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Microcanonical Simulation of Nuclear Disassembly

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Abstract:

We formulate a microcanonical simulation of the disassembly of a finite nuclear system into individually excitable and mutually interacting nuclear fragments. Illustrative results are presented.

There is considerable interst in the disassembly of the hot nuclear matter produced in high-energy nuclear collisions. A particular stimulus has been the prospect of observing a nuclear liquid-gas phase transition. On rather general grounds, such a transition is expected to occur in nuclear matter at sub-saturation densities with temperatures of 10-20 MeV. However, virtually all previous discussions of this phenomenon have been based on thermodynamical considerations valid for infinte, non-interacting systems and the qualitative validity of the results has not been ascertained for the relatively small, finite, interacting systems of practical relevance. Nor is it clear how the occurrence of the phase transition will manifest itself in the asymptotically observed fragment distribution.

To progress in these matters , we have formulated a microcanonical simulation of the disassembly process, *including* interfragment interactions. It is a natural refinement of the grand canonical model first presented in [1] and further developed in [2] and is also an exact version of the model developed in [3] for the generation of complete multifragment events in medium-energy collisions. In this contribution, we give in brief description of the key ingredients in the model and its numerical implementation. A more detailed presentation, and a discussion of calculated results is currrently being prepared for publication [4]; that presentation also contains a discussion of the relationship of our work to those of Gross *et al.* [5] and Bondorf *et al.* [6] which are also based on microscopical simulation.

We consider a system of interacting nuclear fragments confined within some volume Ω. A given state F of the system is specified by

$$F: \ \{N_F; (A_n, \mathbf{r}_n, \mathbf{p}_n, \epsilon_n), \ n = 1, ..., N_F\} \tag{1}$$

Here N_F is the number of fragments present, and $A_n, \mathbf{r}_n, \mathbf{p}_n, \epsilon_n$ are their mass numbers, positions, momenta, and intrinsic excitation energies. The total number of nucleons present in F is

$$A_F = \sum_{n=1}^{N_F} A_n \tag{2}$$

and we take the corresponding total energy to be

$$E_F = \sum_{n=1}^{N_F} \Big[\frac{p_n^2}{2mA_n} - B_n + \epsilon_n + \frac{1}{2} \sum_{n' \neq n} V_{nn'} \Big] \ . \tag{3}$$

Here, the first term is the kinetic energy associated with translational motion, the inertial mass being taken as mA_n, where m is the mass of the free nucleon. The binding energy of the ground state of fragment n may be taken as

$$B_n = a_V A_n - a_S A_n^{2/3} - a_C Z_n^2 / A_n^{1/3} \tag{4}$$

where $Z_n \approx A_n/2$. Furthermore, the intrinsic excitation is denoted by ϵ_n. Finally, $V_{nn'}$ is the interaction energy between the fragments n and n'. This quantity generally includes both the electrostatic (Coulomb) and the nuclear (proximity) energies. A convenient form is

$$V_{12} = e^2 \frac{Z_1 Z_2}{r_{12}} + 4\pi\gamma \bar{R} b \Phi(\frac{s_{12}}{b}) \tag{5}$$

where r_{12} is the distance between the fragment centers and $s_{12} = r_{12} - C_1 - C_2$ is the corresponding surface separation.[7]

In the microcanonical simulation, we consider as equally probable all states F that are accessible to the system when due account is taken of conservation laws. In our present studies, we impose overall conservation of nucleon number and energy, but ignore other conservation laws, such as linear and angular momentum. The relaxation of these latter constraints are not expected to be of importance for our present purposes, but our calculational method can readily be modified to accomodate these features as well.

