Common Aspects of Phase Transitions of Molecules, Nuclei, and Hadronic Matter

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The fragmentation of molecules and that of atomic nuclei, as well as the phase transition between the color-singlet hadrons and a plasma of quarks and gluons are the three most important examples of experimentally attainable phase transitions in systems with only a mesoscopic number of constituents. Thus their common features can provide important insights into extreme finite-size corrections to observables in general phase transitions. Here I will try to point out these common aspects.

1. Phase Transitions in Finite Systems

In the strict thermodynamic sense phase transitions are only defined for "infinite" systems, i.e. systems for which the number of elementary constituents is comparable to Avogadro's number, $N_A = 6.022 \times 10^{23}$. Typically, the task of theoretical calculations based on finite discrete lattices is to extrapolate to infinite lattice size. In order to compare to experiments, the numerical data obtained from lattice calculations have to be scaled. For example, to obtain the relation between the order parameter and the control parameter – a relation that defines the critical exponent β – the distance to the critical value of the control parameter has to be scaled by L^ν, and the value of the order parameter by $L^{\beta/\nu}$, where L is the number of lattice sites, and ν is the finite-size scaling exponent.

In nature there are, however, a few mesoscopic system with numbers of constituents on the order of 10^2 to 10^5. Here, extreme finite-size scaling effects should become visible. The importance of studying these systems lies also in the possibility to experimentally verify the finite-size scaling laws that have so far only been determined in computer-based simulations. Here I would like to discuss three different physical systems which we expect to experience phase transitions under certain conditions, and for which mesoscopic finite-size effect should play very important roles.

The first such system is the fragmentation of atomic nuclei. For now more than two decades, there have been speculations that we may be able to see a first-order phase

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coexistence between the Fermi liquid of ground state nuclei and the hadronic gas phase of individual nucleons and/or small clusters [1]. Of particular interest is the perspective that this first-order transition will terminate at a critical point, where the transition becomes continuous and the critical exponents of nuclear matter can be determined experimentally. In particular, the work of the Purdue group was pursuing this point of view [2,3], following the so-called "Fisher droplet model" [4]. In this context, particular attention was focussed on the power-law dependence of the yield of nuclear fragments of size A as a function of that mass number.

If nuclei can be fragmented and a resulting phase transition can be studied experimentally and theoretically, it might also be possible to pursue a similar lines of research for molecular fragmentation. In particular, for the most fashionable molecule of the last decade, the C_{60} ("Buckyball") with soccer-ball geometry, these studies were undertaken. In the framework of a molecular dynamics calculation coupled to a fixed temperature heat bath (Hoover-Nosé molecular dynamics), Kim and Tomanek [5] found evidence for several structural transitions. Interestingly, when examining a the relationship between temperature and total energy, they did not find the plateau conventionally associated with a first-order transition, but only a gradual rise. This is due to the fact that the condition of constant pressure is not fulfilled in this case. This observation should serve as a warning against interpreting such a plateau as evidence for a first-order transition, as previously postulated for nuclear fragmentation [6].

