GANIL

GRAND ACCELERATEUR NATIONAL D'IONS LOURDS - CAEN
LABORATOIRE COMMUN IN2P3 (CNRS) - D.S.M. (CEA)

PHASE TRANSITION IN FINITE SYSTEMS

Ph.Chomaz[1] and V.Duflot[1,2] and F.Gulminelli[2]
(1) GANIL (DSM-CEA/IN2P3-CNRS), B.P.5027, F-14021 Caen cedex, France
(2) LPC Caen, (IN2P3-CNRS/ISMRA et Universite), F-14050 Caen cedex, France

XXXVIIIth Winter Meeting on Nuclear Physics
Bormio, Italy, 24-29 January 2000

GANIL P 00 13

PHASE TRANSITION IN FINITE SYSTEMS

Ph.Chomaz[1] and V.Duflot[1,2] and F.Gulminelli[2]
(1) GANIL (DSM-CEA/IN2P3-CNRS), B.P.5027, F-14021 Caen cedex, France
(2) LPC Caen, (IN2P3-CNRS/ISMRA et Universite), F-14050 Caen cedex, France

Abstract

The general problem of the definition of a phase transition without employing the thermodynamical limit is addressed. Different necessary conditions are considered and illustrated with examples from different nuclear and general physics phenomenologies.

1 Introduction

Phase transitions are universal properties of matter in interaction. They have been widely studied in the thermodynamical limit of infinite systems. However, in many physical situations this limit cannot be accessed and so phase transitions should be reconsidered from a more general point of view. This is for example the case of matter under long range forces like gravitation[1]. Even if these self gravitating systems are very large they cannot be considered as infinite because of the non saturating nature of the force. Other cases are provided by microscopic or mesoscopic systems built out of matter which is known to present phase transitions. Metallic clusters can melt before being vaporized[2]. Quantum fluid may undergo Bose condensation or super-fluid phase transition[3]. Dense hadronic matter should merge in a quark and gluon plasma phase[4] while nuclei are expected to exhibit a liquid -gas phase transition[5]. For all these systems the experimental issue is how to characterize a possible phase transition in a finite system. In this paper we will present new results and ideas about the theoretical definition of phase transitions in finite systems as well as experimental observables which may allow their identification.

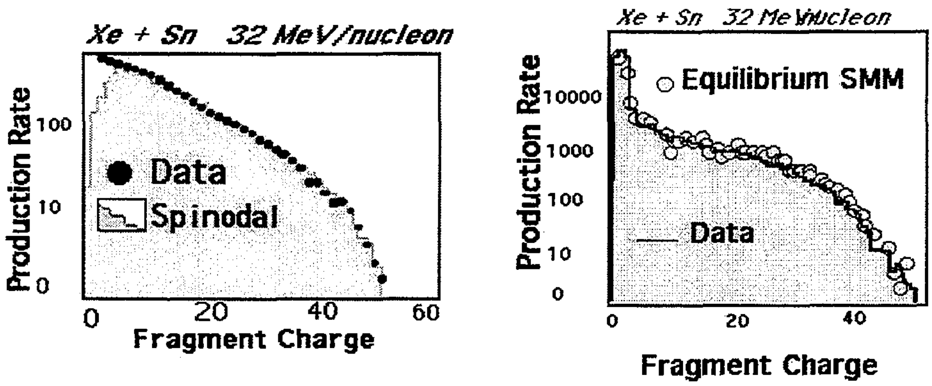

Figure 1: Charge distribution of central events measured for the Xe+Sn reaction at 32 Mev/u by the INDRA collaboration compared to a dynamical spinodal decomposition (left) and a statistical partition at freeze-out (right).

2 Dynamics versus thermodynamics

One of the most important challenges of heavy ion physics at intermediate bombarding energies is the identification and characterization of the nuclear equation of states. At high density and temperature the matter should be a plasma of quarks and gluons. Cooling down or being decompressed hadrons should appear. In the low temperature and density region one expects a transition from a Fermi liquid to a gas. Different events are expected to explore the phase diagram. In particular, heavy ion reactions may allow to reach the liquid-gas coexistence zone.

