DETERMINATION OF CRITICAL EXPONENTS IN NUCLEAR SYSTEMS *

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Signatures of critical behaviour in nuclear fragmentation are often based on arguments from percolation theory. We demonstrate with general thermodynamic considerations and studies of the Ising model that the reliance on percolation as a reference model bears the risk of missing parts of the essential physics.

1 Introduction

The existence of phase transitions in nuclear matter was proposed more than 20 years ago in conjunction with the description of the structure of neutron stars [1,2]. This led to the question whether phase separation [3], dynamical instabilities [4] or critical phenomena [5] play a role in the disintegration of highly excited nuclei produced in proton or heavy ion induced collisions. The observation of a power law for the fragment size distribution [6,7] was the first experimental hint for a second order phase transition, but the determination of critical exponents [8] or other parameters [9] turned out to be difficult with the mostly inclusive data available at that time [10,11,12]. In the past 3 years, however, data from a new generation of experiments with an almost complete coverage for the decay products of an excited system allowed for rapid progress. The observation of potential signals of a

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first order phase transition [13,14] and the attempt of a quantitative determination of critical exponents [15] sparked an intense discussion on what reliable signatures for a first or second order phase transition in a small and dynamically evolving system are.

In the following we will take the recent claim [15,16], that a continuous phase transition with critical exponents consistent with those of a liquid-gas system has been observed in the fragmentation of nuclei, at face value and revisit the theoretical arguments used in this analysis.

2 Critical Phenomena in a Nutshell

Near a critical point, the order parameter ϕ, associated susceptibility χ, specific heat c, and the correlation length ξ exhibit a power law dependence on two reduced control parameters ϵ and h:

$$\begin{aligned}
\phi_{(\epsilon,h=0)} &= B\epsilon^{\beta} \\
\phi_{(\epsilon=0,h)} &\sim h^{1/\delta} \\
\chi_{(\epsilon,h=0)} &= \Gamma\epsilon^{-\gamma} \\
c_{(\epsilon,h=0)} &= A\epsilon^{-\alpha} \\
\xi_{(\epsilon,h=0)} &= \xi_0\epsilon^{-\nu}
\end{aligned}
\qquad \text{with} \qquad
\begin{array}{cccc}
 & \text{Liquid-Gas} & \text{Magnet} & \text{Percolation} \\
\phi & \rho-\rho_c & M & P_\infty \\
\chi & \frac{1}{\rho^2}\frac{\partial\rho}{\partial\mu} & \frac{\partial M}{\partial H} & \sum s^2 n_s \\
\epsilon & \frac{T-T_c}{T_c} & \frac{T-T_c}{T_c} & p_c-p \\
h & \mu-\mu_{0(T)} & H & p_g
\end{array}$$

For liquid-gas, magnetic and percolation systems the order parameter ϕ is the difference between liquid and critical density, magnetization per spin M or the fraction of sites in the largest cluster P_∞, respectively. The susceptibility χ corresponds to the isothermal compressibility $\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial p}$ and the second moment of the cluster size distribution for the liquid-gas and percolation case. The 'thermal' control parameter ϵ is the difference of the temperature T or bond probability p to the critical value while the 'field' control parameter h is given by the chemical potential μ, the external field H or the ghost bond [17,18] probability p_g.

3 From Thermodynamics to Percolation and Back

The exponents β and γ can be determined from a measurement of $\phi_{(\epsilon,h=0)}$ and $\chi_{(\epsilon,h=0)}$. For liquids it is indeed possible to determine $\Delta\rho = \rho-\rho_c$ and $\frac{\partial\rho}{\partial\mu}$ directly, e.g. by measuring the density profile in the gravitational field [19,20,21].

