Order parameter fluctuations and thermodynamic phase transitions in finite spin systems and fragmenting nuclei

J. M. Carmona\textsuperscript{a,1}, J. Richert\textsuperscript{b,2}, P. Wagner\textsuperscript{c,3}

\textsuperscript{a}Departamento de Física Teórica, Universidad de Zaragoza, Pedro Cerbuna 12, 50009 Zaragoza, Spain
\textsuperscript{b}Laboratoire de Physique Théorique, Unité de Recherche Mixte Université - CNRS UMR7085, Université Louis Pasteur, 3, rue de l’Université 67084 Strasbourg Cedex, France
\textsuperscript{c}Institut de Recherches Subatomiques, Unité de Recherche Mixte Université - CNRS UMR7500, BP28, 67037 Strasbourg Cedex 2, France

Abstract

We show that in small and low density systems described by a lattice gas model with fixed number of particles the location of a thermodynamic phase transition can be detected by means of the distribution of the fluctuations related to an order parameter which is chosen to be the size of the largest fragment. We show the correlation between the size of the system and the observed order of the transition. We discuss the implications of this correlation on the analysis of experimental fragmentation data.

Key words: Order of phase transition, finite systems, nuclear fragmentation
PACS: 05.70Fh, 25.70.Pq, 75.40.Cx

There exist by now several indications that nuclear matter can appear in different phases which may be produced by means of energetic nuclear collisions. Signs for the possible existence of a phase transition have been found experimentally through the construction of the caloric curve which relates the temperature $T$ to the energy $E$ of the system, the extraction of the specific heat and the analysis of the behaviour of fragment size distributions [1–8]. Simple minded approaches like percolation and lattice gas models generate...

\textsuperscript{1} E-mail: jcarmona@posta.unizar.es
\textsuperscript{2} E-mail: richert@lpt1.u-strasbg.fr
\textsuperscript{3} E-mail: pierre.wagner@ires.in2p3.fr
relevant quantities like fragment size distributions and thermodynamic observables whose features are characteristic for such transitions \[9–18\]. Experiments are seemingly able to reproduce these features. However, there remains a need for further experimental confirmation and for clarification of some points as it will appear below.

The aim of the present work is twofold. First we want to show that under the assumption of thermodynamic equilibrium a judicious choice of observables related to fragment size distributions may be an efficient tool to detect a phase transition in small systems. Second we shall show that the order of the transition which comes out of the present investigations can be different when the system is small or large. Similar effects have been observed in other systems \[19\].

Two facts will guide our investigations. First, Botet and Ploszajczak suggested very recently that the distribution of order parameter fluctuations can be helpful for the detection of a phase transition in a finite system, at least when the transition is continuous \[20\]. Such distributions show a different behaviour at and off a transition point and are scale invariant with respect to the size of the system at that point. An experimental test on Xe+Sn for different bombarding energies reveals indeed scaling properties of the measured events \[21\].

Second, there exists by now some hope and even hints that simple models like lattice models and other related approaches work as generic frameworks which provide a realistic, even though possibly only qualitative description of nuclear fragmentation \[22\]. The lattice gas model (LGM) \[11\] is the paradigm of this type of models. Its basic variables are the temperature \(T\) and the density \(\rho\) of particles. Formulated in the grand canonical ensemble, it can be mapped onto the Ising model with a magnetic field \(h\) \[23\], which, as it is well known, presents a discontinuity in the equation of state involving the magnetization, \(M(T, h)\), for \(T < T_c\) at \(h = 0\), where \(T_c\) is the critical temperature. This corresponds in the LGM to a first-order transition line (the ’coexistence line’) in the \((\rho, T)\) phase diagram, which separates the homogeneous phases from the ’liquid’ and ’gas’ coexistence region. On this line, there is a critical point at \(\rho = 0.5, T = T_c\). The LGM in the canonical ensemble was considered in ref. \[14\]. In finite systems the previous discontinuity evolves into a backbending in the chemical potential as a function of \(\rho\) at subcritical temperatures, which produces a negative branch in its derivative \[14\].

In this context we developed the so called IMFM (Ising Model with Fixed Magnetization) \[16\]. The Hamiltonian reads

\[
H_{\text{IMFM}} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + V_0 \sum_{<ij>} \sigma_i \sigma_j
\]
where $A$ is the number of particles, $\{\sigma_i = \pm 1\}$ is related to the occupation of site $i$ through $s_i = (1 + \sigma_i)/2$, $\{s_i = 0, 1\}$, and the interaction acts between nearest neighbours $< ij >$. The total number of particles $\sum_i s_i = A$ is fixed, so that the canonical partition function can be written as

$$Z(T) = \sum_{\{\sigma\}} e^{-\frac{1}{\beta} H_{\text{IMFM}} \delta \sum_i s_i, A}.$$ 

The determination of the order of the transition is however harder when one considers the behaviour of observables as a function of $T$ while maintaining $A$ as a fixed parameter of the model. Both the specific heat [16] and the fragment distributions [14,16] present an apparent scaling for small systems, and some characteristic features of a smooth transition [24].

