Coalescence, Percolation and Nuclear Multifragmentation

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Abstract

We show that the coalescence model for fragment formation leads to an approximate site percolation model. Features characteristic of a percolation model also appear in microscopic models of disassembly.

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Multifragmentation continues to be one of the most important aspects of heavy ion collisions. Speculations have been made that the observed distribution of mass fragments may indicate that during disassembly finite amounts of nuclear matter passed through a critical region of liquid-gas phase transition. On the other hand, there have been practical calculations which directly attempt to calculate mass distributions using different models which typically have only indirect links, if any, to the question of phase transition. For example, there is a modern version of the evaporation model, statistical models both simultaneous and sequential (with and without radial expansion built in), and a fully microscopic model proposed in ref. 6 which is based upon the BUU model but with the inclusion of fluctuations. Applications of this BUU-with-fluctuations model agree reasonably well with experimental data but these calculations are very computer intensive so it is difficult to extract simple physics from such calculations. However, a critical study of the validity of this model has been made.

The percolation model was introduced by Bauer et al. and Campi et al. in an attempt to model nuclear fragmentation. Numerous applications to data have been made and Campi has argued that one can use this model to find out how, in spite of finite particle number, signatures of phase transitions can be extracted from experiments. Both Campi and Bauer have provided some physical arguments for the parameters of percolation models. For bond percolation model in three dimensions, the six bonds refer to the attractive bonds a given nucleon will feel because of short-range attractive nuclear interaction. These bonds are then broken with a probability $p$, which is the percolation parameter and depends linearly on the excitation energy per nucleon. While this picture is intuitively very pleasing and easily understandable for bonds between atoms in a molecule, for example, it is harder to understand it in terms of mean-field theories of nuclei (Hartree-Fock or Thomas-Fermi) which are usually employed to describe finite nuclei. In this paper we attempt to overcome this difficulty. We will show that a simple coalescence model for fragment formation leads to an approximate site percolation model in three dimensions. Although the arguments presented
for the connection between the two models are based on many approximations they seem to hold nonetheless as substantiated by results of a mean field calculation that we will present at the end. That calculation as well establishes contact between percolation and microscopic models.

A popular version of the coalescence model is the following: If, after hard collisions are over, \( n \) nucleons appear within a short momentum distance \( P_0 \) of each other then these nucleons will coalesce into one composite because of mutual attractive interactions. This simple idea is incomplete. Two nucleons with about the same momenta might be spatially separated by a large distance clearly prohibiting them from coalescing to form a deuteron. The real statement should be that nucleons must appear close to each other in phase-space\(^{15} \). On a semi-classical level the volume of a cell in phase-space is \( h^3 \). In any one of these phase-space cells at most one nucleon with a given spin-isospin can appear. We will assume for simplicity our system has \( N = Z \) and no spin excess. After hard collisions are over nucleons will then find themselves in the six-dimensional space which we partition into cubes each of volume \( h^3 \). A given cube then has six labels \( i, j, k, l, m, n \) where the last three labels refer to momenta and the first three to configuration space. A given cube can accommodate more than one nucleon (up to four) but then they must belong to different spin-isospin classes. We might argue that nucleons in the same cell and in adjoining cells with one common wall form a cluster; different clusters have empty walls between them. This leads to a site percolation model in six dimensions. However, the physics of the problem leads to a simpler situation.