In the nuclear physics case, the only directly measured quantities are the size and momenta of clusters produced in an interaction. The standard argument to deduce $\Delta\rho$ and κ_T from the cluster size distribution uses the Fisher droplet model [22]. In this Ansatz the grandcanonical partition function $\mathcal{Z}$ is expressed as a sum over cluster yields $Y_{(A)}$ which depend on a surface energy s and chemical potential difference between liquid and gas phase μ:

$$\ln\mathcal{Z} = \sum Y_{(A)} \qquad \text{with} \qquad Y_{(A)} = q_0 A^{-\tau}\exp\left(-\frac{1}{T}\left(sA^{\sigma}+\mu A\right)\right)$$

From this follows immediately that κ_T is proportional to the second moment of the cluster size distribution

$$\kappa_T = \frac{T}{V\rho^2}\frac{\partial^2}{\partial\mu^2}\ln\mathcal{Z} = \frac{1}{TV\rho^2}\sum A^2 Y_{(A)}. \tag{1}$$

It can also be shown [22] that $\Delta\rho$ is proportional to the fraction of constituents belonging to the largest cluster P_∞. This strong similarity to percolation, where P_∞ and the second moment also play the role of order parameter and susceptibility, has led to a widespread use of percolation in the modeling and interpretation of nuclear physics experiments. In particular, percolation has served as reference model for the development of methods to extract critical exponents [23,24].

Even though there is a mathematical connection between percolation and the thermodynamics of interacting systems (the $q \to 1$ limit of the Potts model corresponds to bond percolation [25]) there are also some significant differences:

- Percolation is usually discussed in terms of only one control parameter, the bond or site probability, leaving the impression that the 'field' control parameter, corresponding to chemical potential or average density in interacting systems, is of minor importance.
- Finite size effects depend strongly on the ensemble in interacting systems [26,27,28], but there is no direct equivalent to the concept of an ensemble in percolation.
- Percolation theory simply starts with the definition of what a cluster is. Thermal systems, on the other hand, are usually defined in terms of the interaction between their constituents and the appropriate definition of a cluster is, as will be shown, nontrivial.

The almost exclusive reliance on percolation as a reference model bears therefore the risk that important parts of the physics are missed. In the following we will consequently turn back to the thermodynamic basics and use the Ising model as guidance.

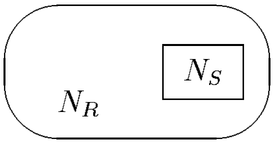
4 From Constituents to Clusters

As a first step it is interesting to establish the connection between κ_T and the cluster size distribution with minimal assumptions and without using a specific model. We follow an idea given by Alexandrowicz [29] for the Ising model but generalize it to an arbitrary system. In the grand canonical ensemble, κ_T is related to the fluctuation of the particle number σ_N^2 by

$$\sigma_N^2 = kT\left.\frac{\partial N}{\partial\mu}\right|_{T,V} = kT\frac{N^2}{V}\kappa_T$$

In the following, we consider a system with N_S constituents coupled to a reservoir with N_R constituents:

N_S: System
N_R: Reservoir
$N = N_R + N_S$



Define for constituent i:

$$q_i = \begin{cases} 1 & \text{if in } S \\ 0 & \text{if in } R \end{cases}$$

To express $\sigma^2_{N_S}$ in terms of clusters we assume that the constituents are grouped into clusters with the properties:

P1 A cluster is either completely in S or in R.

P2 Constituents in different clusters are uncorrelated.

$\sigma^2_{N_S}$ can now be rewritten as a q correlation. The sum over constituent pairs can be split into two parts, one where the pair is in the same cluster and one where it is in different clusters:

$$\begin{aligned}
\sigma^2_{N_S} &= \left\langle N_S^2 \right\rangle - \langle N_S \rangle^2 \\
&= \left\langle \sum_{ij} (q_i - \overline{q})(q_j - \overline{q}) \right\rangle \qquad \text{with } \overline{q} = \tfrac{\langle N_S \rangle}{N} \\
&= \left\langle \sum_{\substack{ij \\ \text{same}}} (q_i - \overline{q})(q_j - \overline{q}) \right\rangle + \underbrace{\left\langle \sum_{\substack{ij \\ \text{diff}}} (q_i - \overline{q})(q_j - \overline{q}) \right\rangle}_{\overset{(\text{P2})}{=}\, 0} \\
&\overset{(\text{P1})}{=} (1-\overline{q})^2 \left\langle \sum_{\substack{c_i \\ \text{S}}} |c_i|^2 \right\rangle + \overline{q}^2 \left\langle \sum_{\substack{c_i \\ \text{R}}} |c_i|^2 \right\rangle
\end{aligned}$$

