Phase Transitions in Nuclear Systems

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Abstract

The influence of finite size and surface effects on the determination of critical exponents is investigated in the context of the Ising model. A new method for the determination of critical parameters is presented.

1 Introduction

Based on the similarity between van der Waals and nucleon - nucleon forces the existence of phase transitions in nuclear matter and neutron stars was proposed more than 20 years ago [1, 2]. The observation of a power law for the fragment mass distribution in proton induced reactions was interpreted as an indication of a critical phenomenon [3] and sparked much interest in the role of the liquid-gas phase transition in the disintegration of highly excited nuclei [4, 5]. It was proposed to deduce critical parameters [6] and critical exponents [7]. This goal remained elusive, despite some early efforts [8, 9, 10], until the recent attempt

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System	τ	σ	β	γ	ν
3d percolation	2.18	0.45	0.41	1.80	0.88
3d Ising	2.21	0.64	0.327	1.239	0.629

Table 1: Critical exponents for 3d percolation (from [14]) and Ising models (from [25]). The Ising values for τ and σ were deduced from the scaling relations Eq. (3). Note that the liquid-gas phase transition has the same exponents as the Ising model.

of the Purdue group to determine the full set of critical exponents from exclusive fragmentation data [11, 12]. Even if one ignores the fact that a decaying fragment is a transient system, e.g. by minimizing dynamical effects [13] by studying light-ion induced reactions or peripheral collisions in more symmetric systems, one still faces the question of what the unambiguous signatures of critical behavior and robust methods for the determination of critical parameters and exponents in small systems with only 100 - 200 constituents are.

Following a proposal of Campi [7, 10], it has become customary to use percolation as a testing ground for analysis methods. Percolation on a large lattice exhibits many signatures of a second order phase transition [14], describes the formation of clusters and thus relates directly to observables of fragmentation experiments. Furthermore, calculations on small lattices show remarkable similarities to nuclear data [15, 16]. However, the percolation transition is not a thermal phase transition. The critical exponents - especially ν, which describes the divergence of the correlation length, and σ, which relates to the cluster shape - are substantially different from the values for the liquid-gas phase transition (see Table 1). This might translate into different finite size effects for small systems and raises the question whether methods tested in the percolation case can be generalized to the nuclear case. It is therefore interesting to investigate the finite size effects in other models. In the first part of this contribution we study the determination of critical exponents in small Ising lattices in the hope of learning more about the limiting factors of such an analysis. In the second part we focus on the determination of critical parameters.

2 Finite Size Effects in the Ising Model

One of the simplest systems with a thermal phase transition is the Ising model. It describes a two-state spin system ($s_i = \pm 1$) on a regular lattice with the Hamiltonian

$$\mathcal{H} = -J \sum_{<i,j>} s_i s_j - \mu_B H \sum_i s_i$$

containing a next-neighbor interaction and a coupling to an external field H. For zero external field the Ising model exhibits a ferromagnetic to paramagnetic phase transition where the order parameter, here the magnetization per spin $M = \frac{1}{N}\sum s_i$, vanishes and susceptibility $\chi = \frac{\partial M}{\partial H}$ and correlation length ξ diverge when the temperature approaches a critical value T_C:

$$M \sim t^{\beta} \qquad \chi \sim |t|^{-\gamma} \qquad \xi \sim |t|^{-\nu} \qquad \text{with} \quad t = \tfrac{T}{T_C} - 1. \tag{1}$$

Invoking a model which describes a spin system seems farfetched, but the equivalence of the Ising and lattice gas models, where the magnetization maps to the density difference between liquid and gas phase and the susceptibility to the isothermal compressibility, provides a direct connection to the liquid-gas phase transition [17]. Furthermore, the Ising model is, unlike percolation, in the same universality class as the liquid-gas phase transition, and has thus the same critical exponents.

