampling of the lattice occupations in the canonical ensemble [19].

FIG. 1. Left: distributions of the canonical events at two temperatures (full lines) as a function of the energy for a cubic lattice of size $L = 6$ compared to a random sampling (dashed line). Right: Estimation of the temperature from the inversion of eq. (2) (see text).

The thermodynamics of the model is calculated from a direct evaluation of the partition sum Z via an iterative procedure analogous to the one used in ref. [20]. At a temperature T , the number of sampled realizations of the system with an energy state E as given by the Boltzmann probability is

$$N_T(E) = N \frac{1}{Z_T} W(E) e^{-E/T} \quad (2)$$

where $W(E)$ is the degeneracy of the state and N the total number of sampled states. An exemple is given in the left part of fig.1. From the comparison of the occupation probabilities at two different temperatures T_1, T_2 one then has

$$Z_1 = Z_2 \frac{N_1(E)}{N_2(E)} e^{-E(\frac{1}{T_2} - \frac{1}{T_1})} \equiv z_1(E) \quad (3)$$

which is valid for all the different energy bins. In order to profit from all the available data we can compute the partition sum as a weighted averaged of the above relation over the various energy bins

$$Z_1 = \sum_E z_1(E) \sqrt{N_2(E) N_1(E)} / \sum_E \sqrt{N_2(E) N_1(E)} \quad (4)$$

Then, Z_1 is obtained iteratively with an initial normalization to the infinite temperature limit where the partition sum is analytical. A check of the precision of this method is shown in fig.1: once the partition sum is known, eq.(2) can be inverted leading to an a posteriori estimation of the temperature

$$T^{-1} = \frac{1}{E} \left(\ln Z_\infty - \ln Z_T - \ln \frac{N_T(E)}{N_\infty(E)} \right) \equiv T_{calc}^{-1}(E) \quad (5)$$

via a comparison (presented in the left part of figure 1) of the occupation $N_T(E)$ at temperature T with the occupation in the infinite temperature limit $N_\infty(E)$, which is given by a random sampling. Eq.(5) is again valid for all energy bins. The fact that the calculated temperature T_{calc} for each energy bin is independent of E is a strong test of the numerical sampling of the canonical ensemble and is demonstrated in the right part of fig.1. Even the tails of the canonical distribution are clearly sampled in a very precise way. Moreover, the fact that the a posteriori estimation of the temperature T_{calc} is statistically consistent with the input one T shows the precision of the calculation of the partition sum.

FIG. 2. Pressure as a function of density for different temperatures inside and above the coexistence region calculated from the exact partition sum (symbols) and with the mean field approximation (dashed lines). The full line indicates the coexistence line (see text).

The equations of state can then be obtained from a numerical derivative of the logarithm of the partition sum. As an example, figure 2 presents the extracted pressure as a function of the density. We can recognize a typical $P - V$ diagram of a liquid gas phase transition. In the same figure, the mean field equation of state [16,18] is shown. Only at high supercritical temperature the mean field approach reasonably reproduces the exact calculation, but it badly fails in the phase transition region. It is important to remark that the observed back-bending behavior of the isotherms in the coexistence region has a very different physical meaning in the mean field and in the exact calculation. In the mean field case, this region of negative compressibility reflects the instability of the homogenous system respect to phase separation, which has to be cured through the usual Maxwell construction. On the other hand, in the exact calculation which includes inhomogeneous partitions, the stable equilibrium configurations in the coexistence region are characterized by a negative compressibility. This is analogous to the well documented presence of a negative heat capacity in microcanonical systems undergoing a first order phase transition [21]. This behaviour can only be observed if in the considered sampling a conservation law applies to an extensive variable (here the volume). This point is further explored in figure 3,

FIG. 3. Chemical potential (a) and free energy (c) as a function of the particle number at temperature $T = 5.5$ MeV for a cubic lattice of size $L = 6$. The free energy as a function of the associated pressure is also shown (b).