We have stated that the volume of each phase-space cell is \((\Delta r)^3(\Delta p)^3 = h^3\) but we have not set the relative length scales for \( \Delta r \) or \( \Delta p \). We can choose them to our advantage. A remarkable feature of nuclear physics is that as the mass number \( A \) grows so does the volume in configuration space but the volume in momentum space remains roughly constant; it is always given by \( \frac{4\pi}{3}p_F^3 \) where \( p_F \) is independent of the mass number \( A \). Hence we choose \( \Delta p \) from \((\Delta p)^3 = \frac{4\pi}{3}p_F^3 \). For clusters to form, the nucleons must belong to the same momentum cell (otherwise there is far too much momentum in the system for it to stay together) although they can be in adjoining configuration
space cells. Thus for each value \( l, m \) and \( n \) of momentum indices, we have a site percolation model in three dimensions in configuration space. Refs. 12 and 13 use a bond percolation model in three dimensions; for problems in nuclear physics the bond percolation bond is easier to use as the number of nucleons is always fixed independent of how many bonds are open or closed. The situation is more complicated for site percolation; one assigns an occupation probability \( p \) and, if the number of lattice sites is \( N \), then the average number of nucleons is \( Np \). Thus if the value of \( p \) changes, \( N \) must also change if we want to model the same nucleus. Since most studies use Monte-Carlo simulations the number of occupied sites will usually fluctuate around the value \( Np \) unless special care is taken. Nonetheless, in the spirit of drawing an analogy between percolation and coalescence as discussed above, the parameters for site percolation take physical meaning. The parameter \( p \) becomes related to entropy which can be computed in numerical simulations as done by Bertsch and Cugnon\(^{16}\). We also see that \( p \) can vary with position in momentum space, for example, \( p \) should drop as the value of the momentum characterizing a momentum cell increases. Finally \( p \) can also vary with position in configuration space. The increase in the value of \( N \) as \( p \) changes merely reflects the fact that more and more of phase-space is becoming accessible as, for example, will happen if the energy of collision increases. We remind the reader that because of universality,\(^{17}\) the conclusions reached by the use of site percolation model remain unchanged.

The Pauli principle plays a crucial role in the equivalence between percolation and coalescence. This may seem surprising at first glance but we remind the reader that the Pauli principle was always respected in other studies of phase-transitions in nuclear matter at intermediate energies. For example, in the mean field studies of ref. 18 a given quantum cell does not contain more than one particle of a given spin-isospin.

We still need to show that the simple coalescence model with the incorporation of spin-isospin can be mapped quite faithfully into another calculation which uses no such indices. Let the first calculation which explicitly uses spin-isospin have \( N \) lattice sites and occupation probability \( p \) for
each spin-isospin species. Here each lattice site may have either no nucleon or between 1 and 4 nucleons. In a corresponding calculation without explicit recognition of spin-isospin let the number of lattice sites be \( N' \) and \( p' \). Here each lattice site has either no nucleon or 1 nucleon. What is the mapping of \( N' \) to \( N \) and \( p' \) to \( p \)?

First of all we want to describe the same nucleus which requires

\[
N'p' = 4Np
\]  

(1)

Secondly, the physics of the problem is dictated largely by the ratio of the number of occupied sites to the number of unoccupied sites; we want these ratios to be the same in both the descriptions; this gives

\[
1 - p' = (1 - p)^4
\]  

(2)

Together these two equations determine \( N \) and \( p \) in terms of \( N' \) and \( p' \).

Figs. 1 and 2 show that the same physics is described whether or not spin-isospin is explicitly included and also shows the validity of the mapping described by eqs. (1) and (2). Here we have used the site percolation model. Fig. 1 is the “Campi” plot. We choose arbitrarily the total number of nucleons to be \( A = 64 \); for a given choice of \( N \), \( p \) is given by \( A/4N \); similarly, for a given choice of \( N' \), \( p' \) is given by \( A/N' \). Monte-Carlo simulation produces \( A' \) particles where \( A' \) fluctuates around \( A \). We define reduced multiplicity \( n \) as the number of clusters divided by \( A' \). For a given \( p(p') \) the quantity \( n \) will vary; nonetheless an average \( < n > \) can be defined for each \( p(p') \) and in figs. 1 and 2 when plotting against \( < n > \) we actually include events differing from \( < n > \) by at most \( \pm 0.03 \). For a theoretical calculation, it is easier to use the variable \( p(p') \), but \( p(p') \) is not an observable whereas \( n \) is a direct observable. Each point in Figs. 1 and 2 are averages over 1000 runs taken for fixed \( N(N'), p(p') \) and the small dispersion about \( < n > \). The second moment \( M_2 \) is defined as

