Phase transition with an isospin dependent lattice gas model

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Abstract

The nuclear liquid-gas phase transition is studied within an isospin dependent Lattice Gas Model in the canonical ensemble.

Finite size effects on thermodynamical variables 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 behaviour 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 [1] (Kertész line) as well as subcritical densities.

For isospin asymmetric systems it is shown that, besides the modification of the critical temperature, isotopic distributions can provide an extra observable to identify and characterize the transition.

1 Introduction

One of the most important challenge of heavy ion physics at intermediate bombarding energies is the identification and characterization of the nuclear liquid-gas phase transition. With the increasing availability of quasi complete and exclusive data on the deexcitation of well identified single nuclear sources in heavy ion reactions [2], different indirect evidences of such a transition are rapidly accumulating. On one side, the sudden opening of the multifragmentation [3, 4] and vaporization [5] channels can be interpreted as the signature of the boundaries of phase mixture [6, 7]. This is reinforced by the fact that at the corresponding excitation energy values the caloric curve [8] shows a structure similar to a first order phase transition in the framework of statistical equilibrium models [9, 7]. On the other side, the observation of critical exponents like power laws in the charge distribution of the multifragmenting system [10] can be interpreted as an evidence of the transition. A problem of interpretation however arises since critical signals are expected in a single specific thermodynamical point, the critical point, and not in the middle of the coexistence region, as the behaviour of the caloric curve would suggest. Campi and Krivine have recently pointed out [1] that a critical behaviour in the clustering properties of a multifragmenting system can be observed also at supercritical densities along the Kertész line [11] thus suggesting the picture of an "early" multifragmentation. This idea is supported by molecular dynamics simulations where however thermodynamical equilibrium is clearly not reached [12]. Conversely statistical equilibrium models, extremely successful in reproducing multifragmentation patterns, systematically suggest low freeze out densities [13, 7]. Therefore 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 behaviour 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.

Another difficulty arises from the fact that theoretical calculations of the phase transition with finite systems are usually performed [1, 14, 15] in the isospin symmetric case. It is well known that in a system with two conserved charges (baryon number and isospin, in the nuclear case) the nature itself of the liquid-gas phase transition is modified: the transition is continuous, phase separation is driven by isovector as well as isoscalar instabilities, the value of critical parameters is modified [16, 17]. Since most of the multifragmenting systems produced by heavy ion collisions are far from being isospin symmetric, the comparison of experimental charge distributions with theoretical size distributions can be misleading. In this work we shall show that if one drops out the mean field approximation, the critical parameters of the phase transition depend only very slightly on the asymmetry and this dependence is probably non detectable for experimentally available N/Z ratios.

The plan of the paper is as follows: in the first section the isospin dependent Lattice Gas model will be introduced and its thermodynamics calculated from an exact evaluation of the canonical partition sum; section 2 will be devoted to cluster observables at subcritical and supercritical densities with a special emphasis on finite size distorsions of the critical parameters; some first results on isospin asymmetric systems will be presented in section 3, and finally section 4 will be devoted to conclusions and outlooks.