Order parameter and susceptibility are not directly accessible in nuclear physics experiments which usually determine cluster size and velocity distributions. The connection can be made using Fisher's droplet model [18] which predicts for the concentration of clusters of size s the relation

$$n_s = q_0\, s^{-\tau}\, X^{s^{\sigma}} Y^{s} \tag{2}$$

with two critical exponents τ and σ and the surface and volume terms

$$X = \exp\left(-\tfrac{\Delta F_s}{k_B T}\right) \qquad\qquad Y = \exp\left(-\tfrac{\Delta F_v}{k_B T}\right)$$

containing the surface and volume free energies F_s and F_v. Below T_C most spins will point into the direction of the spontaneous magnetization. With the ansatz that clusters of reversed spins can be described by Eq. (2), thus

$$M = 1 - 2\sum_s s n_s,$$

and the plausible assumption that the surface free energy F_s is independent of H and the volume free energy F_v is proportional to H (for a derivation see [19]) one obtains

$$\chi \propto \tfrac{1}{k_B T}\sum_s s^2 n_s.$$

The second moment of the cluster size distribution is therefore a measure of the susceptibility. With a little more algebra one gets the exponent relations

$$\tau = 2 + \frac{\beta}{\beta+\gamma} \qquad\qquad \sigma = \frac{1}{\beta+\gamma}. \tag{3}$$

An analogous argument can be derived for the liquid-gas phase transition [18] and forms the basis of the determination of γ and β from the second moment of the cluster size distribution and the size of the largest cluster, respectively [12].

For simplicity and numerical efficiency, but also because the proper definition of a cluster is non-trivial for the Ising model [20, 21, 14], we restrict this study to the determination of exponents from the magnetization.

2.1 Finite Size Scaling

In a finite system with a linear size L the divergences found in an infinite system will be reduced to a mere peaking. Since correlations cannot grow larger than L, it's a natural ansatz [22] to assume that L/ξ is the relevant variable to describe the size dependence. Since $L/\xi \sim Lt^\nu$ one expects that

$$x = tL^{1/\nu} \tag{4}$$

is a good scaling variable. Rewriting Eq. (1) in terms of x yields

$$ML^{\beta/\nu} \sim x^\beta \qquad\qquad \chi L^{-\gamma/\nu} \sim x^{-\gamma}$$

and introducing scaling functions X and Y gives the finite size scaling relations [23, 25]

$$M = X_{(x)} L^{-\beta/\nu} \qquad\qquad \chi = Y_{(x)} L^{\gamma/\nu} \tag{5}$$

with $X_{(x)} \sim x^\beta$ and $Y_{(x)} \sim x^{-\gamma}$ for $L \to \infty, t \to 0$. The size dependence of magnetization and susceptibility is therefore determined by the same exponents which describe the temperature dependence for the infinite system. It is important to note that Eq. (5) is valid not only at the critical temperature ($x = 0$) but at any value of x as long as scaling holds, e.g. at the position x_m of the susceptibility maximum given by $\frac{\partial Y}{\partial x}_{|x_m} = 0$.

The relations (5) allow only the determination of the exponent ratios β/ν and γ/ν. However, it has been shown [24] that the temperature derivative of the renormalized coupling constant g_r defined by

$$g_r = \frac{< M^4 >}{< M^2 >^2} - 3$$

varies like $L^{1/\nu}$ and therefore allows to determine ν. Evaluating Eqs. (4) and (5) at x_m and introducing another scaling function G for $\frac{\partial}{\partial T} g_r$

$$\begin{array}{rcl} \chi_{m(L)} = \chi_{(x_m,L)} & = & Y_{(x_m)}\, L^{\gamma/\nu} \\ M_{(x_m,L)} & = & X_{(x_m)}\, L^{-\beta/\nu} \\ \frac{\partial}{\partial T} g_{r\,(x_m,L)} & = & G_{(x_m)}\, L^{1/\nu} \\ T_{m(L)} & = & T_C\,(1 + x_m L^{-1/\nu}) \end{array} \tag{6}$$

leads then to a method of deducing the exponents ν, β and γ and the critical temperature T_C from the size dependence of m and χ:

$$\begin{array}{llrlrll} \text{1. determine } M_{(T)} \text{ and } \chi_{(T)} \text{ for different system sizes } L & & & & & & \\ \text{2. find position } T_m \text{ and height } \chi_m \text{ of the susceptibility maximum} & & & & & & \\ \text{3. plot} & \ln \chi_m & \text{vs} & \ln L & \text{slope} & \Longrightarrow & \gamma/\nu \\ & \ln M_{(T_m)} & \text{vs} & \ln L & \text{slope} & \Longrightarrow & -\beta/\nu \\ & \ln \frac{\partial}{\partial T} g_{r(T_m)} & \text{vs} & \ln L & \text{slope} & \Longrightarrow & 1/\nu \\ & T_m & \text{vs} & L^{-1/\nu} & \text{intercept} & \Longrightarrow & T_C \end{array} \tag{7}$$