\[
M_2 = \frac{\sum s^2d(s)}{A}
\]

where \( d(s) \) is the average value of the number of
clusters of size $s$ and the largest cluster in each event is left out when this averaging is computed. The definitions follow those of ref. 13. Fig. 2 shows the average value of the mass number of the largest cluster once again as a function of $n$ in order to show that results with explicit spin-isospin can be mapped onto results without explicit spin-isospin. We have shown in Figs. 1 and 2 results from two-dimensional site percolation rather than three in order to gather more points ($N = L^3$ grows very quickly with $L$ so that the number of points in the interesting region will be sparse). Three dimensional percolation model calculations were also done; with fewer available points they confirm the conclusions presented here.

The simple coalescence model with which we have established a one-to-one correspondence to the percolation model is not sufficiently realistic. One may wonder if features seen in percolation model can emerge in more realistic microscopic models which nonetheless depend upon particles being near each other in phase-space coalescing to form clusters. We will follow numerically the time development of a blob of nuclear matter which is initially at excitation energy and compression appropriate for about 40 MeV/nucleon beam energy for equal ion collisions. We assume that because of hard collisions a phase-space density with fluctuations has been produced which then disassembles; during disassembly matter is moving outward so there are fewer collisions. We take into account only a mean-field during the disassembly. This model was first employed by Knoll and Strack\textsuperscript{19} who used time-dependent Hartree-Fock theory in two dimensions. The model here is identical with that of ref. 14 except the initial stage in ref. 14 was produced by the cascade model. At the initial time, the $i$–th nucleon is represented by a phase-space density

$$f(\vec{r}, \vec{p}) = \frac{1}{(\hbar\pi)^3} \exp(-\alpha^2(\vec{r} - \vec{r}_i)^2) \exp(-((\vec{p} - \vec{p}_i)^2)/\hbar^2\alpha^2).$$

This is a Wigner transform of a Gaussian wave-function and retains the quantum uncertainty between $\vec{r}$ and $\vec{p}$, i.e., if the nucleon is localized in configuration space, then it is spread out in momentum space. The value of $\alpha$ is kept at $0.5 \text{fm}^{-1}$ which is a standard value used before in similar
calculations\textsuperscript{14,20}. We choose the initial positions $\vec{r}_i$ by Monte-Carlo sampling within a radius $R$ which is fixed such that the average density $\bar{\rho} = \int \rho d^3 r / \int \rho d^3 r$ is $0.18 fm^{-3}$. The initial momenta $\vec{p}_i$ are chosen by Monte-Carlo sampling an occupational probability distribution obtained from a nuclear matter Fermi-gas calculation at density $0.18 fm^{-3}$ and a given temperature. Small adjustments (detailed later) are made so that the initial energy of the generated phase-space density has a pre-assigned value. Ideally in subsequent Vlasov propagation this energy is exactly conserved. We use the test particle method and the Lenk-Pandharipande prescription\textsuperscript{21} which gives quite accurate energy conservation. We use 50 test particles per nucleon. The calculation is done in a configuration space $(40 fm)^3$ and the size of each cube is $1 fm^3$. A Skyrme interaction $U(\rho) = A(\rho/\rho_0) + B(\rho/\rho_0)^{7/6}$ is used where $A = -356 MeV, B = 303 MeV$ and $\rho_0 = 0.16 fm^{-3}$. We start with a small and compact piece of nuclear matter and let it evolve for $81 fm/c$. At this time we count clusters. Test particles which share a common wall are part of the same cluster; the number of real particles in each cluster will usually turn out to be non-integral. We disregard initially all the clusters whose number of particles adds up to less than one; they will contribute to single nucleons. The clusters with particle number greater than one are integerized to the next integer. The number of single nucleons is then the total number of nucleons minus the number of nucleons bound in composites. One could also let the system evolve for longer times but this would necessitate expanding the dimension beyond $(40 fm)^3$ as some nucleons begin to leave the box.