2 Thermodynamics of the Lattice Gas Model

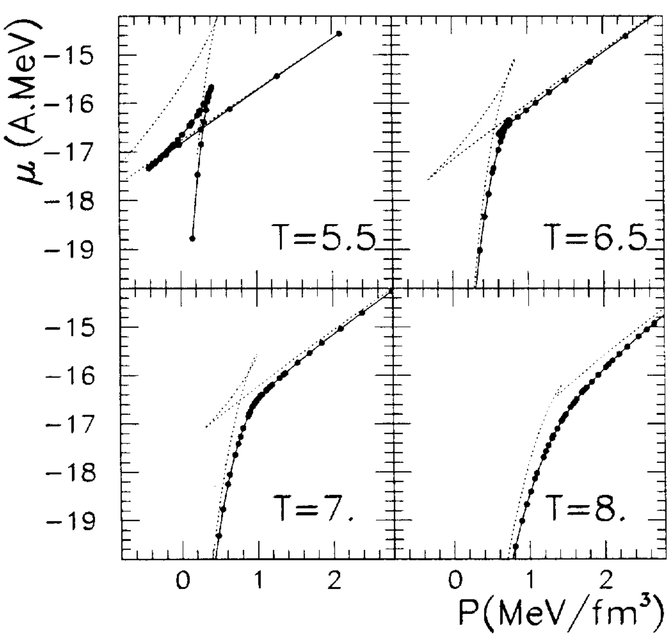

Figure 1: Chemical potential as a function of pressure at different temperatures for a cubic lattice of size $L = 6$ calculated from the exact partition sum (circles) and with the mean field approximation (dotted line).

The Lattice Gas Model of Lee and Yang [18], where the grancanonical 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, has successfully described the liquid-gas phase transition for atomic systems. This same model has already been applied to nuclear physics for isospin symmetric systems in the grancanonical ensemble [15, 1], with an approximate sampling [19] of the canonical ensemble [14], and for isospin asymmetric infinite nuclear matter in the mean field approximation [17]. 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 $\tau = 1(-1)$ for a proton(neutron). Particles occupying nearest neighbouring sites interact with an energy ϵ_{τ_i,τ_j}. The hamiltonian is given by

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} |\tau_i| + \sum_{i \neq j} \epsilon_{\tau_i,\tau_j} \tau_i \tau_j \tag{1}$$

The coupling constants ϵ_{τ_i,τ_j} are fixed such as to reproduce the volume and symmetry part of the liquid drop model parametrization, $\epsilon_{1,1} = \epsilon_{-1,-1} \equiv \epsilon_d = 0.$ MeV, $\epsilon_{1,-1} \equiv \epsilon_s = 5.5$ MeV. 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 size L, a number of particles $A = N + Z$ (or equivalently a density $\rho/\rho_0 = A/L^3$) and a temperature T. Statistical averages are taken over events obtained with a standard Metropolis sampling of the lattice in the canonical ensemble. In this section and in the following one we shall limit our analysis to isospin symmetric systems $N = Z = A/2$.

The thermodynamics of the model is calculated from a direct evaluation of the partition sum Z via an iterative procedure. At a temperature T, the occupation probability of an energy state E as given by the Metropolis algorithm is

$$P(E) = \frac{1}{Z_T} W(E) e^{-E/T} \tag{2}$$

where $W(E)$ is the degeneracy of the state. We have checked that an inversion of eq.(2) leads to an a posteriori estimation of the temperature differing from the input one of at most 0.1 MeV for the tails of the probability distributions [20]. From the comparison of the occupation probabilities at two different temperatures T_1, T_2 one then has

$$Z_1 = Z_2 \frac{1}{N_E} \sum_{E}^{N_E} \frac{P_1(E)}{P_2(E)} e^{-E\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} \tag{3}$$

which can be solved iteratively with an initial normalization to the infinite temperature limit where the partition sum is analytical. Once the partition sum is known, all thermodynamical quantities can be computed from the standard statistical definitions in the canonical ensemble. As an exemple, in figure 1 a few isothermes 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 $A = 210$). Even for such small systems, a very clean liquid and gas branch is seen for temperatures up to about 6.5 MeV. Since the crossing point of the two branches represents the coexistence boundary, the coexistence line can be evaluated very precisely from figure 1 leading to a critical temperature $T_c = 6.7$ MeV and a critical exponent for the temperature dependence of the order parameter $\beta = 0.31$. This value has to be compared with the mean field approximation [14] (shown as dotted line in figure 1) $\beta = 0.5, T_c = 8.1$ and with the expected value in the thermodynamical limit $\beta^{\infty} = 0.33, T_c^{\infty} = 6.16$. 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 $\beta = 0.31$). However the speed of convergence towards the thermodynamical limit strongly depends on the observable studied [1], therefore the question remains wheather critical exponents are accessible through measurable quantities, *i.e.* observables of fragments not necessarily produced at the critical density. This question is addressed in the next section.