It should be noted that the determination of the exponents is independent of the determination of T_C. Furthermore, any other definition of the size dependent transition temperature $T_{m(L)}$, e.g. using the maxima of the specific heat, $\frac{\partial}{\partial T} g_r$ or $\frac{\partial}{\partial T} \ln M$, is conceptually equivalent and only means using Eqs. (6) at a different value of x_m.

The procedure (7) is a simplified variation of the method used in a recent precision study by Ferrenberg and Landau [25]. They determined exponents and T_C with a precision of about 1% and 10^{-5} respectively by using lattices in the range $L = 8, \ldots, 96$ and taking first order corrections to scaling into account. In the following we use their results, denoted as 'correct' values, as a reference representing the properties of an infinite lattice and investigate whether exponents can also be determined from systems with a size typically found in nuclear physics experiments.

We will study lattices with periodic boundary conditions - the first and last spin in each direction are treated as neighbors - as well as with open boundary conditions. The former case treats only the finite size effects caused by the cutoff in the correlation length whereas in the later case also explicit surface effects are taken into account.

2.2 Simulation Results

The finite size behavior of the 3d Ising model on a simple cubic lattice was studied numerically with a standard Metropolis sampling algorithm [26]. The units were fixed with $J = \mu_B = k_B = 1$. The 'finite lattice' susceptibility was determined from magnetization fluctuations at $H = 0$

$$\chi = \frac{N}{T} \left(\left\langle |M|^2 \right\rangle - \langle |M| \rangle^2 \right)$$

whereas temperature derivatives of any quantity Q were deduced from the correlation with the total energy U

$$\frac{\partial Q}{\partial T} = \frac{1}{T^2} \left(\langle UQ \rangle - \langle U \rangle \langle Q \rangle \right) .$$

The temperature dependence of magnetization and susceptibility is presented in Fig. 1 for system sizes in the range $L = 2, \ldots, 24$. The data for periodic boundary conditions show