The results of our calculation are shown in Fig. 3. We plot the second moment $< M_2 >$ as function of energy per nucleon rather than $< n >$ since in the calculation the energy can be specified at the beginning whereas $n$ is determined only at the end when Vlasov propagation stops. We find that $< M_2(n) > = f(n, E/A)$ and thus for a meaningful plot against $n$ we need to choose a weighting function $g(E/A)$. There is of course an average value $< n >$ for a given $E/A$ which is shown also in Fig.3. If we plotted $< M_2 >$ against the calculated $< n >$ the graph would look very much like Fig.2 in ref. 13. In Fig. 3 we have shown the results for systems with particle numbers
40 and 64. Not only does one find the appearance of a maximum, the height of this maximum increases as the number of particles in the system increases much like in the percolation model in 3 dimensions. The value of $E/A$ can be converted into a beam energy remembering that with our forces and approximations the energy per nucleon in a cold nucleus of 40 nucleons is $\approx -11 \text{MeV}$. It is probably not surprising that the maximum in $M_2$ is obtained when the available beam energy is close to that which is enough to liberate all the nucleons. Each point in Fig. 3 is an average of 40 runs at a given $E/A$.

Although at initialization the momenta in $\vec{p}_i$ (eq.3) were chosen from a nuclear matter Fermi gas calculation at a given temperature, neither the kinetic energy nor the potential energy per particle in our system will be the same as in nuclear matter. The potential energy is different because in our system the density fluctuates; the kinetic energy per particle is also different because the folding done in eq.3 increases the kinetic energy. In addition Monte-Carlo sampling leads to usual small fluctuations in the value of $E/A$ from one event to another. In the numerical simulation once the Monte-Carlo for positions and momenta of test particles is done for one event a slight readjustment of the momentum scale is imposed so that we always have a fixed energy per particle.

It is possible to see that the appearance of a maximum in Fig. 3 (or Fig. 2 in ref. 13) is closely related to composite formation. Imagine a scenario where a piece of hot nuclear matter containing $A$ nucleons can only shed nucleons but not composites. If the excitation energy is small it sheds none or a few nucleons. On the other extreme for high excitation energy it will explode into $A$ nucleons. In the low excitation energy limit $n$ is $1/A \approx 0$ and $M_2 = 0$ since the largest cluster is left out when computing $M_2$. On the high energy side $n \approx 1$ and $M_2 \approx 1$. The value of $M_2$ grows monotonically from 0 in one extreme to 1 in the other; thus the appearance of a maximum in the plot of $M_2$ against $n$ and a value higher than 1 can only happen if fragments are formed.

It will be interesting to check whether the features seen in figures 1 and 3 also appear in phenomenological models such as considered in ref. 22.
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Figure Captions

Fig. 1. Plots of second moment against reduced multiplicity done without explicit consideration of spin-isospin (solid dots) and with explicit consideration of spin-isospin (hollow dots). The bracketed numbers opposite solid dots give the value of $p'$; the bracketed numbers opposite hollow dots do not refer to $p$ but to equivalent $p' = 1 - (1 - p)^4$. This curve therefore shows that the second moment and multiplicity are mapped by eqs. (1) and (2).

Fig. 2. The average value of the mass number of the largest cluster plotted against reduced multiplicity for the two calculations in Fig. 1. The same horizontal axis is chosen to facilitate the correspondence between points in Figs. 1 and 2.

Fig. 3. Second moment (left axis) as it depends on the energy per particle. Also shown (on the right axis) is the average reduced multiplicity against the same variable, namely, the energy per particle.