3 Finite Size Scaling

The definition of clusters in the lattice gas combines a site and bond percolation algorithm: two particles are bonded if they *a)* occupy neighbour sites and *b)* the kinetic energy of their relative motion $\vec{p}_r^2/2\mu$ does not exceed the binding energy ϵ_{τ_i,τ_j}. For details about the definition of clusters we report the reader to refs.[1, 14]. Remark that condition *b)* implies that the fragments produced are relatively cold, *i.e.* their thermal excitation energy is lower than the threshold of particle emission; their finite excitation energy is given by their shape rather than by internal degrees of freedom. This definition of clusters guarantees that the thermodynamical critical point exhibits critical fragment size distributions and that in the proximity of the

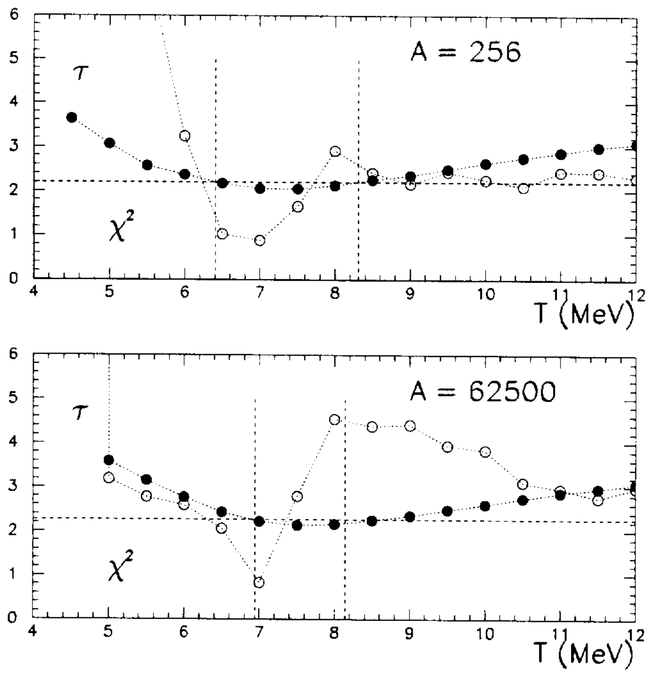

Figure 2: Slope (filled circles) and corresponding χ^2 (open circles) of the size distribution as a function of temperature for two different system sizes at the critical density. Dashed lines: τ_{max} extracted from the maximum production yields (see text) and corresponding critical temperature interval.

critical point the size distribution scales as [21]

$$\frac{dN}{dA}(A,T) = A^{-\tau} f(A^{\sigma}(T - T_c)) \tag{4}$$

where f is a universal scaling function and τ, σ are critical exponents.