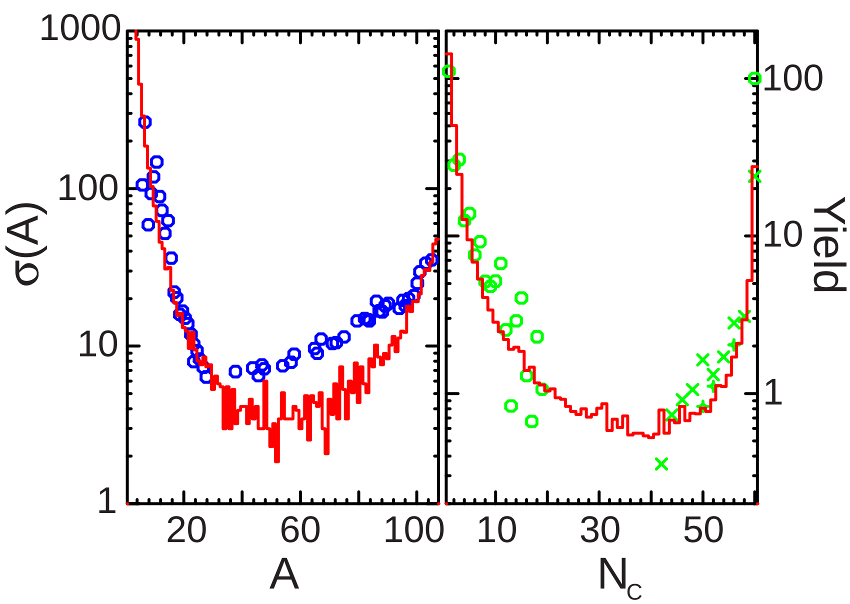

Figure 1. Comparison of experimental mass yield data (circles) for high-energy proton induced nuclear [8] (left) and high-energy heavy-ion induced buckyball [7] (right) fragmentation to percolation models (histograms) of fragmentation.

On the experimental side, the group of D. Gemmell at Argonne National Laboratory bombarded a gas target consisting of C_{60} molecules with high-energy Xe^{35+} ions, resulting in the experimental observation of mass yield spectra very similar to the ones observed in the case of nuclear fragmentation [7].

The experimental data for the mass-yield functions are displayed in Fig. 1. On the right, we show the data for the case of the fragmentation of C_{60} molecules with high-energy (625 MeV) Xe^{35+} ions, and on the left the case of the fragmentation of silver nuclei after bombardment with 300 GeV protons. Clearly, in both cases we can see the U-shaped mass yield spectra and the power-law dependence of the yield of the low-to-medium mass fragments on the size of the fragments – the fragment mass number, A, in the case of nuclear fragmentation, and the number of carbon atoms in the fragment molecule, N_c, in the case of the buckyball fragmentation.

The third phase transition postulated for finite systems is that between a hadron gas, in which quarks and gluons are confined in color singlets, and a plasma of quarks and gluons, in which they can move freely across the entire volume [9–13]. Unlike the two cases mentioned previously, this phase transition has implications for the evolution of the early universe, but again only in the case that is extrapolated to infinite systems. Under laboratory conditions, this phase transition should be able to be explored by central collisions of high-energy heavy ions at beam energies above 10 GeV per nucleon.

This phase transition is believed to be of first order for all finite values of the net-baryon density and only continuous for zero net baryon density, with the Polyakov loop as its order parameter [14]. This case is presently the only one that can be addressed by lattice QCD calculations and is not believed to be attained in present-day accelerator experiments. With the operation of RHIC however, this statement may change. We are thus all awaiting the first data from this new collider. At high baryon densities, a whole new set of phenomena may await us, and indeed a color-superconducting phase has been postulated in QCD [18,19]. In addition, instantons may cause the gap to be much larger than initially anticipated [20–22]

The non-abelian character of QCD is complicating the direct observation of this phase transition and has – up to now – prevented the kind of moment analysis that will be touched on later. Thus one has to rely on indirect experimental evidence for the phase transition. The favorite experimental signatures are presently that of chemical composition, hard photon and soft di-lepton production, suppression of the J/ψ resonance, and strangeness enhancement [15], and – very recently – the "balance function" [16]. While all presently available data are compatible with the formation of this deconfined state of matter (see the recent CERN press-conference), there is also in each case a whole list of theoretical papers that manages to interpret the findings in a purely hadronic scenario. Indeed, it may not be possible at all to unambiguously decide between a set of purely hadronic basis states and a set of sub-hadronic basis states which of the two is "better" in describing the experimental data [17].

What all of these mesoscopic systems have in common is that their thermodynamic state variables, (pressure, volume, temperature, and entropy) cannot be observed directly. All systems are only transiently excited to the energies that are (hopefully) sufficient to explore the phase transitions. The time intervals during which this occurs are much to short for a direct observation. The fact that anything approaching thermodynamic equilibrium is approached is by no means assured. And even if equilibration occurs, the system cannot be kept a fixed values of the state variables. Our ability to perform experimental observation is restricted to the detection of the asymptotic momentum states, and no coordinate space information is available. In addition these asymptotic momentum states are the product of time integrations over the entire history of the reaction, during which the system experiences pre-equilibrium and (hopefully) equilibrium stages, and migrates along a path in the phase diagram.

2. Theoretical Tools

To explore the issues raised above, we employ two kinds of theoretical tools. In order to study the approach to equilibrium and non-equilibrium phenomena, we need to rely on transport theories such as Boltzmann-type of theories at intermediate [23] and high energies [24], or molecular dynamics calculations [25].