The main problem concerning the possibility to observe a phase transition in the reactions is the fact that collisions are dynamical processes between finite systems which means that collisions are not directly related to the static properties of infinite matter at equilibrium. In the recent years a lot of work has been devoted to the theoretical description of heavy ion collisions. In particular, stochastic mean-field approaches have been able to describe the dynamics of a phase transition in the spinodal region where diluted matter is unstable against small density fluctuations[6]. These approaches are now fully operational and have been used to explain the data obtained in most central events of heavy ion reactions around the Fermi energy. An example

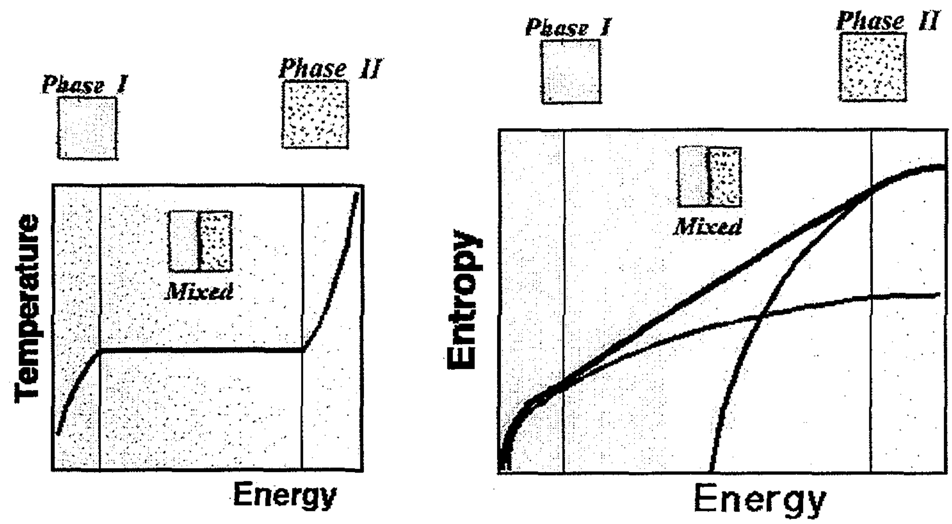

Figure 2: Schematic caloric curve of a system at the thermodynamical limit undergoing a liquid-gas phase transition (left). The right part corresponds to the associated entropy.

of the quality of the reproduction of data is shown in the left part of Figure 1. Calculations of dynamical phase transitions are able to reproduce fragment partitions and also kinetic energy spectra [7]. The puzzling observation is that the main features of the results of dynamical simulations can be fitted using statistical models. In fact statistical approaches assuming equilibrium are known to do an excellent job in reproducing the data as shown in the right part of Figure 1.[1] This tends to demonstrate that spinodal decomposition is a fast way to reach an equilibrium in the sense that it populates the whole phase space. In this sense spinodal decomposition may be compatible with a freeze-out picture even if in dynamical calculations it is difficult to spot a well defined time associated with fragment production. In other words, a dynamical phase transition can lead to an ensemble of events which almost uniformly populate a phase space associated with a freeze-out configuration: if this is true the statistical properties of this configuration and hence the

[1]Only recently considering high order correlations it has been possible to show that a fossil signal of the dynamics of the phase transition was present in the data[8].

equation of state associated with it, can be experimentally accessed. In the rest of this paper we will concentrate on the properties of a statistical ensemble of events without discussing the possible ways to produce it. In particular we would like to study genuine properties of phase transitions in finite systems.

3 From infinite to finite systems

Phase transitions are well defined in infinite systems. They can be identified by non analytical behaviours in thermostatistical potentials. When the first derivative of the potential adapted to the physical situation under study is discontinuous, we are facing a first oder phase transition; conversely when the second derivative is diverging the phase transition is second order. Let us consider a typical first order phase transition such as the liquid-gas phase transition at constant pressure. Bringing more energy in the system the liquid temperature continuously increase up to the transition point were the temperature remains constant until all the liquid is transformed into vapor. The energy cost of this transformation is the latent heat. Then the temperature rises at the typical rate of the gas, as schematically represented in the left part of Figure 2. This behavior comes from a specific anomaly of the entropy of the system. Indeed, in the phase transition region the system can maximize its entropy by mixing a linear combination of the liquid and gas phase. The system should be at the thermodynamical limit meaning that energies and entropies are additive. The result, displayed in the right part of Figure 2, is that the entropy presents a linear behavior in the phase transition region. This corresponds to the well-known Maxwell construction. Since the temperature is the inverse of the energy derivative of the entropy

$$T^{-1} = \partial_E S \tag{1}$$

the temperature is constant during the phase transition.