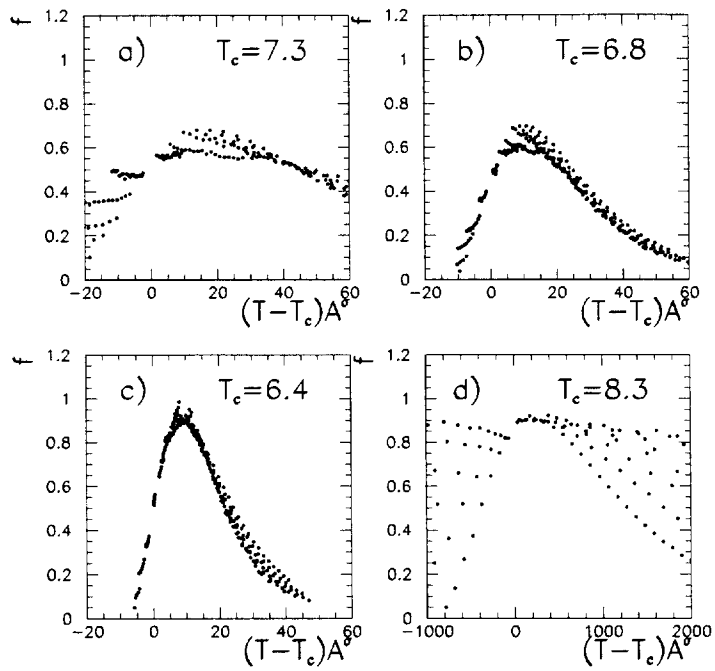

Figure 3: Scaling function for clusters of size ranging from 4<A<30 and temperature 2<T<20 obtained from eq.(4) with critical exponents extracted with methods 1 (a), 2 (b), and 3 (c,d) described in the text. In figure 3c (d) T_c is given by the lower (upper) bound of the critical temperature region of figure 2.

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 [1] and at some subcritical densities at lower temperatures [14]. In order to better quantify this statement and study the distorsions due to finite size effects we have checked the validity of eq.(4) for different densities and lattice sizes. Different tecniques can be proposed to extract the value of the τ exponent. A first possibility[10] (method 1) is to plot the slope of $ln(dN)$ versus $ln(A)$ as a function of temperature; the minimum of this curve (τ_{min}) gives the exponent τ

and the corresponding temperature is identified with T_c. Alternatively[14] (method 2) 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. Another method (method 3) consists in plotting the maximum production yield $dN_{max}(A)$ of a species of size A as a function of A; one can see from eq.(4) that this quantity should behave as a power law of exponent τ_{max}. 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 $\tau = \tau_{max}$.

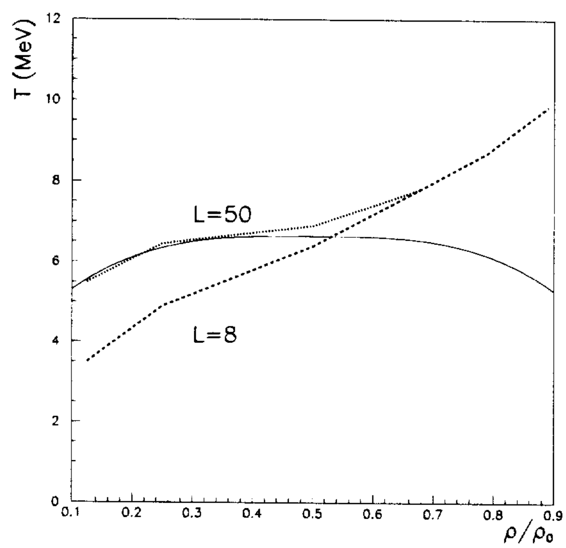

Figure 4: Full line: coexistence line from thermodynamics (see section 1); dashed line: critical curve from fragment size distributions for a cubic lattice of linear dimension $L = 8$; dotted line: as the dashed line, but $L = 50$

These three methods lead to approximately the same value of τ, as it is shown in figure 2; 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 2) obtained with the third 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 clearly violated by the use of method 1 (figure

3) and the critical temperature can be determined within 0.5 MeV even for a system of a typical nuclear size.

The result of the same analysis at different freeze out densities and lattice sizes is shown in figures 4 and 5. For all data points presented the quality of finite size scaling is comparable to the one of figure 3c.