FIG. 4. The exact (symbols) and mean field (dotted lines) free energy as a function of the associated pressure as in fig. (3b) for various T around the critical temperature ($T_c = 6.7$ MeV).

where thermodynamical variables are shown for a lattice of size $L = 6$ at a subcritical temperature. The Van Hove theorem assures that in the infinite system the thermodynamical potential must be convex. However, for the free energy of the finite system (fig. 3c) we observe a concave pattern due to the surface energy between the liquid and the vapor in the mixed phase. This behaviour induces a back-bending of the chemical potential μ (fig. 3a). In infinite systems one would expect the chemical potential to stay constant inside the coexistence region. This corresponds to a non-analytical behaviour of F which can only be obtained in the thermodynamical limit when the volume and the number of particles diverge. In a finite system the partition sum is always analytical and the chemical potential

presents a smooth back-bending which will become a flat plateau as $V \rightarrow \infty$. This "anomaly" of an intensive variable (e.g. μ) as a function of its extensive conjugated variable (e.g. A_0) or equivalently the non-convex behaviour of the thermodynamical potential can be considered as the signature of the phase transition in a finite system. Again, this behaviour comes from a conservation law on the extensive variable and the observed back-bending is analogous to the negative heat capacity or the negative compressibility as reported above.

In the presented results the limit of the coexistence zone can be accurately spotted on the chemical potential versus pressure plane as shown in fig. 3b and fig. 4 where a few isotherms are shown in the chemical potential versus pressure plane for a lattice of size $L = 6$ (i.e. a number of particles varying from $A = 10$ to $A = 210$). At low temperature, one can clearly observe two branches characteristic of a gas phase at low pressure and of a liquid phase at high density. The point where the two branches met defines the coexistence since the two solutions have the same pressure and chemical potential. This coexistence of two phases disappears above a critical temperature leaving a single fluid isotherm. Making a systematic analysis of the crossing point of the two branches, the coexistence zone can be evaluated very accurately leading to a critical temperature $T_c = 6.7$ MeV and a critical exponent $\beta = 0.31$ for the temperature dependence of the order parameter

$$\rho - \rho_c = (T - T_c)^\beta \quad (6)$$

This value has to be compared with the mean field approximation [16] (shown as dotted lines in figure 4) $\beta = 0.5$, $T_c = 8.1$ and with the expected value in the thermodynamical limit $\beta^\infty = 0.33$, $T_c^\infty = 6.16$. Once again we can see that the mean field approach fails in the phase transition region but becomes rather reasonable when the temperature increases. Moreover it is clear that the finite size of accessible nuclear systems does not imply a drastic deformation of thermodynamical parameters (the corresponding values for $L = 8$ are $T_c = 6.6$ and $\beta = 0.31$).

III. FRAGMENT PRODUCTION AND FINITE SIZE SCALING

The definition of clusters has been extensively discussed in the literature [10,16]. The first idea is to group all the connected sites (Ising clusters). However, it is known since a long time that this is not the proper way to define clusters in the lattice gas model since it does not fulfil the requirement that the correlation length should diverge at the critical point (see [10] for a discussion of the literature). Using renormalization group arguments, Coniglio and Klein proposed to combine the site percolation with an additional bond percolation algorithm using a temperature dependent bond breaking probability [22]:

$$p(T) = e^{-\epsilon/2T} \quad (7)$$

An alternative and almost equivalent way to define clusters [10] is to break the bond between two nucleons as soon as the kinetic energy of their relative motion $\tilde{p}_r^2/2\mu$ exceeds the binding energy ϵ . Remark that this bond breaking stage of the fragment definition can be understood as a secondary decay of the Ising Fragments.