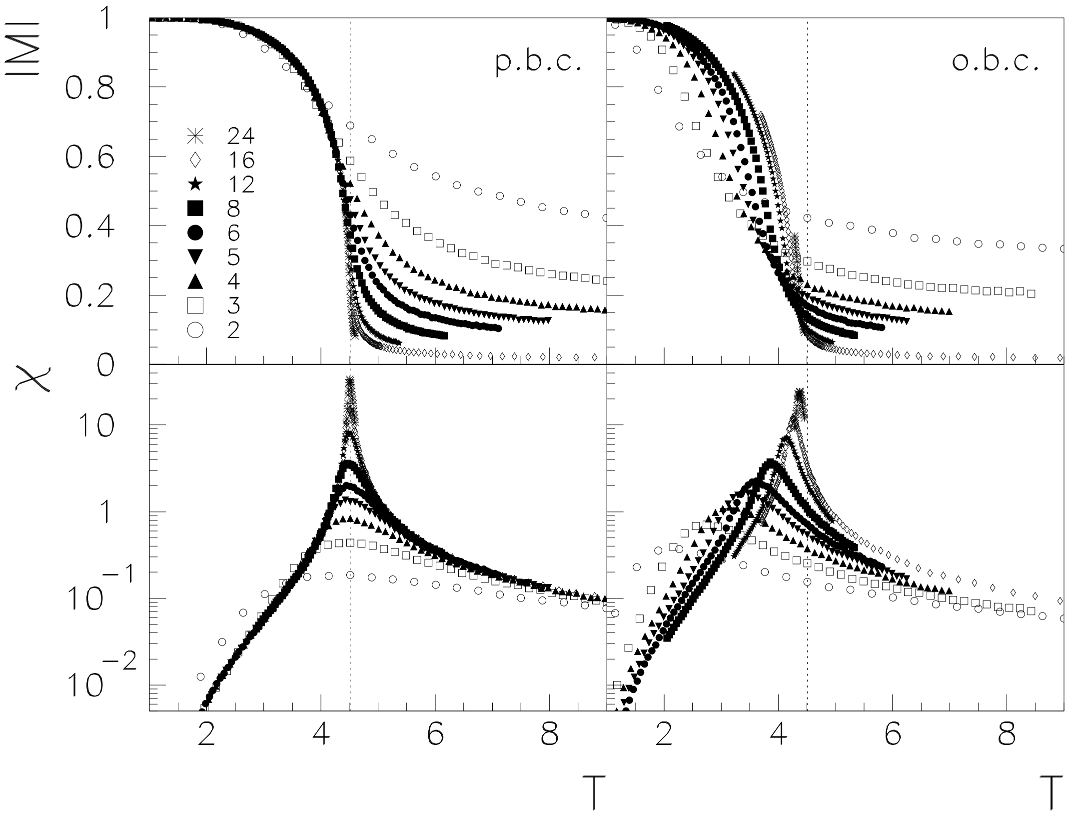

Figure 1: Magnetization $|M|$ (top row) and susceptibility χ (bottom row) for system sizes in the range $L = 2, \dots, 24$ with periodic (left column) and open (right column) boundary conditions. The correct value of T_C is indicated by a dashed line.

only a more pronounced rounding of the susceptibility peak for smaller systems, whereas for open boundary conditions one observes, in addition, a shift of the peak position towards lower temperatures.

Fig. 2 shows the four plots listed in (7). The exponents and T_C were determined with a fit for the system sizes $L = 4$, 5 and 6, which is representative for typical nuclear sizes of 64 to 216 constituents. For periodic boundary conditions one finds, except for the T_m vs $L^{1/\nu}$ plot, remarkably small deviations from a linear correlation even down to the smallest system size of $L = 2$. For open boundary conditions, the deviations tend to be larger, especially for the correlation which determines the exponent ν. The extracted exponents and T_C are summarized in Table 2. The values for periodic boundary conditions agree within about 10% with the precision values from [25], whereas the values for open boundary conditions differ by up to 35% and are systematically too high. The last row in

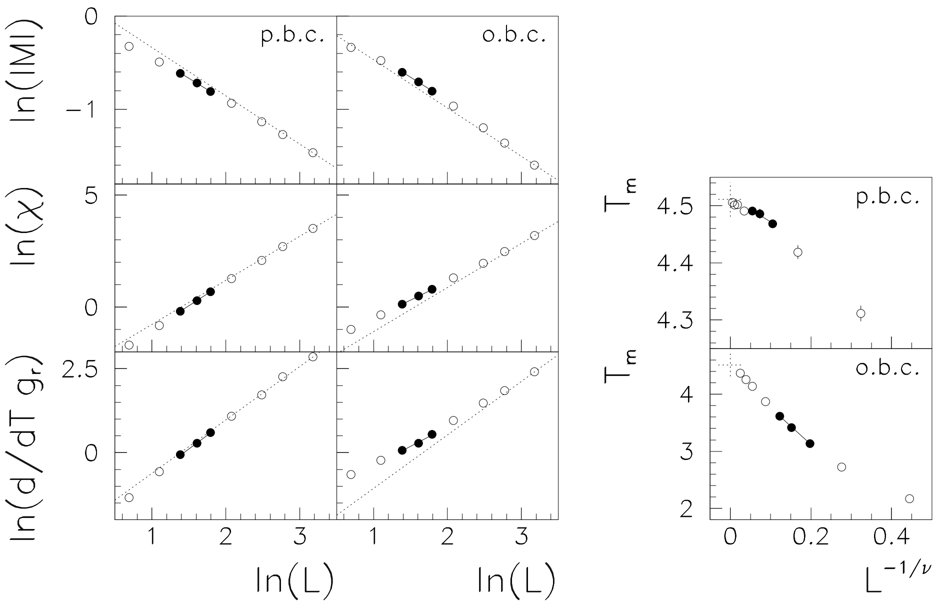

Figure 2: Relations used to extract the exponents and T_C. The full dots denote the data points used in the fits (L = 4, 5 and 6), the solid line the linear fit. The dotted lines in the left panel indicate the slope corresponding to the correct values of the exponents. The dotted crosses in the right panel indicate the correct value of T_C.