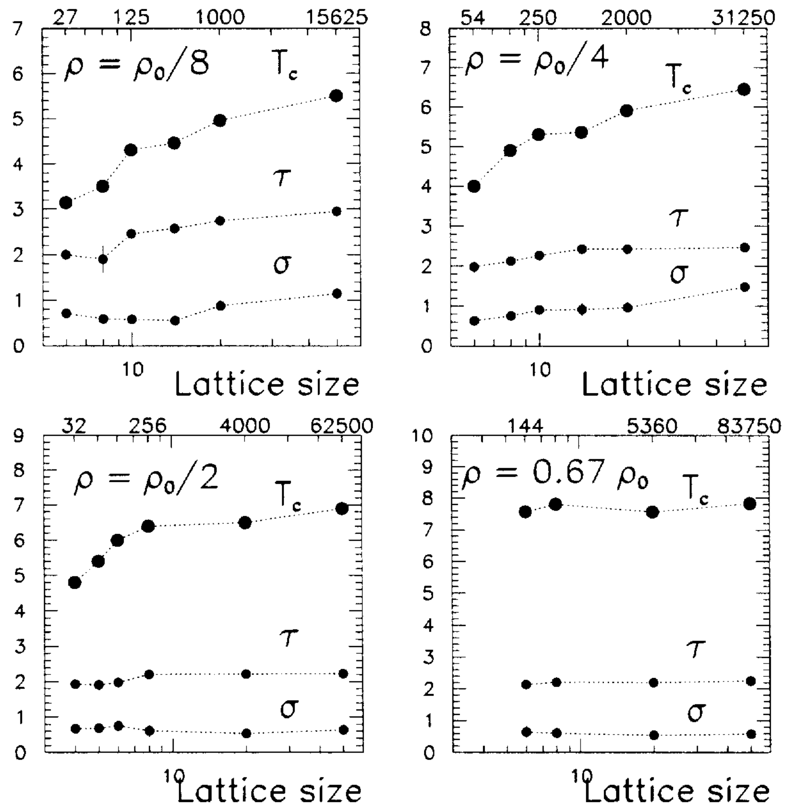

Figure 5: Critical parameters as a function of the linear size of the lattice (lower scale) or of the mass of the system (upper scale) at different freeze out densities.

A critical behaviour is clearly seen at supercritical densities as well as at sub-critical densities (dashed line in figure 4). 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. Moreover, if the critical temperature is extracted from data by verifying that finite size scaling is respected, critical parameters depend only very slightly on the mass for typical nuclear sources ranging from $A \approx 50$ to $A \approx 300$ and relevant thermodynamical informations can be extracted in spite of finite size effects (figure 5). On the other hand, the physical origin of critical behaviour at subcritical densities lies on the finite size of the system. In the (experimentally inaccessible) limit of very large systems, in the subcritical regime power laws are connected to the disappearence of the infinite cluster on the coexistence line (dotted line in figure 4) and not to the existence of critical fluctuations of all sizes, as it can be seen by directly looking at the fragment size distribution and as it is shown by the fact that the critical exponents deviate from the expected value of their universality class (figure 5a, 5b).

4 Isospin Asymmetric Systems

The results presented in the preceding section have been obtained by assuming an isospin symmetric system, $I = (N - Z)/A = 0$. Even in this case, unrealistic for the experimentally available fragmentation data concerning heavy sources, of course the measurable quantity is the charge rather than the mass distribution. However we have verified that critical parameters extracted from finite size scaling of the charge distribution are the same as the ones presented in section 2, and this keeps being true for isospin asymmetric systems.

For an $I \neq 0$ system in the presence of a symmetry energy, *i.e.* different coupling for isoscalar and isovector pairs (see section 1) the nature itself of the phase transition is modified [16]. Just to mention a few well known features from macroscopic thermodynamics with two conserved charges, the coexistence curve is transformed into a surface which implies that the transition is second order instead of first order; phase separation is triggered by isovector as well as isoscalar instabilities; the isotopic composition of the liquid and gas phase differ.

As a first application of the model to isospin asymmetric systems we have studied the asymmetry dependence of the critical parameters at the critical density. The results are displayed in figure 6 for a system of mass $A = 256$. The critical temperature has been obtained with the methods 2 and 3 of section 2. One can see that the isospin dependence of the parameters is less important than in mean field