If A is the total nucleon number of the system and E is its total energy, the associated microcanonical *density of states* is

$$\begin{aligned} \rho(\Omega, A, E) &= \sum_F \delta(A_F - A)\, \delta(E_F - E) \qquad (6) \\ &= \sum_{N_F} \frac{1}{N_F!} \prod_{n=1}^{N_F} [\sum_{A_n} \int \frac{d\mathbf{r}_n d\mathbf{p}_n}{h^3} \int \rho_n(\epsilon_n) d\epsilon_n]\, \delta(A_F - A)\delta(E_F - E) \end{aligned}$$

where ρ_n is the intrinsic level density. The integrals over the N_F fragment momenta can be carried out analytically and the expression for ρ can be reduced to

$$\rho(\Omega, A, E) = \sum_N \prod_{n=1}^{N} [\sum_{A_n} \int \frac{d\mathbf{r}_n}{\Omega} \int d\epsilon_n]\, w\ . \tag{7}$$

Here the *statistical weight* of a particular configuration is given by

$$w = \frac{1}{N!} \frac{1}{\Gamma(\frac{3N}{2})} \prod_{n=1}^{N} \left[\Omega \left(\frac{2\pi m A_n}{h^2}\right)^{\frac{3}{2}} \rho_n(\epsilon_n)\right] \delta(\sum_{n=1}^{N} A_n - A)\ K^{\frac{3N}{2}-1}\ , \tag{8}$$

where K is the kinetic energy,

$$K = E - \sum_{n=1}^{N} [-B_n + \epsilon_n + \frac{1}{2} \sum_{n' \neq n} V_{nn'}] \tag{9}$$

The above form of the density of states ρ is suitable for a Monte Carlo treatment, in which expectation values of observables are calculated as averages over a statistically determined sample of configurations. To select this sample, we employ the Metropolis method, in which a sequence of configurations is generated by a markovian process in configuration space. To generate the next sample member of this sequence, a candidate configuration is first generated from the current one by one of several possible random "moves": change of position or excitation energy of a fragment, exchange of

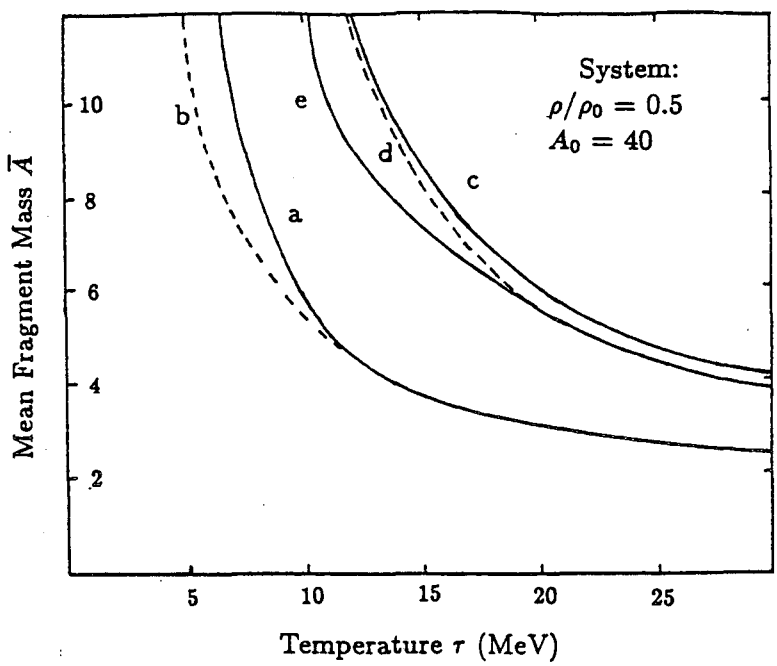

Figure 1: Illustrative results in a schematic model.

This figure displays the mean fragment mass number $\bar{A}$ as a function of the temperature τ in a microcanonical system containing a total of 40 nucleons. These nucleons may coalesce into composite fragments without any internal excitation, and the mean nucleon density is equal $0.08/\text{fm}^3$, *i.e.* half the nuclear matter saturation value. The labeled curves correspond to the following five schematic scenarios:

(*a*) The fragments are totally independent (and thus may overlap) and no Coulomb forces are acting (neither within nor between the fragments).