If one wants to study equilibrium aspects of the phase transition, it is better to use one of the modern tools of many body physics, such as lattice gas models, percolation models, or lattice QCD. Here I will concentrate in particular on the percolation model, which has found application in the study of the fragmentation phase transition in nuclei [26,27] and in molecules [7]. Recently, the percolation approach has also been discovered in the study of the deconfinement phase transition [28].

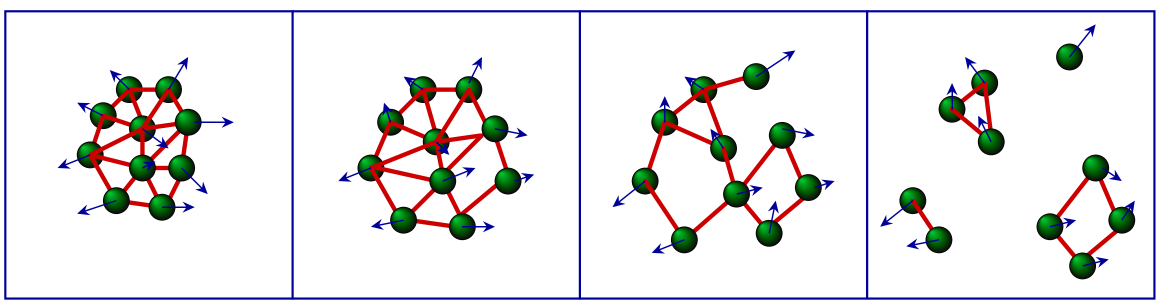

Figure 2. Schematic representation of a fragmentation process in for an expanding system of constituents with nearest neighbor interactions. This sequence of four frames represents different phases of the expansion, with time running from left to right. Nearest neighbor interactions are represented schematically by the straight lines, and the velocity vectors of the constituents by the arrows.

To understand the motivation for the bond percolation model of nuclear fragmentation, consider the schematic representation of a fragmentation process in the presence of short-range nearest neighbor interaction shown in Fig. 2. In systems with short-ranged nearest neighbor interactions, such as atomic nuclei or molecules, the injection of excitation energy in form of thermal or collective expansion energy results in constituents moving apart from each other beyond the range of the interaction. This "bond breaking" causes neighbors to loose contact with each other. Constituents that are still connected via bonds will end up as clusters in the detectors. It is then a reasonable approximation to the dynamical fragmentation process to employ a model based on bond percolation theory. Of course this implies the universality class of the percolation model, and only a careful comparison with experimental data can decide if this assumption is correct. An additional advantage of the percolation model is that the extrapolation to infinite lattices is understood quite well, and that we can perform detailed numerical studies of the finite size corrections.

In passing I note that this time sequence shown in Fig. 2 could have also been generated by a molecular dynamics simulation. This implies a deeper overlap between these two model classes, beyond the usual mean field assumptions that are employed in the microscopic justification of molecular dynamics simulations for nuclear collisions. Additional research into this promising potential connection seems indicated.

The histograms in Fig. 1 were generated by calculations with the percolation model and reproduce the overall features of the fragment mass distribution. The power-law falloff exponents for the low-to-medium size fragments are well reproduced in both cases, with exponents of -1.3 and -2.6 in the cases of the buckyball and nuclear fragmentation, respectively. They are, however, not directly related to the fundamental scaling exponent τ, but are a consequence of the integration over different event classes at different impact parameters with different amounts of excitation energy deposited.

For self-bound systems of Fermions, one can also calculate the probability that a given bond is broken. Li et al. have shown that this yields the relationship [29,30]

$$\begin{aligned} p_{\mathrm{b}}(T) &= \int_{E_b}^{\infty} \sqrt{\epsilon_b} e^{-\epsilon_b/t_b} d\epsilon_b \Big/ \int_0^{\infty} \sqrt{\epsilon_b} e^{-\epsilon_b/t_b} d\epsilon_b \\ &= \int_{B}^{\infty} \sqrt{E_s} e^{-E_s/T_s} dE_s \Big/ \int_0^{\infty} \sqrt{E_s} e^{-E_s/T_s} dE_s \\ &= 1 - \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, 0, \frac{B}{T}\right) , \end{aligned} \tag{1}$$

where Γ is the generalized incomplete gamma function, B is the binding energy per constituent in the residue, and T is the temperature, which has to be calculated in the framework of a model able to describe the dynamics of equilibration, or which can be deduced from the total excitation energy deposited. This ansatz is intimately related to the formula derived by Coniglio and Klein [31],

$$p(\epsilon/T) = 1 - \exp(-\epsilon/2T) \tag{2}$$

This formula also provides a connection to another class of models more and more used in the description of the nuclear fragmentation phase transition, the lattice gas model [32]. It has the universality class of the Ising model [33], though.