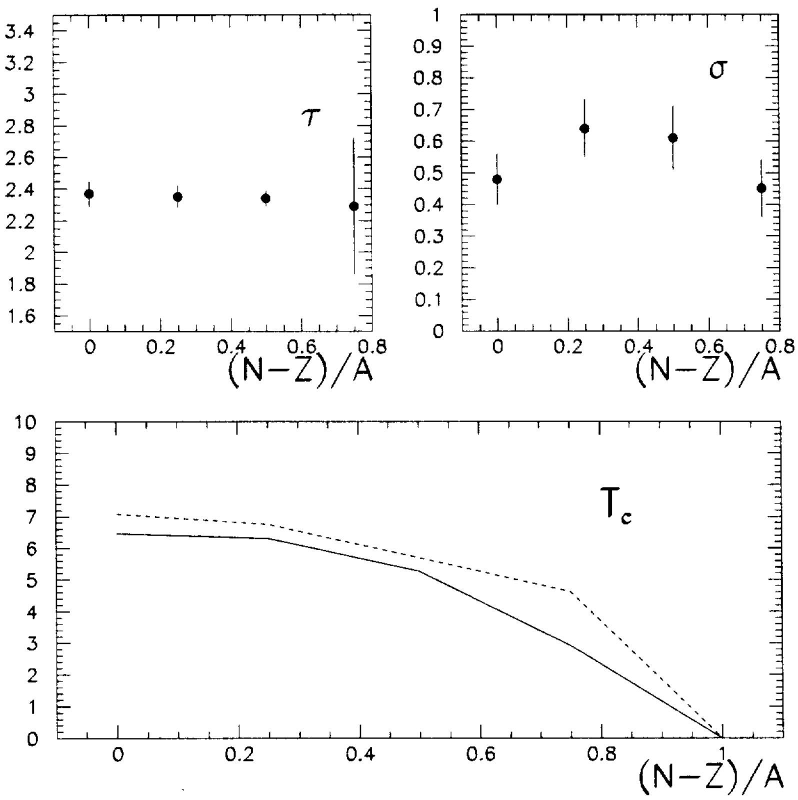

Figure 6: Critical parameters as a function of the isospin asymmetry of the system for a 8x8x8 cubic lattice at critical density. Full (dashed) line: critical temperature obtained from method 3(2) of section 2.

calculations [17]: even for very exotic nuclei and extremely precise measurements the asymmetry dependence of the critical temperature would be barely visible. On the other hand, this result implies that fragmentation data obtained with different systems can be analysed together for a better determination of critical parameters.

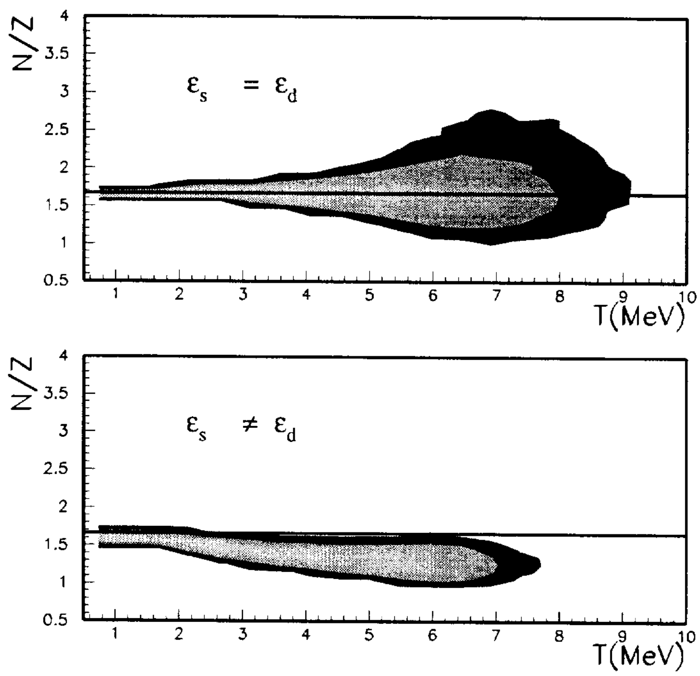

Figure 7: Ratio between neutron N and proton Z number of produced clusters with $N > 40$ as a function of temperature for a fragmenting system with $N = 96$ and $Z = 64$. Upper part: interaction energy $\epsilon_s = \epsilon_d = -5.5$ MeV. Lower part: interaction energy $\epsilon_s = -5.5$, $\epsilon_d = 0.$ MeV.