In the last line, the sum over constituents was rewritten as a sum over clusters $\sum_{\substack{ij \\ \text{same}}} \to \sum_{c_i} |c_i|^2$ and split into two parts, running over S and R, respectively. In the thermodynamic limit, $N_R \to \infty$, $\overline{q} \to 0$, the second term goes to zero if the largest cluster in R grows slower than N_R (in other words: No condensation in R) and one finally gets

$$\kappa_T = \frac{V}{kT} \frac{\sigma^2_{N_S}}{\langle N_S \rangle^2} = \frac{1}{kT\rho} \sum_s s^2 n_s \tag{2}$$

where n_s is the concentration of clusters of size s. This is equivalent to Eqn. (1) but was derived with only one essential assumption, that constituents in different clusters are uncorrelated.

5 The Ising Model

One of the simplest thermodynamic models with a phase transition is the Ising model, given by the Hamiltonian:

$$\mathcal{H} = -J \sum_{<i,j>} \sigma_i \sigma_j - H \sum_i \sigma_i \tag{3}$$

It can be interpreted as a model for a magnet, with $\sigma = \pm 1$ representing up and down spins, or as a lattice model of a gas [30] where $\sigma = \pm 1$ now indicates whether a site is occupied or empty. The number of sites N, magnetization M and external field H correspond in the lattice gas interpretation to the volume V, density ρ and chemical potential μ, respectively.

Order parameter $\langle |M| \rangle$ and susceptibilities χ and χ' for $T \geq T_c$ and $T < T_c$, respectively, are defined in terms of constituents as:

$$\begin{aligned} \langle |M| \rangle &= \left\langle \left| \tfrac{1}{N} \textstyle\sum_i \sigma_i \right| \right\rangle \\ \chi &= \tfrac{N}{kT} \langle M^2 \rangle = \tfrac{N}{kT} \left(\tfrac{1}{N^2} \left\langle \textstyle\sum_{ij} \sigma_i \sigma_j \right\rangle \right) \\ \chi' &= \tfrac{N}{kT} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right) \end{aligned} \tag{4}$$

M and χ can be expressed in terms of clusters using arguments which are for χ analogous to the ones in the previous section. A detailed derivation along those lines was given by de Meo [31] while other authors arrived at the same result from different viewpoints [29,32,33,34]. One obtains for the cluster observables $\widetilde{M}$, $\widetilde{\chi}$ and $\widetilde{\chi'}$:

$$\begin{aligned} \widetilde{M} &:= \langle P_\infty \rangle & &\leq \langle |M| \rangle \\ \widetilde{\chi} &:= \tfrac{1}{kT} \chi_p & &= \chi \\ \widetilde{\chi'} &:= \tfrac{1}{kT} \left(\chi'_p + N(\Delta P)^2 \right) & &\geq \chi' \end{aligned} \tag{5}$$

with the fluctuation of largest cluster $(\Delta P)^2 = \langle P_\infty^2 \rangle - \langle P_\infty \rangle^2$ and the percolation susceptibility $\chi_p = \sum_m m^2 < n_m >$ where n_m is the number of clusters per site with magnetization m.

While the order parameter is indeed given by the relative size of the largest cluster, we observe two significant differences between $\widetilde{\chi}$ and χ_p:

- The trivial $\frac{1}{kT}$ factor (see also Eqn. (1) and (2)) makes sure that the paramagnetic or ideal gas limit $\chi \propto \frac{1}{kT}$ is approached for $T \to \infty$ where $\chi_p \to 1$. Even though it does not affect the asymptotic power law behaviour for $T \to T_c$ it will change the effective exponents if a wide temperature range is considered, like in the nuclear exponent analysis [15].
- The susceptibitity $\widetilde{\chi'}$ for $T < T_c$ is given by the sum of χ'_p, the second moment taken without the largest cluster, and the fluctuation of the largest cluster $(\Delta P)^2$.

Numerical results for the 3d Ising model with periodic boundary conditions are shown in Fig. 1. The calculations were done with the Swendsen-Wang [36] and Wolff [37] algorithms in implementations similar to Ref. [38] using a random number generator proposed by Ziff [39,40]. In the left two columns we compare the cluster observables to the true values given by Eqn. (4). Consistent with Eqn. (5) we find $\widetilde{M}$ slightly smaller than $\langle |M| \rangle$ and $\widetilde{\chi}$ equal to χ while $\widetilde{\chi'}$ is only close to χ' for $T < T_c$.