The entropy is the best concept to discuss phase transitions in finite systems. Indeed, it is directly related to the density of states W of the system through the relation

$$S = k \log W \tag{2}$$

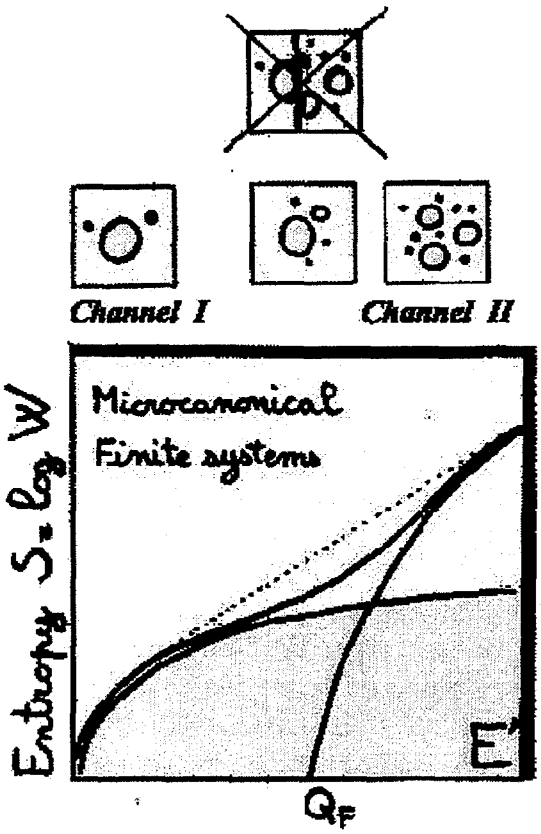

Figure 3: The entropy of a state of a finite system which can exist in two types of states. Since the total number of states is the sum over the different types the density of states is additive and not the entropy which is the logarithm of it.

In this context a phase transition can be seen as an anomaly in the evolution of the density of states. In particular, a new phase can be seen as the opening of a new type of states. Indeed, let us imagine that we can sort the states of a system in two classes differentiated according to a given observable.In the liquid-gas case this observable can be for example the fragment multiplicity or the size of the largest cluster. For each energy bin, the total number of states is then the sum of the states in the first channel and the states in the second one. Since the total entropy is the logarithm of this sum, the Maxwell construction between the two phases is not recovered as shown in Figure 3. This is due to the finite size of the system. Indeed, the Maxwell construction would correspond to consider partitions which are linear combinations of the two channels. At the thermodynamical limit of an infinite system, their entropy will be simply the weighted sum of each channel entropy as well as their energy would be the weighted sum of their respective energies. However, in a finite system the energy of a mixed event cannot be the sum of the two partial energies because of the presence of a surface term. The same reasoning holds for the entropy which should contain a surface contribution. This results in a depletion in the number of states in the phase transition region and leads to a convex intruder in the system entropy (see Figure 3).

The convex intruder gives a characteristic back-bending in the caloric curve and hence produces negative heat capacities[9]. The presence of such anomalies in the entropy has been proposed to be the generic definition of phase transitions in finite systems[10, 11]. In this respect the microcanonical ensemble plays an essential role since the energy and entropy are its natural state variables and thermodynamical potentials. One can generalize such a definition to the presence of anomalies in any thermostatistical potential, i.e. in the logarithm of any partition sum [11]. In such a case at least one conserved quantity should be controlled and considered as an extensive[2] state variable in order to allow a sampling of partitions in the coexistence zone. Then anomalous convexities can be considered as a signal of phase transitions. The associated equation of states, i.e. the intensive conjugate of the controlled extensive variable which is computed from the derivative of the considered thermodynamical potential, will present a characteristic

[2]We define here an extensive variable in its weak sense of a conserved quantity which is defined for any individual statistical realization of the system. An extensive variable has not necessarily to grow linearly with the size of the system. This will however be the case if the system has a thermodynamical limit.

