About the determination of critical exponents related to possible phase transitions in nuclear fragmentation

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Abstract. We introduce a method based on the finite size scaling assumption which allows to determine numerically the critical point and critical exponents related to observables in an infinite system starting from the knowledge of the observables in finite systems. We apply the method to bond percolation in 2 dimensions and compare the results obtained when the bond probability $p$ or the fragment multiplicity $m$ are chosen as the relevant parameter.

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1. Introduction

Phase transitions are phenomena which are related to infinite systems. Hence the quantities which characterize these phenomena must be related to infinite systems. In fields like solid state physics this can be more or less easily realized since the systems which are considered can most of the time be assimilated to infinite systems. But this is not the case in nuclear physics where nuclei contain at most a few hundred constituents.

Among the most striking features which are observed in the study of nuclear fragmentation emerges the fact that there are signs for the existence of a phase transition. This phenomenon is commonly under scrutiny nowadays, both experimentally and theoretically. There are indications for the existence of a first order transition but its existence is not clearly established up to now [1-4]. On the other hand, charge distributions of fragments obtained in peripheral collisions show universal properties [5] which are conspicuously compatible with bond percolation [6] and phase space models which describe excited and disordered systems [7,8]. If one relies on a percolation-type interpretation of these results, it is tempting to conclude that one is confronted with the existence of a second order phase transition whose characteristic features are smoothed by finite size effects.

The fascinating perspective that it might be possible to unravel the existence of a phase transition in nuclear matter motivated the attempt to extract more precise information about this kind of phenomenon. Such information is given by the numerical values of critical exponents which allow to fix the class to which the observed phase transition belongs. The most important exponents are $\nu$ which governs the correlation length $\xi$, $\sigma$ which characterizes the behaviour of $m_2/m_1$ ($m_k$ is the moment of order $k$ of charge or mass distributions), $\beta$ which fixes the behaviour of $m_1$ close to the critical point, $\tau$ which gives the slope of the power law distribution at the critical point and $\gamma$ which governs the strength of the singularity of $m_2$ at this point. These quantities are connected by universal relations [16].

The determination of critical exponents raises however two intimately related points. The first one concerns the obtention of these quantities from observables which characterize finite systems and hence do not show any singularity as they do for infinite systems. This is a conceptual problem which, to our opinion, is fundamental. The second point which is directly linked to it concerns the direct extraction of exponents from finite size model results or experimental data necessarily obtained from systems of finite size $L$, especially in the case of nuclei. Any
such attempt leads inevitably to a size-dependence of any “exponent” say $\alpha$, i.e. $\alpha = \alpha (L)$. As a consequence, it gets difficult if not impossible to compare these quantities to corresponding reference exponents characterizing well-known systems, like the liquid-gas, percolation or magnetic systems, which have been worked out in the infinite limit and fix the universality class to which the considered system belongs. The possibility to extract critical exponents from finite size systems has been attempted in refs. [9-11] and was followed by controversial debates [12,13].

In the sequel we aim to present and use a new numerical approach which has been worked out recently in order to analyze finite size calculations in the 2D and 3D Ising models [14]. The method relies on the finite size scaling (FSS) assumption [15].

2. The method

We sketch here the essential steps which lead to the determination of the critical point and critical exponents for infinite systems starting from finite systems of different sizes $L$ in spaces of any physical dimension.

Consider an observable $O_L(\Delta t)$ characterizing a finite system of linear size $L$ where $\Delta t$ measures the distance of the variable $t$ to its value at the critical point $t_c$, $\Delta t = (t_c - t)/t_c$, $\Delta t > 0$. Define $x(L, t) \equiv \xi_L(t)/L$, where $\xi_L(t)$ is the correlation length in the system of size $L$ for a fixed value $t$ of the relevant variable. Then the FSS assumption states that

$$O_L(\Delta t) = O(\Delta t) \cdot Q_O(x(L, t))$$

where $Q_O(x(L, t))$ is a so called scaling function and $O(\Delta t)$ fixes the value of the observable in the corresponding infinite system. The remarkable property of $Q_O(x)$ is the fact that it is universal, which means here that it is independent of $t$ for different values of $x$ in the range $[0, t_c]$ of the variable $t$.