(*b*) The fragments are still non-interacting, but the Coulomb energy is included in the fragment binding.

(*c*) No Coulomb forces are acting at all, but hard-sphere potentials are imposed between the fragment pairs.

(*d*) In addition to the hard-sphere potential, both intra- and inter-fragment Coulomb forces are included.

(*e*) In addition to the hard-sphere potential, the intra-fragment Coulomb forces are included (*i.e.* $a_C > 0$ in (4)), but the inter-fragment Coulomb forces are not.

nucleons between two fragments, fusion of two fragments, or fission of a fragment. This candidate is accepted as the next configuration in the sequence if its weight, w', is greater then that of the current configuration, w. If $w < w'$, the candidate is accepted with the probability w'/w, and otherwise the current configuration is used again. It is easy to show that, in the limit of long sequences, any configuration appears with the appropriate probability. However, since the candidate configuration is usually very similar to the current one, the sampling procedure diffuses rather slowly through configuration space and subsequent configurations are highly correlated. To obtain the required sample of sufficiently uncorrelated configurations, only a small fraction of the configurations in the sequence are employed (for example every lth member, with l to be determined empirically).

In terms of the state density, the *entropy* of the system is $S = \ln \rho(\Omega, A, E)$. While we cannot calculate S by our method, we can find many other quantities of interest. In particular, the basic thermodynamic relation $dE = \tau dS + \mu dA - P d\Omega$ allows the *inverse temperature* $\beta \equiv 1/\tau$, the *chemical potential* μ, and the *pressure* P to be written as

$$\beta = \frac{\partial S}{\partial E}, \quad \mu = -\tau \frac{\partial S}{\partial A}, \quad P = \tau \frac{\partial S}{\partial \Omega} \tag{10}$$

Each of these derivatives leads to the expectation value of some "observable" over the sample of configurations described above. For example, from (7-9), we find $\beta = \langle (\frac{3N}{2} - 1)/K \rangle$.

The simplest non-trivial situation occurs when the fragments are assumed to be uncharged, non-interacting and cold. The character of the ensemble is then determined by the balance between the

fragment kinetic energies (which drive the system towards many, hence small, fragments) and the fragment surface energies (which drive the system towards large, and hence few, fragments).

To illustrate the characteristic features of the multifragmentation process in this simplest situation, we consider the fragments distribution as a function of the imposed temperature, for a specified value of the nucleon density. The result is shown by curve *a* in the figure. As the temperature is decreased, the composition changes from many small fragments to a few large ones. If the Coulomb energy is included in the fragment binding energy, very little change occurs at higher temperature, while the mean fragment size drops somewhat at lower temperature, as shown by curve *b*; that is because the total binding is increased by partitioning a given amount of matter into small fragments.

Several refinements of the above simplest scenario can be considered. The first one is to take approximate account of the high nuclear incompressibility by imposing a high penalty for configurations with overlapping fragments, corresponding to considering the fragments to be hard spheres. The effect of this (excluded volume) refinement is shown by curve *c*. At the same temperature, the system prefers larger fragments. This is because the volume available to a fragment is effectively smaller (and in general the fragments grow larger when the system is compressed).

Next we consider the effects of including the electrostatic energy. The Coulomb forces between the constituent nucleons have two effects: One is to reduce the binding energy of each individual fragment, and the other is to generate a repulsive force between fragment pairs. A consistent treatment must incorporate both of these effects. The result is given by curve *d*. As would be expected, only little change results, and towards slightly smaller fragments. The effect of including only the self energy, but *not* the interaction, is shown by curve *e*. While no effect occurs at high temperature, where the multiplicity is high, there is an enhanced preference for higher multiplicity at the lower temperatures, as would be expected.

The presented model establishes a well-founded formal basis for quantitative studies of a variety of aspects relating to the properties of hot and dilute nuclear matter. In particular, it is expected to be of value in ascertaining the quantitative applicability of thermodynamical methods and certain approximate microcanonical models (such as that of [3]).

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