With the above definition of clusters one expects that the thermodynamical critical point exhibits critical fragment size distributions and that in the proximity of the critical point the size distribution scales as [23,24]

$$\frac{dN}{dA}(A, T) = A^{-\tau} f(A^\sigma(T - T_c)) \quad (8)$$

where f is a universal scaling function and τ, σ are critical exponents. Two values of the universal function are of particular interest:

- its value at the origin $f(0)$ since it is associated with the critical point

$$\frac{dN}{dA}(A, T_c) = A^{-\tau} f(0) \quad (9)$$

- its maximum value $f(x_{\max}) = f_{\max}$. For each mass A it exists a temperature for which the production is maximum for a given temperature $T_{\max}(A) = T_c - x_{\max} A^{-\sigma}$

$$\left(\frac{dN}{dA} \right)_{\max}(A) = \frac{dN}{dA}(A, T_{\max}(A)) = A^{-\tau} f_{\max} \quad (10)$$

FIG. 5. Fragment production yield as a function of the temperature for different fragment sizes for a lattice size $L = 8$ at the critical density. The dashed line connects the maximum production probabilities.

FIG. 6. Evolution of the maximum production yield as a function of the fragment size (dots) and the corresponding power law fit (line) with the critical exponent $\tau = 2.2$ for a lattice size $L = 8$ at the critical density.

FIG. 7. Top part: Slope of the exponential decay (filled circles) and corresponding χ^2 (open circles) of the size distribution as a function of temperature for a lattice size $L = 8$ at the critical density. Dashed lines: τ_{max} extracted from the maximum production yields (see text) and corresponding possible critical temperatures. Bottom part: size distribution for 3 temperatures around the critical one.

FIG. 8. Temperature of the maximum production yield for each fragment as a function of the fragment size (dots) and the corresponding power law fit (line) with the critical exponent $\sigma = .6$ for a lattice size $L = 8$ at the critical density.

Therefore a possible method (method 1) to extract critical exponents consists in plotting the maximum production yield $(dN/dA)_{max}$ of a species of size A as a function of A as shown in figure 5; one can see from eq.(10) that this quantity should behave as a power law of exponent τ_{max} . This analysis is presented in figure 6. Then T_c can be obtained as the temperature at which the power law fit to the size distribution $dN/dA(A)$ gives an exponent $\tau = \tau_{max}$. On figure 7 one can see that in finite size systems two temperatures fulfil this condition. In order to decide which temperature should be associated with a critical behavior we have to extract the σ critical exponent and check the

existence of a universal scaling function f by plotting $A^\tau \frac{dN}{dA}(A, T)$ as a function of $A^\sigma (T - T_c)$ for all values of A and T . If all these different data points collapse on a single curve the validity of the finite size scaling will be demonstrated. If T_c is known, the σ exponent can be obtained by a power law fit of the maximum production temperature $T_{\max}(A)$ as a function of the fragment mass as illustrated in figure 8 for the lowest "critical" temperature defined in figure 7. The scaling analysis is shown in figure 9 for the different possible definitions of the critical temperature. Comparing fig.9c and 9d one can see that only the lowest critical temperature can be associated with a scaling behavior.

FIG. 9. Scaling function for clusters of size $4 < A < 30$ and temperature $2 < T < 20$ MeV obtained from eq.(8) with critical exponents extracted with methods 2 (a), 3 (b), and 1 (c,d) described in the text. In figure c (d) T_c is given by the lower (upper) bound of the critical temperature region of figure 7. The lattice size is $L = 8$ and the system is at the critical density.

Other alternative techniques have been proposed to extract the value of the τ exponent. One possibility [9] (method 2) is to plot the slope of $\ln(dN)$ versus $\ln(A)$ as a function of temperature; the minimum of this curve ($\tau_{\min}$) gives the exponent τ and the corresponding temperature is identified with T_c . Alternatively [16] (method 3) one can use the fact that at $T = T_c$ the χ^2 of the power law fit should be minimum, and the corresponding slope τ_χ of the fit gives the value of τ .

The three methods lead to approximately the same value of τ , as it is shown in figure 7; however the corresponding T_c (and consequently the value of σ) are quite different. The values found systematically lie inside the "critical region" (bounded by the dashed vertical lines of figure 7) obtained with the first method introduced above. This is not a smoothing effect due to the finite size of the system (a well defined critical point of an infinite system being replaced by a wider critical region in the finite one) but it is rather due to the intrinsic imprecision of the methods. As a matter of fact finite size scaling is violated by the use of method 2 (figure 9a) and is slightly better with method 1 than with method 3 (figures 9c,9b). Therefore, the critical temperature can be determined within 0.5 MeV even for a system of a typical nuclear size.