It comes out that quantities like $\xi_L(\Delta t)$ and other observables $O_L(\Delta t)$ converge to a finite value with increasing $L$. Hence, if $O_L(\Delta t)$ is known for different values of $L$ and if its asymptotic value with increasing $L$, $O(\Delta t)$, can be numerically reached the scaling function $Q_O(x(L, t))$ can be obtained through (1). Once this quantity is known for different values of $x \equiv \xi_L(t)/L$, it can be used to get

$$O(\Delta t) = O_L(\Delta t)/Q_O(x) \sim \Delta t^{-\alpha} \sim (t_c - t)^{-\alpha}$$

where $t_c$ is the critical point and $\alpha$ the corresponding exponent.
In practice, once $Q_O(x)$ is numerically known it can be easily parametrized in terms of polynomials in $x$ or some other function of $x$ [14]. The knowledge of $Q_O$ and $O_L(\Delta t)$ gives $O(\Delta t)$ through (2), the numerical result can be fitted to an expression like $(t_c - t)^{-\alpha}$ through which $t_c$ and $\alpha$ can be determined. The accuracy of the fits can be controlled by means of $\chi^2$ tests.

3. Application to 2D percolation

We have checked the applicability of the method presented above on the 2D bond percolation problem on a square lattice for which the numerical values of the critical exponents are well known [16]. In the sequel we restrict ourselves to the explicit calculation of $\nu$, $\gamma$, $\sigma$ and the critical point. We try to obtain these quantities through the determination of $\xi_L(\Delta t)$, $m_{2L}(\Delta t)/L^2$ and $m_{2L}(\Delta t)/m_{1L}(\Delta t)$ where $L$ is the linear size of the 2D lattice and $t$ stands either for $p$ (bond probability) or $m$ (cluster multiplicity).

The choice of $m_{2L}(\Delta t)/L^2$ deserves a comment. In practice we are interested in $m_{2L}(\Delta t)$, but this quantity does not converge to any finite value when $L$ goes to infinity, whatever $t$ (extensive quantity). We found no rigorous mathematical proof for the convergence of the aforementioned quantity to a constant asymptotic value with increasing $L$. It is however trivial to see that $m_{2L}/L^2 = 1$ when $t = p = 0$. It is equal to 0 when $t = p = 1$ (the heaviest cluster is not taken into account). Furthermore, numerical tests indicate that this quantity may indeed reach an asymptotic value, although this value is reached for larger and larger values of $L$ when $t (p, m)$ gets closer and closer to $t_c$. We discuss this point in the sequel. If this convergence property is fulfilled, one faces a second point which is the question whether the exponent and location of the critical point are the same for $m_{2L}$ and $m_{2L}/L^2$ when $L$ is infinite. One can convince oneself that the corresponding scaling functions $Q$ are not the same. The tests presented below confirm that $t_c$ and the exponent are in numerical agreement with the known values [17]. Finally, it is easy to show that $m_{1L}/L^2$ tends to 1 with increasing $L$. Hence $m_{2L}/m_{1L}$ reaches a constant limit for very large systems and allows to extract in principle the exponent ($\sigma$ or $\tilde{\sigma}$, see below).

Calculations and the results which will be shown correspond to systems without periodic boundary conditions. Comments about calculations made for systems with periodic boundary conditions will be made below.
3a. Calculations with the bond probability $p$

We have determined the correlation length $\xi_L(\Delta p)$, the normalized second moment $m_{2L}(\Delta p)/L^2$ and the ratio $m_{2L}(\Delta p)/m_{1L}(\Delta p)$ for $L$ up to 1 000 and different values of $p$ in the interval $[0.40, 0.48]$ in steps of $\Delta p = 0.01$. For each value of $p$ we generated $10^4$ events. The critical value is $p_c = 0.5$. Fig. 1 shows the behaviour of the observables. As it can be seen, these quantities tend to reach a constant value. One may notice that this saturation effect is better realized for smaller values of $p$ and more effective for $\xi_L$ than for $m_{2L}$. As it can be seen on the figure, it is not effectively reached for the highest value of $p$. The consequences of these observations will be seen below.