Fig. 1. Caloric curve $E$ vs. temperature $T$ for 3D systems with a) $L = 10$ and b) $L = 30$ at density $\rho = 0.13$. The configuration energy $E$ has been scaled by $3V = 3L^3$. The calculations are made in the framework of the IMFM model [16].

Fig. 2. Phase diagram in the $(\rho, T)$ plane. The solid line shows the locus of $T_{tr}$, the dashed line the locus of $T_f$. 

3
Fig. 1 shows typical caloric curves for $\rho = 0.13$ and different linear sizes $L$. Microcanonical and canonical calculations are indistinguishable up to $L = 30$. It is not possible to conclude about the order of the transition. This observation agrees with the microcanonical calculations of Pleimling and Hüller who showed that the first order nature of the transition appears only for $L \geq 60$ [25].

We have used the IMFM and systematically determined the values of the transition temperature $T_{tr}$ corresponding to the maximum of the specific heat and the temperature $T_f$ corresponding to the maximum of the second moment of the fragment size distribution. The specific heat does not diverge in the thermodynamic limit (except for the critical point at $\rho = 0.5$), but in finite systems it presents maxima which can indeed be observed experimentally [4]. These maxima define a transition line $(\rho, T_{tr})$ which however differs from the liquid-gas coexistence line obtained by the usual Maxwell construction [14]. In fact for finite systems it lies systematically below the coexistence line [11,14], but both lines are expected to coincide in the thermodynamic limit [25]. The use of $C_V$ is of interest in correlation with the fact that this quantity may be experimentally accessible [4,5].

The locus of $T_{tr}$ and $T_f$ corresponds respectively to the full and the dashed line in the $(\rho, T)$ phase diagram shown in Fig. 2. For $\rho > 0.5$ $T_f$ is always larger than $T_{tr}$, but for $\rho < 0.5$ the temperatures $T_f$ and $T_{tr}$ come very close to each other, their distance decreases with decreasing $\rho$ and increasing $L$. Hence both maxima are correlated and different aspects of the same transition.

Fig. 3. Evolution of $\langle A_{\text{max}} \rangle / A_{\text{tot}}$ ($A_{\text{tot}}$ = total number of particles) with the temperature for $\rho = 0.13$, $L = 10$ (open dots), 20 (squares), 30 (triangles). The calculations are performed in the framework of the microcanonical ensemble.
Fig. 3 shows the behaviour of the mean value of the size of the largest cluster \( < A_{\text{max}} > \) as a function of the temperature. It appears that \( < A_{\text{max}} > \) like the second moment varies more or less abruptly in an interval of temperatures which lies close to \( T_{tr} \). If the IMFM provides a realistic picture of the underlying physics of nuclear fragmentation it comes out that for low densities \( \rho \) the observable \( A_{\text{max}} \) can be used as an order parameter which signals the presence of a thermodynamic phase separation point. We use \( A_{\text{max}} \) in order to implement scaling tests. Following the arguments of ref. [20] we consider the function

\[
\Phi(z) \equiv \frac{A_{\text{max}} - A_{\text{max}}^*}{< A_{\text{max}} > \Delta} \equiv < A_{\text{max}} > \Delta P(A_{\text{max}})
\]

where \( A_{\text{max}}^* \) is the most probable value of \( A_{\text{max}} \), \( \Delta \) a real positive number and \( P(A_{\text{max}}) \) the normalised probability distribution function of \( A_{\text{max}} \). At a continuous transition point and \( \Delta = 1 \) the distribution \( \Phi \) which shows the properties of the fluctuations of the order parameter \( A_{\text{max}} \) is a scale invariant quantity.

This is indeed the case in our model for systems of linear size \( L \leq 40 \) as it can be seen in Fig. 4. The functions \( \Phi \) show the characteristic scale invariance of the fluctuations for systems with different linear sizes \( L \) at a temperature which corresponds to the value of \( T_{tr} \) for the infinite system. Above \( T_f \) scale invariance can be observed for \( \Delta \neq 1 \), even though the overlap between the scaling functions for different values of \( L \) is not perfect as it can be seen in Fig. 5.