FIG. 10. Same as the upper part of figure 7 but at the subcritical density $\rho = \rho_0/3$.

FIG. 11. Evolution of the critical exponent τ with the density for a lattice size $L = 8$.

FIG. 12. Scaling function at various densities for clusters of size $4 < A < 30$ and temperature $2 < T < 20$ MeV obtained from eq.(8) with critical exponents extracted with method 1 described in the text.

FIG. 13. Fragment size distribution for a lattice size $L = 8$ for different densities and temperatures around the critical one: $T=9, 10.5$ and 12 MeV for $\rho = 0.97\rho_0$; $7.5, 8.5$ and 9.5 for $\rho = 0.75\rho_0$; $4.5, 5$ and 5.5 for $\rho = 0.25\rho_0$ and finally $T=4, 4.5$ and 5 MeV for $\rho = 0.16\rho_0$.

We have performed the same analysis at different freeze out densities. As an exemple the determination of τ and T_c at a subcritical density presented in figure 10 shows no qualitative difference from the study at $\rho = \rho_c$. Most amazingly, the value of τ extracted is almost independent of the density (figure 11) showing only a small increase over the wide range of densities. Moreover, the quality of finite size scaling at all densities is comparable to the one observed at the critical density as illustrated in figure 12. Finally, typical fragment size distributions around the respective density dependent critical temperatures exhibit a power law behavior as shown in fig. 13.

FIG. 14. Full line: coexistence line from thermodynamics (see section 1); Points: critical curve from fragment size distributions using method 1 for a cubic lattice of linear dimension $L = 6$. Star: thermodynamical critical point. The shaded surfaces show the χ^2 quality test of a power law fit.

FIG. 15. As figure 14, but for a lattice size $L = 8$.

Signals of criticality are thus clearly seen at supercritical densities as well as at subcritical densities. Figures 14 and 15 present the evolution of the critical temperature as a function of the density for two different lattice sizes. One can see that the critical temperature draws a line of criticality rising from low temperature at low density to high temperature at $\rho = \rho_0$. This critical line with increasing size of the system rapidly converges towards the thermodynamical critical point of the second order phase transition at the critical density but clearly dives into the coexistence region at low densities. From figures 14,15 one can also see that the line of criticality defined by method 1 is always close to the minimum χ^2 requirement, and the two criteria tend to converge by increasing the size of the

system.

It has already been observed that power laws in the size distribution are not characteristic of the critical point solely, but occur also at supercritical densities along the Kertész line [10] and at some subcritical densities at lower temperatures [17]. However the possibility to observe finite size scaling in small systems was never demonstrated. In this sense there is no contradiction between the scenario of fragmentation at low density inside the coexistence or the spinodal region (first order phase transition) and the observation of critical signals characteristic of a second order phase transition.

The physical origin of critical behavior at subcritical densities lies on the finite size of the system. As a matter of fact, in the subcritical regime power laws are connected to the disappearance of the infinite cluster on the coexistence line and not to the existence of critical fluctuations of all sizes. To clearly show this point we have studied the critical behavior by increasing the size of the system. As an example, the fragment distributions at temperatures close to the critical one at the subcritical density $\rho_0/4$ are shown in figure 16 for different lattice sizes. In large systems, a large fragment, reminiscent of the infinite percolating cluster of the thermodynamical limit, is always present in the coexistence region. Raising the temperature, when the infinite cluster disappears we observe an exponential fragment size distribution without ever passing through a power law. On the other side in small systems the "infinite" cluster gets a size comparable to the vapor fraction and populates the tail of the small fragment distribution before disappearing when the system crosses the coexistence line. Therefore, in small systems it exists a temperature for which the contribution of the largest fragment induces a behavior which resembles to a critical behavior. It is amazing to see how well this behavior fulfills the requirement of finite size scaling (see figure 12 above): this might indicate a more fundamental reason for the observation of criticality in finite systems undergoing a first order phase transition.