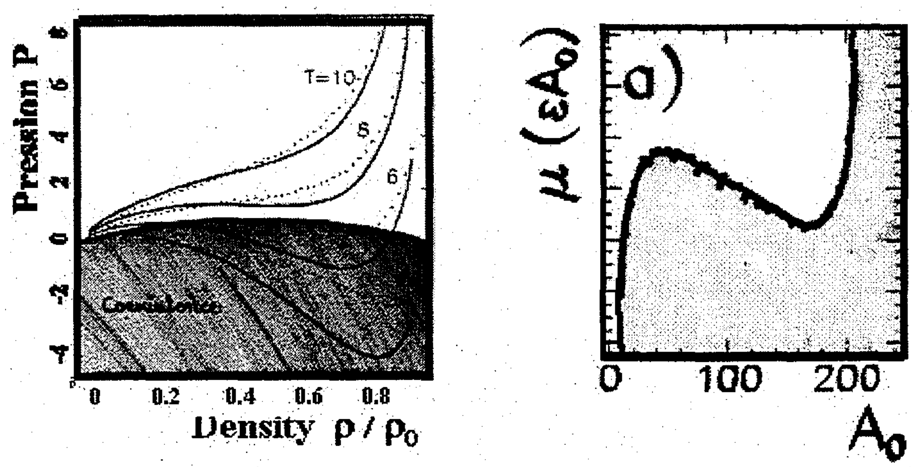

Figure 4: Back-bending behavior in subcritical isotherms in the pressure versus density (upper part) and chemical potential versus mass (lower part) plane for the canonical Lattice-gas model.

back-bending behavior in the case of a first order phase transition. Two examples calculated in the framework of the Lattice-gas model are presented in Figure 4[12, 13]. If the volume of a fluid is used as a sorting variable, the pressure presents a back-bending behavior as a function of the density. Then the compressibility shows a negative branch surrounded by two divergences. Similarly if the number of particles is controlled, a back-bending of the chemical potential will be obtained. It should be noticed that because of the correspondence between the Ising and Lattice-gas model this back-bending is also a back-bending of the magnetic field as a function of the magnetization. This means that the magnetic susceptibility of a finite system in a first order phase transition presents two divergences and a negative branch. Finally, when energy is used as a sorting variable, a back-bending is seen in the caloric curve corresponding to a negative branch for the heat capacity[9, 12, 14].

4 A simple model for a state change

In order to clarify the physics involved in the back-bending of the caloric curve let us consider the simplest possible case : the state change from one dimer to two monomers. This is a system with only two particles in a box which can exist in two states :

- a bound state bounded by an energy $-e$, this dimer can move in the box of volume V so that its density of states is $W_1(E) \propto V\sqrt{E+e}$
- a state with two free monomers which corresponds to a free density of states $W_1(E) \propto V^2E^2$

Then the total density of states is $W(E) = W_1(E)+W_2(E)$. For negative energies from $-e$ to 0 the system can exist only as a dimer while at 0 a new channel opens in competition with the first one (see Figure 5). Depending upon the volume the entropy $S(E) = \log W(E)$ may present an anomaly and a convex intruder as shown in the same Figure 5.

Having computed the entropy we can derive the microcanonical caloric curve using equation (1) above. The result is presented in Figure 6 as a function of the density. At low density the caloric curve presents a back-bending characteristic of a first order transition of state. Indeed the heat capacity there presents two divergences and a negative branch. The negative heat capacity region corresponds to a transition region in the state diagram. At low densities (large volumes) the transition from one dimer to two monomers proceeds via an anomalous region.

The important question now is the link between the observed anomaly in a small system and the possible phase transition which is rigorously defined only in an infinite system. The observed anomaly is indeed related to a transition between two types of states but this is not sufficient to claim that it is associated with a phase transition. As a matter of fact, this model can be extended to a larger and eventually an infinite number of constituents in two different ways:

- On one hand we can allow many body correlations connecting an arbitrary number of particles together to form a polymer or a liquid-like phase. In such a case when we go to the thermodynamical limit the transition observed in the two body system goes towards a phase transition.