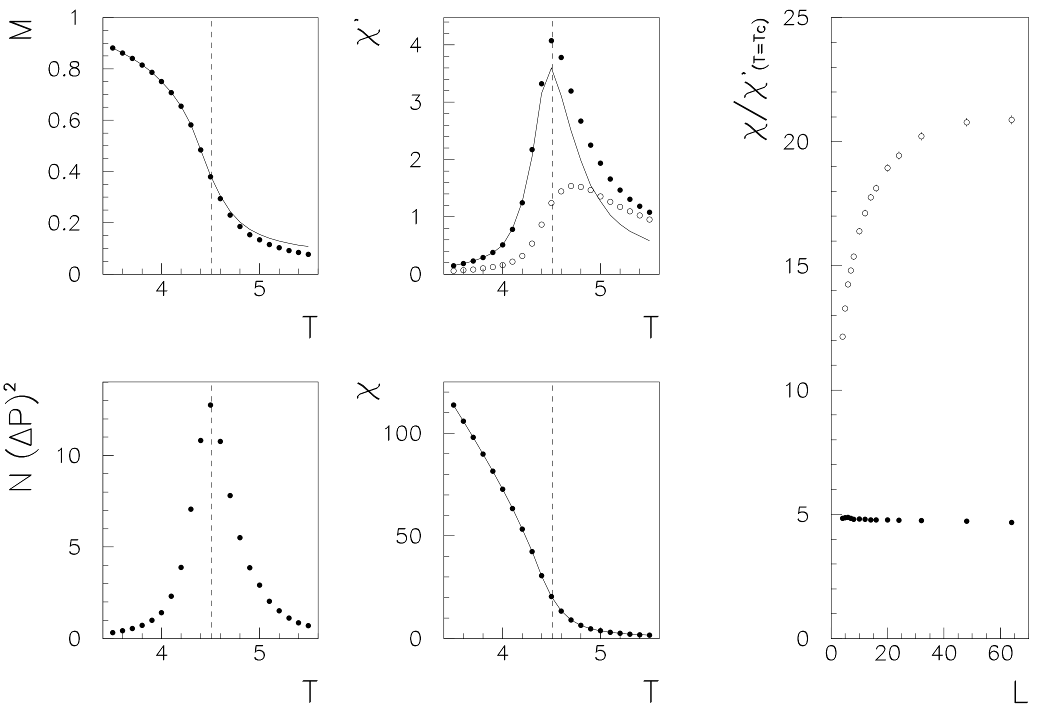


Figure 1: Left two columns: Comparison of cluster observables (Eqn. (5), full dots) and true values (Eqn. (4), full lines) for an Ising model with 8^3 sites. The dotted lines indicate the bulk critical temperature $T_c = 4.51152$[35].
Right column: Susceptibility ratio $\widetilde{\chi}/\widetilde{\chi'}$ at T_c as a function of the linear system size L with (full dots) and without (open dots) the $(\Delta P)^2$ contribution to $\widetilde{\chi'}$.

It is interesting to note, that the main contribution to $\widetilde{\chi'}$ is the fluctuation term $(\Delta P)^2$ while the second moment term $\frac{1}{kT}\chi'_p$ (indicated by open dots in the top middle frame of Fig. 1) carries only a small part of the signal. This can be seen more quantitatively in the right panel of Fig. 1 where the susceptibility ratio $\widetilde{\chi}/\widetilde{\chi'}$ at T_c is shown as a function of the linear system size L with (full dots) and without (open dots) the $(\Delta P)^2$ contribution to $\widetilde{\chi'}$. Depending on system size, between 60 and 75% of the susceptibility are carried by the fluctuation term.

6 Critical Clusters

Clusters can be defined in interacting systems in many different ways. We call the result of a definition 'critical clusters' if order parameter and susceptibility correspond to size of largest cluster and second moment, or formally, if Eqn. (5) holds. We saw in the previous two sections that a necessary condition is the noncorrelation of constituents in different clusters but have not given so far an explicit definition.