3. Moment Analysis

Already more than a decade ago, the first theoretical studies of the moment analysis of the fragment distribution were conducted on an event by event basis [27]. The i^{th} moment of the fragment size distribution is defined as

$$M_i = \sum_{k=1}^{\infty'} k^i \, n(k) \tag{3}$$

where $n(k)$ is the number of fragments with mass number k in that particular event. Here the upper limit in this sum is meant to indicate that the largest fragment – the "infinite cluster" – is not included. For example, in the limit of an infinite system the second moment diverges as $|p_b - p_c|^{-\gamma}$ in the vicinity of the critical value p_c of the control parameter p_b.

Recently, the EoS collaboration has produced data for the fragmentation of a 1A·GeV gold fragmentation on a carbon target. Since they used a time projection chamber (TPC), they were able to collect a large number of events (10^4) for which they were able to more-or-less completely account for all of the 79 charges of the gold nucleus and therefore detect all of its fragments [34]. They then assumed that the control parameter of the phase transition (temperature, or – in our case – breaking probability) is strictly proportional to the total charged particle multiplicity and plotted the second moment, M_2 vs. multiplicity. They found that for certain ranges of multiplicity it was possible to fit a power law to their data and concluded that the numerical value of the power observed in this fashion is the exponent γ for nuclear fragmentation. In a similar manner, they proceeded to extract the critical exponent β from their data for the charge of the largest fragment as a function of charged particle multiplicity. Their analysis suggests values are $\beta = 0.29$ and $\gamma = 1.4$.

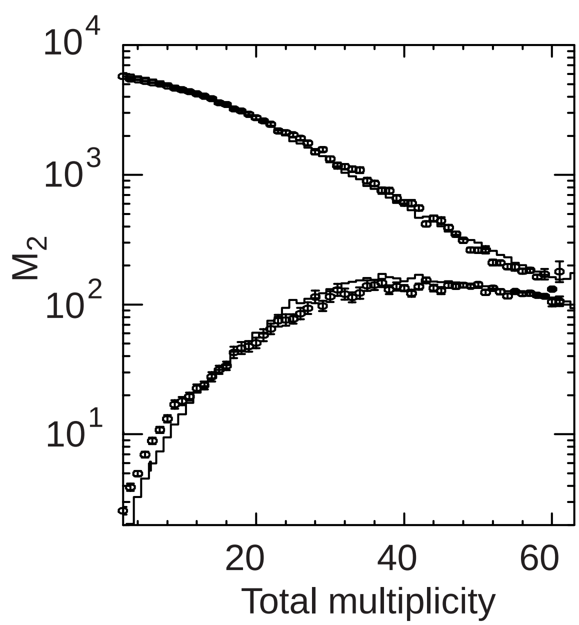

Figure 3. Second moment of the charge distribution vs. total charged-particle multiplicity in the reaction 1 A·GeV Au + C. The data are from [34] (plot symbols with error bars). The histograms are the results of our model calculations [30]. The upper data set and histogram are obtained by including all fragments, and the lower ones by omitting the largest fragment in each event.

We have compared our calculations based on the percolation model of [30] to the data of the EoS collaboration. The results are shown in Fig. 3. The data are shown by the plot symbols, and the results of the calculations are indicated by the histograms. The upper curves are for the case where the largest fragment is included in the summation for the second moment, and the lower curves for the case where it is not. We obtain almost perfect agreement. This agreement is a strong indication that the percolation model contains the right features to reproduce the data. If one accepts this, then one finds that the relevant exponents are those of the percolation universality class, $\beta = 0.41$ and $\gamma = 1.8$.

As one can see, there is no multiplicity for which the second moment actually diverges, as one would expect for an infinite system at the critical point. Again, this is a consequence of the extreme finite size effects at work here.