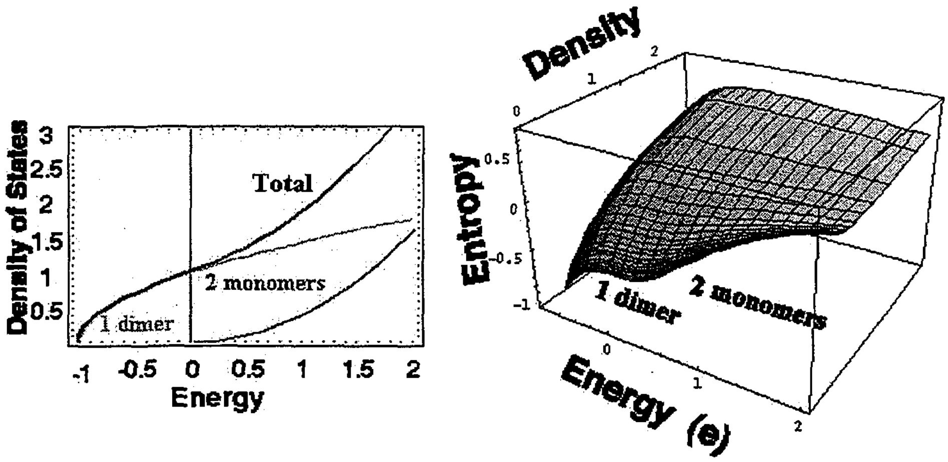

Figure 5: Illustration of a classical two-state two-body thermodynamics. Left side: density of one body and two body states, and total density of states as a function of the system energy. Right side: entropy as a function of density and energy.

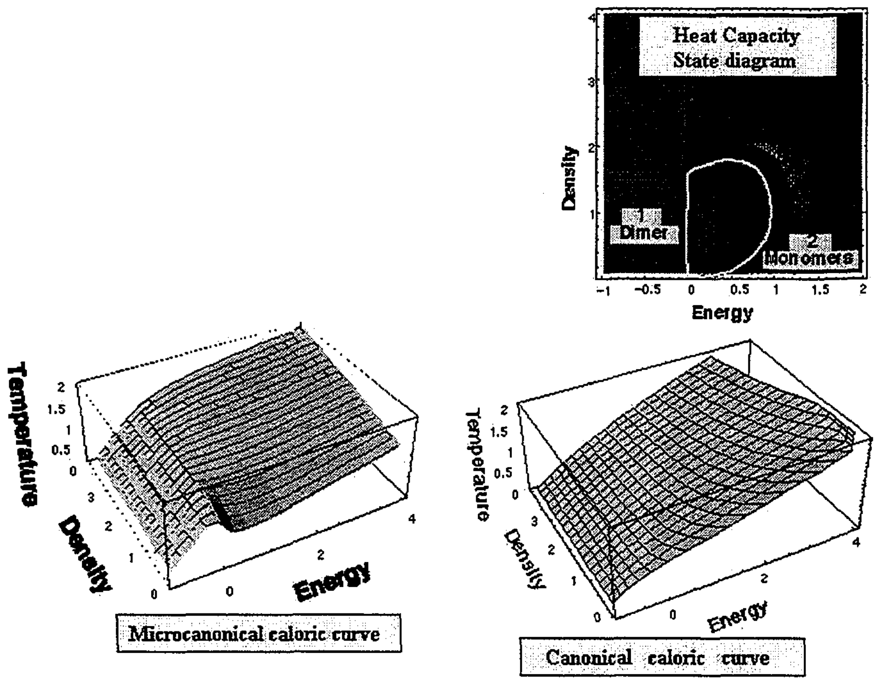

Figure 6: Bottom left: the microcanonical caloric curve of the one-dimer/two-monomers model presenting a back-bending. Top: the associated heat capacity with a negative region at low density. Bottom right: the caloric curve computed in the canonical ensemble.

- In a second model only two body bindings (dimers) can be allowed even for a many body system. Then the situation is analogous to ionization which is known to only present a cross-over from a dimer gas to a plasma without going through a phase transition region.

Therefore it is clear that the presence of a back-bending in an equation of state is not sufficient condition to claim that we observe the scar of a phase transition. Other arguments should be presented.