Isospin can be not only viewed as a degree of freedom but also as an observable: we can hope that next generation detectors for multifragmentation, measuring masses as well as charges of the reaction products, will supply us with a richer two dimensional information reducing the ambiguities of the existing signals for the phase transition. One intriguing possibility is the expectation that for an $I \neq 0$ system inside the coexistence region the vapour phase should be more asymmetric than the liquid phase [16].

The isotopic composition of heavy fragments (*i.e.* of the liquid fraction) is

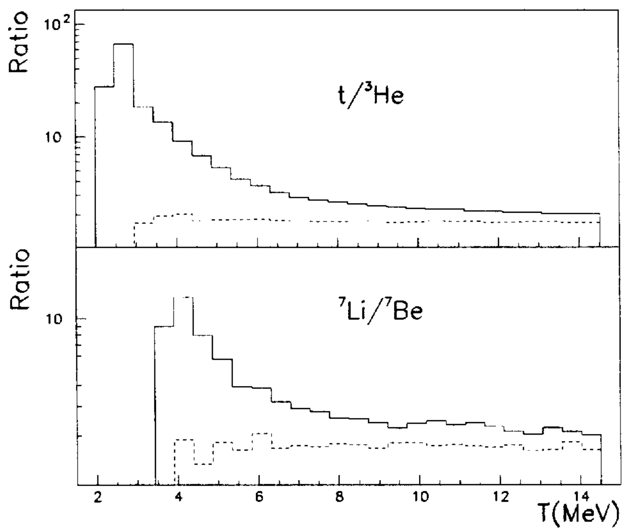

Figure 8: Relative production yield of light isobars as a function of temperature for a fragmenting system with $N = 96$ and $Z = 64$. Full lines: interaction energy $\epsilon_s = -5.5$, $\epsilon_d = 0.$ MeV. Dashed lines: interaction energy $\epsilon_s = \epsilon_d = -5.5$ MeV.

displayed in figure 7 as a function of temperature for a system with $I = 0.25$. If the interaction energy is assumed independent of isospin (upper part), at all temperatures the distribution is centered on the N/Z of the source. This effect is purely combinatorial and the broadening of the distribution approaching the critical temperature reflects the maximum of fluctuations at the critical point. If symmetry energy is taken into account (lower part), the distribution is centered on a value the closer to stability ($N/Z = 1$ in the model, independent on the mass) the higher is the temperature. The large fluctuations at the critical point are washed out by secondary decay and one can wonder if the observed proton richness (relative to the isotopic composition of the source) of the fragments does not trivially reflect secondary decay. However remark that the distribution is shifted respect to the combinatorial expectation even at very low temperatures, where secondary decay is negligeable. Still since more symmetric means also closer to the stability valley, it may be difficult to disentangle the two effects.

A clearer signal of phase coexistence with two conserved charges can be obtained from the analysis of the vapor isotopic composition. Figure 8 shows the ratio between the production yields of different light isobars as a function of temperature with and without isospin dependent interactions. Only at supercritical temperatures the combinatorial value $R = N/Z = 2.1$ is achieved, and the trend is opposite respect to the expected effect of secondary decay.

5 Conclusions

In this contribution we have looked for relevant signals of the nuclear liquid-gas phase transition within an isospin dependent Lattice Gas model. An exact calculation of the canonical partition function has allowed us to compute the critical temperature within 0.1 MeV. We have shown that this variable is only very slightly perturbed by finite size effects. 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 [1] as well as subcritical densities. At variance with the supercritical regime, critical behaviour 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. The fact that the critical behaviour is not confined to a single thermodynamical point, but can be seen along a whole critical line implies that the temperature and density of the multifragmenting source have to be inferred at the same time from experimental data. An interesting observable to better localize the system in the $T - \rho$ plane is given by the isotopic composition of the fragments. We have shown that in the coexistence region the vapor fraction is more asymmetric than the liquid fraction and the signal is not washed out by secondary decay. 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, 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 [20].

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