Table 2 serves to check the hyperscaling exponent relation

$$d = \frac{\gamma}{\nu} + 2\,\frac{\beta}{\nu} \qquad \text{with} \qquad d = \text{dimension.}$$

The finite size scaling relations, Eqs. (5), can be tested by plotting the quantities

$$ML^{\beta/\nu} \quad \text{vs} \quad tL^{1/\nu} \qquad \text{and} \qquad \chi L^{-\gamma/\nu} \quad \text{vs} \quad tL^{1/\nu}$$

as shown in Fig. 3. If scaling holds, the data for all system sizes should fall on two curves, the scaling functions $X_{(x)}$ and $Y_{(x)}$. The periodic boundary condition data in the left column group together very well whereas the open boundary condition data in the middle column exhibit a substantial scatter and only the tendency to group for the largest system sizes. The correct values for exponents and T_C were used for the left and middle column of Fig. 3. In the right column, we have replotted the open boundary condition data using the exponents and T_C deduced from the small lattices. The small system sizes now group fairly well, only the larger sizes tend to deviate from a common curve. However, this is not too astonishing because the data for L = 4, 5 and 6 should group by construction, and serves only to illustrate how difficult it is to test scaling for a small range of system sizes.

	p.b.c.	o.b.c.	Ref. [25]
β	0.29	0.42	0.327
γ	1.29	1.40	1.239
ν	0.61	0.85	0.629
T_C	4.51	4.4	4.511
$\frac{\gamma}{\nu} + 2\frac{\beta}{\nu}$	3.07	2.64	3.009

Table 2: Critical exponents extracted from systems of size $L = 4$, 5 and 6.