First, the canonical case should be studied because in the infinite system canonical and microcanonical calculations should give the same thermodynamics in the phase space regions which are accessible to both approaches. Even in a finite system the canonical equation of states cannot present back-bending regions in the temperature versus energy plane since the temperature is the controlled parameter. However, if the microcanonical back-bending corresponds to a phase transition, the canonical caloric curve should also present a slope change between two different regimes which goes towards a plateau as the number of particles is increased. For our model it is shown in Figure 6 that this is not the case in agreement with the idea that the dissociation of a dimer gas into a monomer "plasma" is not a phase transition.

5 State changes versus phase transitions

This is in fact an old discussion in physics. For example the link between the back-bendings of rotational bands and a superfluid phase transition has been extensively discussed in the literature[15]. However, it has been shown that the back-bending phenomenon in this case corresponds to a single particle effect rather than to a collective transition.

The same discussion holds for the detailed study of the level density which is expected to present fluctuations when measured with enough energy resolution. A very interesting and precise study of the level density at low spin of heavy nuclei between 0 and 10 MeV of total excitation energy is reported in ref.[16]. Many fluctuations are seen related to the threshold effect for the onset of new degrees of freedom (breaking of nucleon pairs and quenching of the pair correlations). These fluctuations induce oscillations of the microcanonical temperature but again they do not correspond to a phase transition because they are associated to single particle effects and not to collective macroscopic changes of the involved state structure. Once again this can be easily understood by looking at the canonical case in which these small anomalies are simply washed out and a Fermi gas density of states is recovered [16]. The observed microcanonical negative heat capacities in this case cannot be considered as a signal of a phase transition.

If we now consider cases for which we know that the infinite system does present a phase transition such as in the melting case[17, 18] and in the liquid-gas phase transition[19, 14] we observe that the microcanonical phase transition signal survives in the canonical case[2]. This is displayed for the liquid-gas phase transition in the context of the Lattice-gas model in Figure 7[12]. If for the canonical calculation the energy is defined as the average over the energy distribution, a smooth behavior is observed linking the liquid to the gas phase with however a clear slope change. If the canonical energy is taken as the most probable value of the energy distribution, the phase transition jump corresponding to the latent heat is visible already for a finite system (216 particles for the calculation presented in Figure 7). When both ensembles reach the same caloric curve, i.e. at the thermodynamical limit, one then observes an anomaly which corresponds to the Maxwell construction. This demonstrates that we are facing a phase transition.

Another important signal of a phase transition is to spot a macroscopic collective change in the states involved in the microcanonical back-bending. For example the existence of an order (symmetry) or an order parameter (such as the density variation or the size of the biggest fragment) which will survive when the thermodynamical limit will be taken and which is already present in the finite system, is a strong signal of the phase transition. As an example the top part of Figure 7 displays the size distribution of clusters in the Lattice-gas model at an energy lower (left) and higher (right) than the back-bending region. In the "gas" phase the distribution is monotonically decreasing, while in the "liquid" phase a peak at high mass is seen corresponding to the reminiscence of the infinite percolation cluster. The region of the temperature back-bending (central panel) corresponds to a liquid fraction composed of fragments of a size comparable to the gas fraction.

6 Conclusions

In this contribution we have looked for relevant signals of a phase transition in a finite system. We have stressed the fact that a necessary condition is that a curvature anomaly should be present in the thermostatistical potential