The most obvious way to define a cluster is the 'geometrical cluster' which corresponds to a domain in the Ising model, or in the lattice gas picture to a connected region of occupied sites surrounded by empty sites. However, it is easy to see that this violates the noncorrelation requirement [29] and it has indeed been shown that in 3d 'geometrical clusters' lead to a percolation transition at temperatures below the thermal transition [43], thus do not fulfill Eqn. (5).

The proper prescription for 'critical clusters' for the Ising model was given by Coniglio and Klein [44] and requires that the geometrical clusters are broken into smaller pieces with a bond percolation with $p_b = 1 - \exp(-\frac{2J}{kT})$.

The definition of a 'physical cluster', based on pairwise binding, proposed by Hill [45] and recently used in a lattice gas model for nuclear fragmentation [46], results in bond probabilities quite similar to the Coniglio-Klein values. Even though both definitions give numerically similar results for small system sizes they are clearly not equivalent in the thermodynamic limit.

7 Summary

Percolation describes remarkably well the cluster distributions and correlations in nuclear fragmentation [47,48]. This, together with its simplicity and ease of use, made it the ideal reference model for the study of signatures of critical behaviour. But given the hints, that we observe a liquid-gas rather than a percolation phase transition, we have to face the limitations of percolation. Even scratching at the surface of a proper thermodynamic description raises many issues:

- **Critical clusters** have rather remarkable properties, they are neither well separated nor compact [†], are interacting but have nevertheless no correlations between constituents of different clusters. So one might wonder whether critical clusters are mere mathematical constructs, like the clusters in Mayer's cluster expansion, or real physical entities. All attempts to infer signatures of critical behaviour in nuclear physics not only imply that critical clusters are observable objects, they also assume that the distribution of clusters formed in the decay of a system is representative of the equilibrium distribution at some freeze-out condition. Even though there are attempts to support this connection with model calculations [49] it remains to be seen whether there is a more rigorous way to justify this.
- **Ensembles:** Although the experimental situation is certainly better represented by a microcanonical treatment we used for simplicity for all arguments in sections 4 and 5 the grand canonical ensemble. While the expectation values of extensive quantities do not depend on the ensemble in the thermodynamic limit it is easy to show that this is not the case for fluctuations [50]. The cluster observables (Eqn. (5)) are therefore likely to be ensemble dependent.
- **Role of control parameters:** The exponent analysis rests on the precondition that the temperature of the system is varied while the second control

[†] they are in general fractals with a dimension $y_h = \frac{1}{\sigma\nu}$ or about 2.5 in the 3d Ising class

parameter, the density, stays constant and close to its critical value. Assuming that we observe conditions along a freeze-out line and taking Papp's schematic model [51,52] as a guide one sees that the reverse might be true, that the temperature is almost constant but that the density varies. In this case one would determine different exponents, e.g. $1/\delta$ rather than β (see section 2). One should also keep in mind that the relative size of the largest cluster correlates with the density of the liquid phase (thus the order parameter) only on the critical isochore but is in general more readily interpreted as a measure of the mass fraction of the liquid phase.

- **Corrections to scaling:** The power laws listed in section 2 hold only asymptotically for $\epsilon \to 0$ while a description in a wider range is possible with correction to scaling terms [53] or a crossover approach [54]. The size of the critical region depends strongly on the exact form of the interaction and is rather small in real liquids [54] but substantially larger in models with only next-neighbor or short range interactions. The leading correction term for the order parameter in the Ising model [55] is not only substantially smaller in magnitude but has even a different sign as compared to typical liquids [21]. It is therefore uncertain whether simple schematic models, like percolation or Ising, are adequate for the modeling of finite size and finite control parameter effects in the nuclear case.
- **Field gradients:** The hallmark of critical phenomena is scale invariance which at least requires homogeneous conditions throughout the system under study. A Coulomb or a radial flow [56] field will prevent the growth of fluctuations across the whole system much like the chemical potential gradient caused by the gravitational field is limiting the usable sample size in earthbound experiments on liquids [20].

All those points will have to be addressed before the experimental results can be connected to the parameters of bulk nuclear matter in a quantitative way.

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