We retain the asymptotic values reached by the observables as those which correspond to the infinite system and use them in order to get the universal scaling functions $Q_\xi$, $Q_{m_{2L}/L^2}$ and $Q_{m_{2L}/m_{1L}}$ through (1). Fig. 2 shows examples of these quantities obtained for different values of $p$ and represented as functions of $x = \xi_L/L$. Universality requires that all contributions from different $p's$ lie on each other and asymptotic saturation requires that the $Q's$ reach a constant value (equal to 1) for $x$ close to 0. The universality functions are fit to polynomial in $x$, see eq. (14) in ref. [14]. Finally these quantities are used in order to determine $p_c, \nu, \gamma$ and $\sigma$ by means of a fit procedure to the quantities relevant to the infinite system, i.e.

$$\xi_\infty \simeq (p_c - p)^{-\nu}$$

and

$$m_{2\infty} \simeq (p_c - p)^{-\gamma}$$

and

$$m_{2\infty}/m_{1\infty} = (p_c - p)^{-1/\sigma}$$

The quality of the fits is estimated by means of $\chi^2$ analyses. Fig. 3 shows a typical example of the calculations. In practice we worked with many different intervals of $p$ values in the range $[0.40, 0.48]$ over which we averaged. We retained those results which correspond to the smallest $\chi^2$ values, with a confidence level of 95%.

Results are shown in Table 1 and Fig. 4. The exponents are calculated from systems of different sizes. They are in an overall good agreement with the exact values [17]. One notices however that $\nu, \gamma$ and $1/\sigma$ decreases with increasing $L$, $\nu$ gets closer to the exact value while $\gamma$ and $1/\sigma$ get away from it. Introducing periodic
boundary conditions leads to values which remain very close to those which do not 
take them into account. In practice, the two types of calculations differ essentially 
in the way asymptotic saturation of the observables is reached, the rise being steeper 
when periodic boundary conditions are taken into account.

3b. Analysis and discussion of the FFS method

As mentionned above, we have tested the present method by choosing different 
intervals in $p$ lying more or less close to $p_c$. If the interval is taken for, say between 
0.30 and 0.40, the exponents are robust with respect to the value of $L$ from which 
they are extracted. The exponents are however sizably smaller than the exact known 
values [19]. If the interval approaches $p_c$, they come closer to the exact value but 
they are less robust with respect to $L$, as already mentionned.

These ascertainments have a common origin. In principle, the universal func-
tions $Q_O$ are obtained from the asymptotic constant limit of $O$. This limit with 
increasing $L$ is easily reached when $p$ is small. If however $p$ comes close to $p_c$, higher 
values of $L$ are needed in order to reach this limit. It comes out that this limit is 
more easily reached for $\xi L$ than for $m_{2L}/L^2$ and $m_{2L}/m_{1L}$. This reflects on the 
behaviour of $Q_\xi$, $Q_{m_{2L}/L^2}$ and $Q_{m_{2L}/m_{1L}}$. Indeed, one can observe that for values of 
$L$ up to 1000, $Q_\xi$ reaches a plateau for the smallest values of $x = L/\xi L$, whereas 
one can hardly see this effect for $Q_{m_{2L}/L^2}$ and $Q_{m_{2L}/m_{1L}}$. This means in practice 
that one needs to determine the considered observables for values of $L$ which are 
sizably larger than $L = 1000$. We did not work these cases since it is not our aim 
to work the exponents for 2D percolation which are well known, but rather test a 
method and its efficiency.