The results of the finite size scale analysis on the critical exponents and the critical temperatures as a function of the lattice size at a few selected densities are summarized in figure 17. The scaling functions obtained for different densities and lattice sizes are shown in figure 18. At subcritical densities increasing the size of the system one can see that the critical behavior is lost. The critical exponents deviate from the expected value of their universality class (see figs. 17a, 17b) and the scaling laws are violated as shown in fig. 18c. The situation is different at and above the critical density where the critical behaviors and the scaling remain valid when the size of the system is increased. Therefore, for large systems the critical line abruptly stops at the critical point and does not enter in the coexistence zone.

To conclude, it is interesting to see that at the critical density the critical parameters rapidly converge toward the thermodynamical limit. In particular, for typical nuclear sources ranging from $A \approx 50$ to $A \approx 300$ critical parameters depend only very slightly on the mass and relevant thermodynamical informations can be extracted in spite of finite size effects.

FIG. 16. Fragment size distributions for different temperatures around the critical one and different total sizes of the system $L=6, 14, 20$ and 50 at a density $\rho = \rho_0/4$.

FIG. 17. Critical parameters as a function of the linear size of the lattice (lower scale) or of the mass of the system (upper scale) at different freeze out densities.

FIG. 18. Scaling function at $\rho = \rho_0/4$ (left) and $\rho = \rho_c = \rho_0/2$ (right) for clusters of size ranging from $4 < A < 30$ and temperature $2 < T < 20$ obtained from eq.(8) with critical exponents extracted with method 1 described in the text. The upper (lower) part corresponds to a lattice size $L = 8$ ($L = 50$).

IV. CONCLUSIONS

In this paper we have looked for relevant signals of the nuclear liquid-gas phase transition within the Lattice Gas model. An exact calculation of the canonical partition function has allowed us to define the critical temperature even for very small systems. We have demonstrated that this variable is only very slightly perturbed by finite size effects.

We have shown that in finite systems, in a statistical ensemble with conserved quantities such as here the particle number or the volume, the associated equation of state presents an anomalous back-bending in the first order phase transition region. In particular we have shown that volume and particle number conservation imply that the compressibility becomes negative as well as the variation of the chemical potential as a function of the particle number. This signature is analogous to the proposed presence of negative heat capacities in first order phase transitions in the microcanonical ensemble [21]. When energy is a conserved quantity the associated thermodynamical potential (*i.e.* the entropy) presents a region of abnormal convexity due to the surface energy between the liquid and the vapor in the mixed phase, so that its first derivative respect to the energy (*i.e.* the temperature) presents the characteristic back-bending. This can be generalized to any conserved extensive variable: as a function of this quantity the thermodynamical potential presents a region of abnormal convexity so that the conjugated intensive variable (*i.e.* the derivative of the potential respect to the conserved quantity) shows a back-bending.

The critical temperature is also accessible from the fragment production yield, as well as the universal critical exponents of the transition. A full agreement between thermodynamical and fragment variables is obtained if the parameters are extracted from a systematic analysis of size distributions at different temperatures. In this case finite size scaling is remarkably verified over a wide range of sizes and temperatures at supercritical [10] as well as subcritical densities. At variance with the supercritical regime, critical behavior at subcritical densities is a side effect of the finite size of the system which disappears in the infinite limit. However, the dependence with mass being smooth, the observation of critical signals from multifragmenting systems at low densities can provide useful informations on the characteristics and the parameters of the transition.

For a realistic application to fragmentation data however many important physical ingredients have to be added to the model. Surface effects have to be studied by replacing periodic boundary conditions with a confining Lagrange potential [25], the persistence of signals must be verified respect to the Coulomb interaction, and the possible influence on the results of the chosen thermodynamical ensemble (microcanonical versus canonical) has to be checked [26].

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