Finally, we should point out that this detailed agreement was only possible to achieve by performing the proper integration over impact parameters and with it the distribution of residue sizes and excitation energy deposition.

In our interpretation, the data of the EoS collaboration combined with our model calculation contain the up to now strongest evidence for the observation of a second-order critical point in the nuclear matter phase diagram. While the exact values of the critical exponents of this phase transition are still under debate, there seems to be consensus about the basic fact of the observation of the phase transition. And unlike the case of other possible phase transitions in nuclear matter, there are no competing theories or models that can explain the moment analysis data of the EoS group without invoking a phase transition.

4. Future Studies

If a first-order phase transition has been discovered in the CERN-SPS data, then it is clear that an extensive research program at RHIC will have to study this phenomenon. Most important in this context appears to be the question of the determination of the latent heat of this transition. Experience with the numerical studies of structural phase transitions in buckyballs suggests that this could turn out to become an exceedingly difficult task, as eluded to above.

At present, no data on dn/dy at RHIC have been published yet. So it is not clear how baryon-rich the central region will turn out to be. This will determine to a large degree how the research program, both theoretical and experimental, will have to progress. In the case that there is incomplete stopping and a region of almost zero net baryon density is created, there may be an opportunity to also observe a critical point in the QCD phase transition. If the central rapidity region turns out to be highly populated, then we might obtain a chance to get a glimpse at the instanton-dominated QCD-superconducting phase. The latter appears to also be a possibility at lower beam energies – possibly around 30 GeV per nucleon, as presently contemplated for the upgrade of the GSI.

The main astrophysical relevance of the fragmentation phase transition lies in the physics of neutron stars [35]. To proceed in this field, we need to extend our phase transition studies along the isospin degree of freedom. A proposed new radioactive beam machine with a projectile fragmentation facility, tentatively named RIA, may afford this opportunity – in addition to the existing projectile fragmentation radioactive beam facilities at, for example, MSU or GSI.

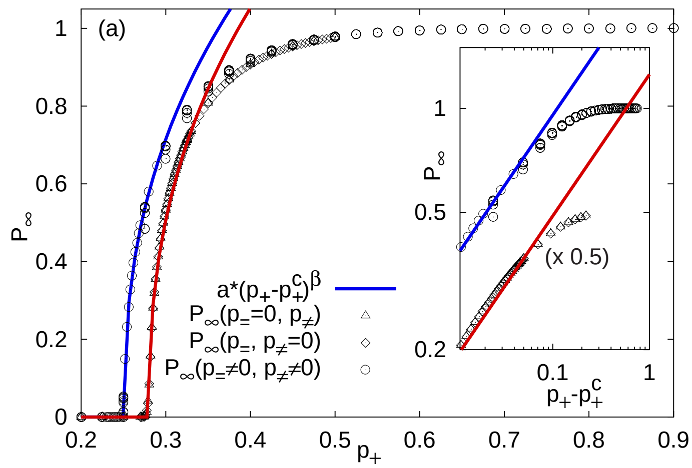

Figure 4. Dependence of the order parameter on the linear combination, p_+, of the individual control parameters for two interacting species, in a percolation model. For the case that the interaction between the two species approaches 0, we observe a shift in the critical value of the control parameter [37].

This research may yield an additional crop of rich new phenomena. As one example, let us just mention the work of Serot and Müller [36], who report a change in the character of the phase transition as one moves away from isospin symmetry, $N = Z$. Another example is shown in Fig. 4, where we report the results of a percolation study with two percolation species (neutrons and protons, for example) [37]. We find that one can generally find a linear combination of the individual control parameters for the two (or more) species that allow a combined description of the phase transition. But as the interaction between the two species approaches 0, there is a shift in the critical value of the control parameter, an effect that was previously not observed.

Increased attention, both experimentally and theoretically, should also be devoted to the investigation of the fragmentation phase transition of molecules. This can be done with table-top-sized experiments, but may yield deep insights into the question of the interplay between the detailed funtional form of the elementary nearest neighbor interaction and the resulting universality class of the fragmentation phase transition.

In summary, it seems clear that the investigation of phase transitions in mesoscopic systems has achieved some real and tangible successes during the last decade. The possibilities for future studies in this most interesting field appear bright.

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