It is possible to find an explanation for the difference in the asymptotic be-
avour of the considered observables. It is easy to observe that the rate of con-
vergence with $L$ decreases with increasing values of the exponents. This fact can 
also be observed in the determination of exponents in ref. [14]. Indeed $\gamma$ and $1/\sigma$ 
are much larger quantities than $\nu$. Larger exponents correspond to steeper increase 
of the corresponding observable, hence a larger sensitivity to the precise numerical 
determination of this observable. One may remark that the exponent $\gamma$ is sizably 
smaller ($\simeq 1.8$) in 3D bond percolation systems. We conjecture that one may need 
smaller values of $L$ in order to reach the asymptotic regime.
A confrontation of a percolation model determination of observables like \( m_2 \) and \( m_2/m_1 \) with experiment [10] is possible if one uses the fragment and particle reduced multiplicity \( m \) [20] (multiplicity divided by \( L^2 \)). It is numerically easy to relate \( p \) to an average value of \( m \), \( \langle m \rangle \). It is then tempting to work out the behaviour of the quoted observables \( \xi_L, m_{2L}/L^2 \) and \( m_{2L}/m_{1L} \) and to confront the exponents \( \tilde{\nu}, \tilde{\gamma} \) and \( \tilde{\sigma} \) with \( \nu, \gamma \) and \( \sigma \) obtained with the bond probability \( p \).

We repeated the preceding calculations with \( m \), following the same procedure as described in section 3a. For a given \( m \) the events were selected out of a uniform distribution in \( p \). For each value of \( m \) we generated 2 500 events. The same remarks as those presented above are valid in the present case. However, as it can be seen in Table 1, the corresponding exponents \( \tilde{\nu}, \tilde{\gamma} \) and \( \tilde{\sigma} \) are no longer numerically compatible with \( \nu, \gamma \) and \( \sigma \). In fact, \( \tilde{\nu} \) and \( \tilde{\gamma} \) are systematically smaller than \( \nu \) and \( \gamma \) whereas \( \tilde{\sigma} \) is larger than \( \sigma \). This result contradicts the findings presented in ref. [12]. One can convince oneself that the discrepancy cannot be attributed to the convergence trouble quoted above, this discrepancy remains for \( \tilde{\nu} \) corresponding to \( \xi_L \), for which the saturation problem is much less acute than for \( \tilde{\gamma} \) and \( \tilde{\sigma} \). In fact, this result is not really surprising for us. Indeed, the relation between \( p \) and \( \langle m \rangle \) is definitely not linear in the neighbourhood of \( p_c \) as it seems to be for 3D percolation on Fig. 7 of [12].

The calculations have been repeated for systems with periodic boundary conditions. As before, the values of the exponents lie within the error bars obtained in the case of open boundaries.

4. Summary, discussion and conclusions

We have used a rather simple method relying on the finite size scaling (FSS) assumption which has earlier been tested on the 2D and 3D Ising model [14]. The method allows the rigorous determination of critical exponents characterizing second order phase transitions in genuine infinite systems.

The method is numerically simple, in principle robust, and should deliver exponents with a very good precision. We verified that it is indeed possible to get values which lie within a few percent of the exact value with a rather modest amount of work. The central point lies in the fact that one must determine the asymptotic value of the corresponding observables as cleanly as possible. This means that it is
necessary to determine these observables for larger and larger systems. The maximum size corresponding to the asymptotic (infinite size) regime depends on the observable itself and empirical experience shows that it depends upon the magnitude of the exponent itself. There exists of course methods which give much more precise exponents [17,18] but they are numerically much more sophisticated than the present one.

In the present work we have concentrated on the academic example of 2D bond percolation and seen that the exponents depend on the relevant parameter (bond probability $p$ or cluster multiplicity $m$) which is used. One may ask oneself whether and how the FSS method could be applied to a realistic physical case such as nuclear fragmentation. As we already said in the introduction, the determination of critical exponents requires rigorous information about the infinite system. This shows that the determination of exponents for nuclear systems may be quite difficult. Indeed nuclei are very small (number of coexisting nuclei $\approx 300 - 400$ in heavy ion collisions), unlike systems found in condensed matter physics where surface effect can be made negligible if the considered samples are large enough.