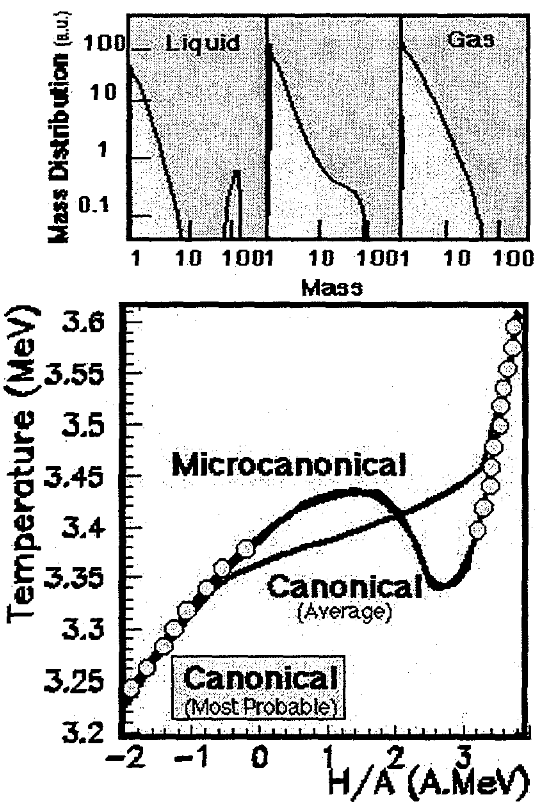

Figure 7: Top part: size distribution of the microcanonical Lattice-gas model at three different energies corresponding to the two increasing branches of the caloric curve (right and left parts) and in the middle of the negative heat capacity region (central panel). Lower part: microcanonical and canonical caloric curve in the subcritical region of the Lattice-gas model phase diagram (see text).

of the finite system. In particular one should consider a statistical ensemble with one extensive variable controlled in order to sample the interior of the phase transition region. In such a case one expects to observe an anomalous back-bending in the conjugated intensive variable which shows the presence of a transition between two types of states.

This observation is a necessary but not sufficient condition for the anomaly to be related with a phase transition. Indeed, one should also look to the behavior of the system in other statistical ensembles (for example the canonical one for the microcanonical back-bending in the caloric curve). At the thermodynamical limit all ensembles should converge to the same phenomenology of the Maxwell construction for a first order phase transition. Therefore, anomalies as a function of an extensive variable should also be associated with a well defined slope change when the conjugate intensive variable is constrained.

Finally, a phase transition is associated with a qualitative change of a macroscopic observable such as an order parameter which should already be present in the finite system and which should be used to spot a phase transition signal in a finite system.

References

[1] W. Thirring, Zeit. Phys. 235 (1970) 339.

[2] M. Schmidt et al., H. Haberland, Phys. Rev. Lett. 79, 99 (1997); Nature 393, 238 (1998);

[3] T. Hijmans, Physics World 12, 20 (1999); A. I. Safanov et al., Phys. Rev. Lett. 81, 4545 (1998); D.G. Fried et al., Phys. Rev. Lett. 81, 3811 (1998).

[4] Proceedings of "Quark Matter 1997", Nucl. Phys. A 638 (1998) 1c-610c.

[5] P.J. Siemens, Nature 305 (1983) 410; M.W. Curtin, H. Toki, D.K. Scott, Phys. Lett. B 123 (1983) 289.

[6] Ph. Chomaz, Ann. Phys 21 (1996) 669

[7] M.F. Rivet et al, Phys. Rev. Lett. B430 (19998) 217

[8] B.Borderie et al., contribution to this conference.

[9] D. H. E. Gross and P.A.Hervieux, Z.Phys. D35 (1995) 27; D.H.E. Gross, Phys. Rep. 279 (1997) 119; D.H.E. Gross and E.Votyakov, cond-mat 9911257 .

[10] D.J.Wales and R.S.Berry, Phys.Rev.Lett. 73 (1994) 2875.

[11] F.Gulminelli and P.Chomaz, Phys. Rev. Lett. 82 (1999) 1402.

[12] F.Gulminelli et al., contribution to this conference.

[13] F.Gulminelli and Ph.Chomaz, Int. Journ. Mod. Phys. E vol.8, n.6 (1999) 1.

[14] F.Gulminelli, P.Chomaz and V.Duflot, preprint LPCC 99-17 and to be published in Europhys.Lett.

[15] P.Ring and P.Schuck, 'The nuclear many body problem', Springer Verlag, NY (1980), chapter 3.

[16] E.Melby et al., Phys.Rev.Lett. 83 (1999) 3150.

[17] P.Labastie and R.L.Whetten, Phys.Rev.Lett. 65 (1990) 1567.

[18] F.Calvo, Ann.Phys.Fr. 24,n.4 (1999).

[19] Ph.Chomaz, F.Gulminelli and V.Duflot, 'Phase transition with an isospin dependent Lattice-gas model', in 'Isospin physics in heavy ion collisions at intermediate energies', B.A.Li and W.U.Schroeder eds, Nova Science Publishers Inc., (2000).