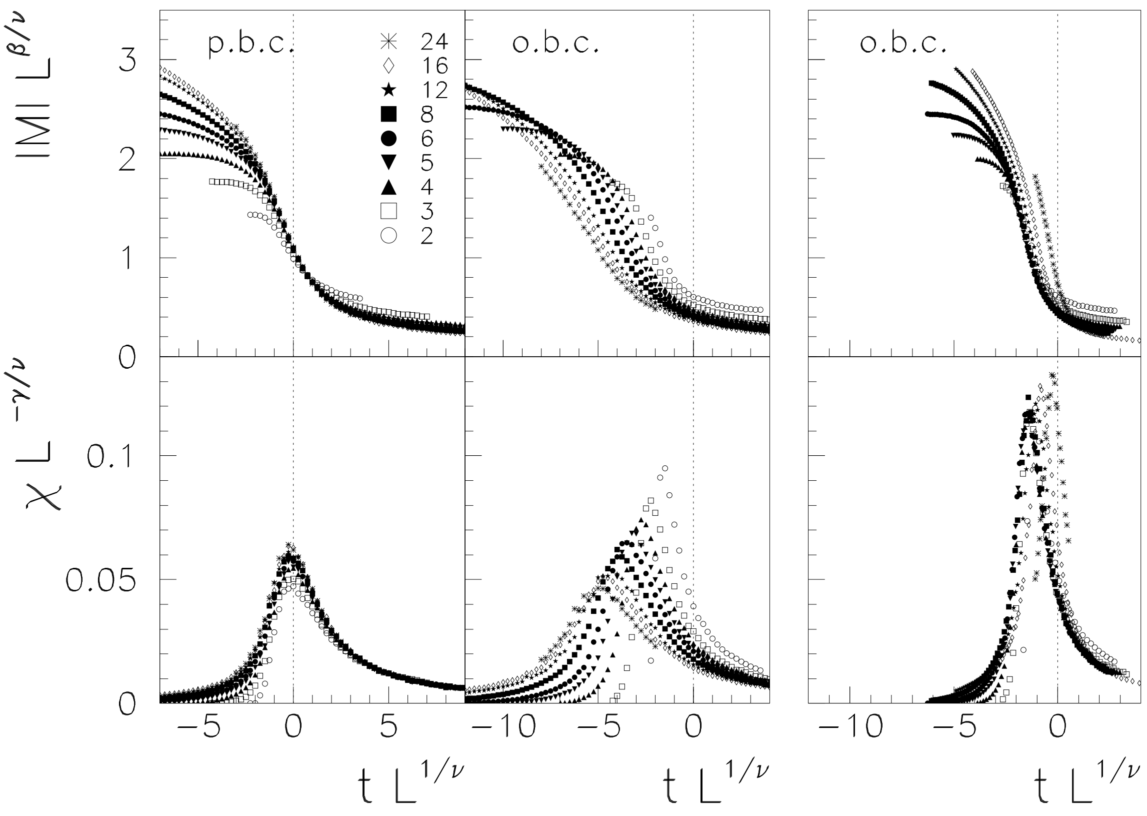

Figure 3: Plots of the scaled magnetization (top) and susceptibility (bottom) as a function of the scaling variable $x = tL^{1/\nu}$. The correct values for the exponents were used for the left and middle column whereas the exponents deduced from open boundary conditions were used in the right column.

In summary, we found that it is indeed possible to obtain quite accurate estimates for the critical exponents from small systems if periodic boundary conditions are used. For open boundary conditions, the extracted exponents show a much larger deviation from the values determined with large lattices. This can be attributed to the fact that lattices with open boundary conditions enter the scaling regime at much larger sizes than lattices with periodic boundary conditions so that corrections to scaling play a much larger role in the former case. It can, at least in part, also be interpreted as the consequence of surface contributions which cause additional terms in the scaling relations with surface exponents $\beta_s = \beta - \nu$ and $\gamma_s = \gamma + \nu$ [23]. This means, if it can be generalized to the nuclear case, that critical exponents extracted from fragment size distributions should be interpreted as effective exponents, containing surface and volume contributions, and not be directly identified with the exponents of bulk nuclear matter.

3 Determination of Critical Parameters

It has long been recognized that the apparent exponent τ_{eff} obtained by the fit of a power law $\sigma_{(Z)} \propto Z^{-\tau_{\text{eff}}}$ to the fragment size distribution exhibits a minimum when plotted versus the temperature or the bombarding energy [8, 9, 27]. It had been suggested to associate the minimum value of τ_{eff} with the critical exponent τ and the position of the minimum with the experimental conditions leading to a second order phase transition [8]. A closer examination of the fragment size distribution given by the Fisher droplet model [18] (see Eq. 2), however, showed that the interplay between surface and volume terms leads to a minimum of τ_{eff} at temperatures substantially below the critical temperature [9]. The correct way to determine the critical temperature using the droplet model is therefore to fit the fragment size distribution with the full expression (2) and search for the conditions leading to $X = Y = 1$. A fit with q_0, τ, σ, X and Y as free parameters is usually not feasible and in practice one or both exponents are fixed to the values of the liquid gas phase transition [9, 28].

A different way to reduce the number of fit parameters is to recognize that the surface tension vanishes at and above the critical temperature. This implies $X = 1$ and Eq. (2) reduces to the product of a power law and an exponential

$$n_s = q_0\, s^{-\tau_1}\ \exp\left(\frac{s}{m_0}\right) \tag{8}$$

with three free parameters q_0, τ_1 and m_0. This functional form should describe the cluster size distribution on the 'gas side' and m_0 should tend to large values, effectively reducing (8) to a power law, when the critical point is approached.

This was tested with data from a percolation simulation on a cubic lattice. Cluster size distributions in the range $2 \leq s \leq L^3/3$ were fitted with Eq. (8) and for comparison with

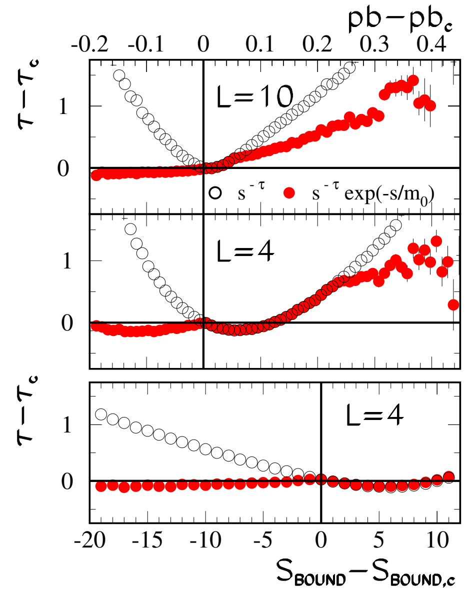

Figure 4: Deviation of the fitted τ values from the correct value $\tau_c = 2.18$ for fits with a pure power law (circles) and Eq. (8) (dots) versus the deviation of the control parameter from its critical value.