In practice, events are collected with a certain experimental width in energies or temperatures. One can then ask whether the scaling signature would survive in a real experiment. In order to evaluate this effect, we simulated systems with \( L = 10, 20, 30, \) and \( 40 \) in a range of temperatures \( T = 3.85 \pm 0.20 \) MeV at \( \rho = 0.13 \) and used these data to produce \( \Phi(z) \). We observed that the \( L = 10 \) and \( L = 20 \) data still lie on the same curve, while this is no longer true for \( L \geq 30 \). The result is not surprising, the smallest systems have a wider transition region and are consequently less sensitive to shifts of the temperature. However, this limitation is not crucial in practice. A system with \( L = 10 \) at \( \rho = 0.3 \) corresponds to 300 particles; \( L = 20 \) at \( \rho = 0.13 \) corresponds to 1040 particles. In fact the scaling signature has already been observed in collision experiments of Xe+Sn (around 245 particles) [21]. In an experiment with much larger number particles and a large temperature dispersion, the signal would effectively be lost.

Fits of the tails of the fluctuation distributions on the transition line are in agreement with the parametrization

\[
\Phi(z) = a \exp(-bz^\nu).
\]
Fig. 4. The scaling behaviour of the fluctuations of $A_{\text{max}}$ for systems of different linear sizes $L$ at $T_f = 3.85$ MeV and density $\rho = 0.13$. Here $\Delta = 1$. The calculations are performed in the canonical ensemble.

At $T_f = 4.5$ MeV one gets $\tilde{\nu} = 1.78 \pm 0.20$ for $\rho = 0.50$ and $\tilde{\nu} = 1.15 \pm 0.15$ for $\rho = 0.30$ which may be compared with $\tilde{\nu} = 1.6 \pm 0.4$ obtained through the experimental analysis of ref. [21].

Fig. 5. Scaling behaviour of the systems of size $L = 10, 20, 30$, $\rho = 0.13$, $T = 4.5$ MeV. Here $\Delta = 0.65$. The calculations are performed in the canonical ensemble.

The present analysis shows that the generation of largest fragment fluctuation distributions may be an efficient tool to detect a thermodynamic phase transition in small finite systems of low density. Fragmentation events which
show scaling properties with respect to the size of the system correspond to events which lie at or in the near neighbourhood of such a transition. They could be used as a tool in an experimental analysis and allow to detect a thermodynamic phase transition in the $(\rho, T)$ plane by selecting events with scaling properties and correlating them with thermodynamic observables like temperature and density.

There remains however an open point. The tools proposed in ref. [20] work for continuous transitions. On the other hand the thermodynamic transition is a first order transition as indicated by simulations of large systems. This can be observed in the framework of the microcanonical ensemble [25]. It may sound contradictory that the transition related to the behaviour of the fragment size distribution and the thermodynamic transition are of different nature. In order to investigate this point we extended our simulations to systems of size $L = 50$ and 60, in the framework of the canonical and microcanonical ensemble. The first order nature of the transition reveals itself in both ensembles. In the case of the microcanonical approach our results confirm those of ref. [25]. In the canonical case, the first order character can clearly be seen. Indeed in the neighbourhood of the thermodynamic transition, the energy distribution shows the characteristic double hump which distinguishes the coexistence of two phases. Working out the distribution of fluctuations $\Phi(z)$ one observes that this observable does no longer scale with the size of the system for $L \geq 50$ as it can be seen in Fig. 4. This also happens with the $\Phi(z)$ derived from microcanonical calculations.

The IMFM offers a possible explanation for the fact that one observes on the one hand features which are consistent with percolation concepts [2] and, on the other hand, a first-order thermodynamic transition. The separation line defined by $T_f$ lies above the thermodynamic transition for $\rho > 0.5$ [11]. But for $\rho < 0.5$ densities, the fragment distribution is intimately related to the thermodynamic behaviour as it is in Fisher’s phenomenological droplet model [8]. Hence, if the freeze-out happens at low densities, fragment formation is controlled by the thermodynamic transition. The scaling observed in experiments could be due to the apparent, transient, continuous behaviour which this transition presents for small systems ($L \lesssim 50, 60$) in the framework of the IMFM. One should however notice that negative values of $C_V$ which should corroborate the observation of a first order transition have been seen experimentally [5,26] in as small systems as nuclei, in agreement with a specific microcanonical treatment of the liquid-gas phase transition [15].