The necessary reference to the infinite system also shows that there exists no direct way to extract exponents from experimental data. One way one may think about consists of working out a model which reproduces the experimental observables obtained for fixed finite sizes $L$. One may then extrapolate the model to $L = \infty$ in the FSS framework and determine the exponents the way which was described above. If the observables can be determined experimentally for several sizes (f.i. $L_1$ and $L_2$) and if they are in agreement with the model then, using the notations of section 2, these observables must verify the scaling relation

$$O_{L_1}^{\text{exp}}(\Delta t)/O_{L_2}^{\text{exp}}(\Delta t) = Q_O(x(L_1,t))/Q_O(x(L_2,t))$$

If this is the case one may conclude that the system is critical in the infinite limit and the exponents determined in this limit effectively characterize the criticality of the system.

Whether such tests can be performed or not in practice is an open question which is strongly related to the precision with which relevant observables can be experimentally determined.
Table 1: Location of the critical point and exponents calculated for different linear sizes $L$ of the 2D percolation system using the FSS assumption (1). The numbers in parentheses correspond to the estimated error on the last figure of the given value.

The exact values are:

$$p_c = 0.5 ; \gamma = 2.389 ; \nu = 1.333 ; \sigma = 0.396$$

| $L$ | $p_c$ | $\gamma$ | $\nu$ | $\sigma$ |
|-----|-------|---------|-------|---------|
| 40  | 0.505(5) | 2.43(6) | 1.42(5) | 0.40(2) |
| 80  | 0.503(5) | 2.43(4) | 1.40(6) | 0.40(2) |
| 120 | 0.501(3) | 2.34(7) | 1.35(3) | 0.42(3) |
|     | 0.505(5) | 2.41(8) | 1.38(7) | 0.41(4) |
| 80  | 0.500(2) | 2.41(5) | 1.39(4) | 0.43(3) |
| 120 | 0.500(2) | 2.28(8) | 1.35(4) | 0.44(3) |

| $L$ | $m_c$ | $\tilde{\gamma}$ | $\tilde{\nu}$ | $\tilde{\sigma}$ |
|-----|-------|-----------------|---------------|-----------------|
| 40  | 0.088(5) | 2.08(4) | 1.26(7) | 0.46(2) |
| 80  | 0.097(3) | 2.01(7) | 1.17(7) | 0.49(3) |
| 120 | 0.098(3) | 1.98(4) | 1.17(3) | 0.50(2) |
|     | 0.100(7) | 1.93(7) | 1.15(7) | 0.51(5) |
| 80  | 0.097(3) | 2.00(6) | 1.14(5) | 0.47(3) |
| 120 | 0.102(3) | 1.97(5) | 1.09(5) | 0.51(3) |

a) bond probability $p$ with open boundaries
b) bond probability $p$ with periodic boundaries
c) reduced multiplicities $m$ with open boundaries
d) reduced multiplicities $m$ with periodic boundaries
Figure caption

Fig. 1: Evolution of $\xi$ and $m_2/L^2$ as a function of the linear size $L$ for different values of $p$.

Fig. 2: Behaviour of the universal functions $Q$ related to $\xi$ and $m_2/L^2$ as a function of $x$ for different values of $p$.

Fig. 3: Typical fit of the second moment represented as a function of $(p_c - p)$ on logarithmic scale for $L = 40$. The dispersion generated through the simulations is smaller than the size of the points.

Fig. 4: Values of the critical exponents from bond probability calculations extracted from the simulations for different values of $L$. The exact known values are indicated by the lines.
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Fig. 1
$L = 40$

2nd order moment

\[ \log \left( \frac{m^2}{L^2} \right) \]

\[ \log (p_c - p) \]

Fig. 3
Fig. 4