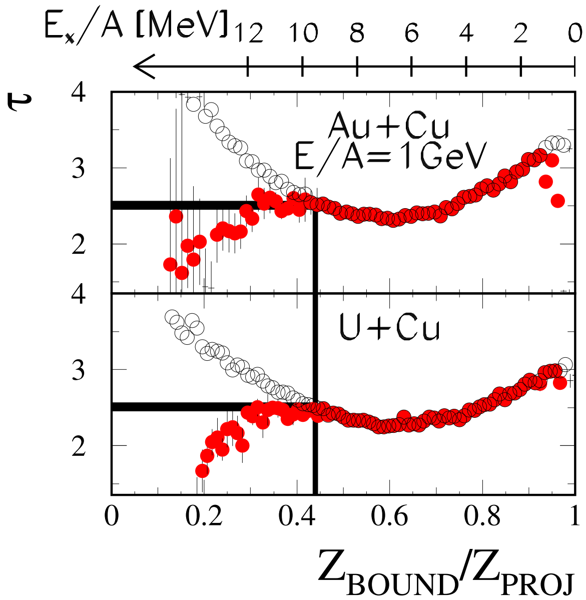

Figure 5: Apparent exponents τ versus reduced Z_{BOUND} for Au + Cu and U + Cu reactions at E/A = 1 GeV.

a pure power law $n_s = q_0\, s^{-\tau_2}$. The relationship between the extracted τ values and the bond probability pb is shown in the upper part of Fig 4. For small values of pb, in the 'gas phase', τ_1 is indeed close to the correct value $\tau_c = 2.18$ whereas τ_2 is substantially larger. When the critical region is approached τ_1 and τ_2 tend to the same value indicating that the cluster size distribution can now be described with a pure power law. Independent of the system size this transition takes place at the critical bond probability $pb_c = 0.249$ of the infinite lattice and exhibits a remarkably clear signature even for systems as small as $L = 4$.

Fragmentation reactions produce a broad distribution of system sizes and excitation energies. Therefore an estimate of the control parameter has to be determined event by event from the data itself. The potential distortions due to such a control parameter substitution were investigated by binning the percolation events according to $S_{\mathrm{BOUND}} = \sum_{s\geq 2} s$, the analogue of the observable Z_{BOUND} used to characterize the energy deposition in nuclear collisions [29]. The bottom part of Fig 4 shows that even in this case one obtains an exponent close to the correct τ value and a critical S_{BOUND} which coincides with the average S_{BOUND} evaluated at the correct critical bond probability pb_c. The transition of the cluster size distribution shape to a pure power law is therefore a robust signature of the critical value of the control parameter in percolation.

The application of this method to projectile fragment distributions of Au and U induced reactions is demonstrated in Fig 5. In both cases we find the transition at $Z_{\mathrm{BOUND}}/Z_{\mathrm{PROJ}} \approx 0.43$, corresponding to an excitation energy per nucleon of approximately 9-10 MeV [29], and a τ value of 2.5 ± 0.1. Caution should be exercised, however, when this result is interpreted in terms of a critical parameter, in this case the critical excitation energy. The relation between temperature and the excitation energy exhibits a plateau - the temperature stays close to 5 MeV for excitation energies per nucleon between 3 and 10 MeV - suggestive of a phase transition of first order with a substantial latent heat [30, 31]. It is intriguing to see that the excitation energy associated with the transition to a pure power law coincides with the upper end of this plateau. Even though it is plausible that in a finite system some observables show signs of critical behavior while others exhibit features of a first order transition [31], it remains a challenging task for the future to develop a consistent picture - including effects of the long range Coulomb force and of the dynamical evolution of the system - and to extract quantitative estimates of phase transition parameters.

J.P. and M.B. acknowledge the financial support of the Deutsche Forschungsgemeinschaft under the Contract No. Po256/2-1 and Be1634/1-1, respectively. This work was supported in part by the European Community under contract ERBCHGE-CT92-0003 and ERBCIPD-CT94-0091.

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