These observations lead to several conclusions. First, different observables may lead to different transition orders if one deals with small systems, and the order may change with the size of the system. Second, in the present case, the canonical and microcanonical treatments lead to the same answer for both small and large systems if one considers the pertinent quantity, here the en-
ergy distribution in the vicinity of the transition point. One should notice that this is not always the case. The nonequivalence between microcanonical and canonical ensembles has been proven in systems with negative specific heat regimes, corresponding to canonically unstable states [27]. Analogously, the backbending in the chemical potential implies nonequivalence between the canonical and grand canonical descriptions of the LGM. In fact this backbending reflects the first order character of the transition [14]. We were interested however in the behaviour of two other quantities, the fragment distributions and the specific heat, which are both experimentally accessible [4,5]. Third, the present behaviour of $\Phi(z)$ seems to indicate that scaling works in the case of a continuous transition as predicted in ref. [20] but not if the transition is first order. Fourth, one observes a consistency between the behaviour of $\Phi(z)$ and the correct thermodynamic limit. The apparent scaling works only when the system is small. When the system is large the first order behaviour reveals itself in this observable and scaling fails.

In summary, we have shown the correlation in the IMFM between observables related to fragment size distributions and a thermodynamic transition. For small systems the distribution function of the largest fragment fluctuations shows the scaling features which may characterise a continuous phase transition. For systems much larger than nuclei, the first order character of the transition appears and the scaling properties of the distribution of the order parameter $A_{\text{max}}$ disappear.

Acknowledgements

The authors acknowledge an interesting discussion with M. Ploszajczak and R. Botet. The work of JMC was partially supported by EU TMR program ERBFMRX-CT97-0122.

References

[1] P. Kreutz et al., Nucl. Phys. A 556 (1993) 672.
[2] Y.M. Zheng, J. Richert and P. Wagner, J. Phys. G 22 (1996) 505.
[3] J. Pochodzalla et al., Phys. Rev. Lett. 75 (1995) 1040.
[4] M. D’Agostino et al., Nucl. Phys. A 650 (1999) 329.
[5] M. D’Agostino et al., Phys. Lett. B 473 (2000) 219.
[6] A. Chbihi, O. Schapiro, S. Salou and D.H.E. Gross, Eur. Phys. J. A 5 (1999) 251.
[7] B. Borderie et al., Phys. Rev. Lett. 86 (2001) 3252.
[8] J.B. Elliott et al., nucl-ex/0104013.
[9] X. Campi, Phys. Lett. B 208 (1988) 351.
[10] B. Elattari, J. Richert, P. Wagner and Y.M. Zheng, Nucl. Phys. A 592 (1995) 385.
[11] X. Campi and H. Krivine, Nucl. Phys. A 620 (1997) 46.
[12] Jicai Pan, Subal Das Gupta and Martin Grant, Phys. Rev. Lett. 80 (1998) 1182.
[13] J. Borg, I.N. Mishustin and J.P. Bondorf, Phys. Lett. B 470 (1999) 13.
[14] F. Gulminelli and Ph. Chomaz, Phys. Rev. Lett. 82 (1999) 1402.
[15] Ph. Chomaz, V. Duflot and F. Gulminelli, Phys. Rev. Lett. 85 (2000) 3587.
[16] J.M. Carmona, J. Richert and A. Tarancón, Nucl. Phys. A 643 (1998) 115.
[17] M. Pleimling and W. Selke, J. Phys. A 33 (2000) L199.
[18] Y.G. Ma, J. Phys. G27 (2001) 2455.
[19] J.L. Alonso et al., Phys. Lett. B 376 (1996) 148; D.H.E. Gross, Microcanonical Thermodynamics, World Scientific, 2001; cond-mat/0004268.
[20] R. Botet and M. Ploszajczak, Phys. Rev. E 62 (2000) 1825.
[21] R. Botet, M. Ploszajczak, A. Chbihi, B. Borderie, D. Durand and J. Frankland, Phys. Rev. Lett. 86 (2001) 3514.
[22] J. Richert and P. Wagner, Phys. Rep. 350 (2001) 1.
[23] T.D. Lee and C.N. Yang, Phys. Rev. 87 (1952) 410.
[24] J.M. Carmona, N. Michel, J. Richert and P. Wagner, Phys. Rev. C 61 (2000) 37304.
[25] M. Pleimling and A. Hüller, J. Stat. Phys. 104 (2001) 971.
[26] M. D’Agostino et al., nucl-ex/0104024.
[27] P. Hertel and W. Thirring, Ann. Phys. 63 (1971) 520; T. Padmanabhan, Phys. Rep. 188 (1990) 285; D. Lynden-Bell, Physica A 263 (1999) 293; I. Ispolatov and E.G.D. Cohen, cond-mat/0101311.