EXACT STATISTICAL CALCULATIONS OF FRAGMENTATION

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Calculations based on the microcanonical distribution [1,2] have provided tremendous insight into the process of nuclear fragmentation. In order to enforce the conservation laws, numerically intensive Monte Carlo procedures have been implemented. Recently, Mekjian and collaborators [3] have discovered a recursive technique which permits the calculation of exact canonical partition functions, Z_A, for non-interacting fragments using a recursive formula.

$$Z_A(T) = \sum_{\langle \sum a_i n_i = A \rangle} \prod_i \frac{\omega_i^{n_i}}{n_i!} \tag{1}$$

$$= \sum_i \frac{a_i}{A} \omega_i(T) Z_{A-a_i}(T) \tag{2}$$

where ω_i is the partition function for a single fragment of type i and mass a_i at temperature T. This formula allows practically instant calculation of the partition function, and therefore of a variety of statistical quantities. The method is applied to any system where the explicit interaction of the individual fragments can be neglected, although mean field and excluded volume effects are easily incorporated. The method exactly sums over every possible division of the A nucleons into fragments.

During the past year, we have made several contributions to this approach [4,5]. First, using the liquid-drop model to generate the partition functions of individual fragments, we have investigated the thermal properties of the model and shown that it gives a discontinuity in the specific heat as a function of temperature at constant volume. The discontinuity is related to a fragmentation transition, where the number of fragments suddenly rises. Secondly, the model was extended to consider multiple conserved charges, thus allowing the exact conservation of both neutron and proton number. It was also found that conservation of energy could be incorporated, thus making microcanonical calculations possible. Finally, recursion relations were developed for the multiplicity distributions which allowed exact calculations of intermediate-mass-fragment (IMF) multiplicity distributions, both for the canonical and microcanonical cases.

To generate the microcanonical distributions, energy was treated like a conserved charge measured as an integer in units of ΔE. The number of ways to arrange a system of mass A at energy E, $N_{A,E}$, satisfies the recursion relation,

$$N_{A,E} = \sum_{i,E_i} \frac{a_i}{A} n_{i,E_i} N(A - a_i, E - E_i). \tag{3}$$

Here, n_{i,E_i} is the number of ways to arrange a single fragment in the volume with energy E_i, which is found by convoluting the internal density of states with the density of states of the fragment's center of mass.

The recursion relation for the multiplicity distributions satisfies the relation,

$$P_{b,A,n}(T) = \sum_{i \in b, E_i} \omega_i(T) \frac{Z_{A-a_k}(T)}{Z_A(T)} P_{b,A-a_k,n-1} \frac{1}{n}. \tag{4}$$

Here, $P_{b,A,n}$ is the multiplicity of fragments in the set defined by b in a system of size A. The microcanonical equivalent is

$$P_{b,A,E,n} = \sum_{i \in b, E_i} n_{i,E_i} \frac{1}{n} P_{b,A-A_i,E-E_i,n-1} \frac{N(A-a_i, E-E_i)}{N(A,E)}. \tag{5}$$

The advantage of the recursion relations relative to Monte Carlo procedures is that the calculations are exact and can be used for quantities which might require an inordinate amount of sampling in a Monte Carlo scheme. One example of such a problem is the calculation of the multiplicity distribution, and it's mean and variance. Fig. 1 displays the multiplicity distribution for a system of size $A = 100$ at three different excitation energies. The liquid-drop model was used to generate the partition functions, with the isospin degree of freedom ignored.

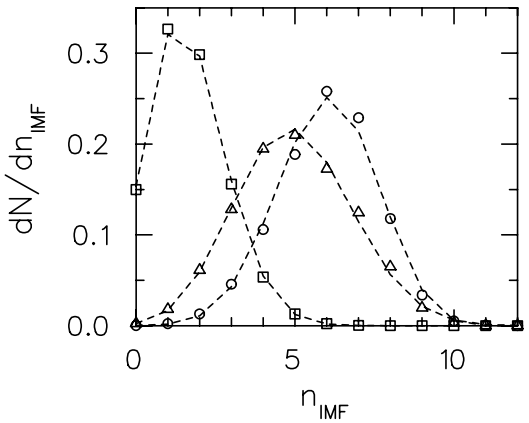

Fig. 1. Multiplicity distributions of IMFs as generated from a microcanonical ensemble are displayed for three excitations, E/A = 7.5 MeV (squares), 12.5 MeV/A (triangles) and 17.5 MeV/A (circles). Calculations assumed a size A=100 and ignored Coulomb effects. The distributions are well described by binomial distributions (dashed lines).

Figure 2 displays the mean multiplicity and the correlation coefficient, which is related to the variance by, $\xi = (\sigma^2 - \langle n \rangle)/\langle n \rangle^2$. The correlation is positive or negative depending on whether the system is super-Poissonian or sub-Poissonian respectively.

Finally, we remark on the numerical requirements of these techniques. Calculations with the canonical ensemble finish within seconds or minutes. However, microcanonical calculations may take on the order of an hour, and if microcanonical calculations are performed while conserving both neutron and proton number, the calculations may require days of CPU time. However, it should be stressed that when such a calculation is finished that the results are generated for all excitation energies, and are exact.

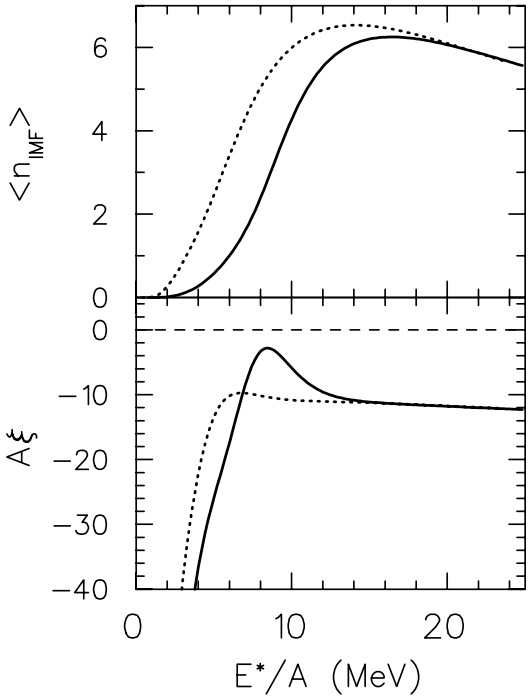

Fig. 2. The average number of IMFs and the correlation coefficient as generated from a microcanonical calculation for a mass A=100 system are shown with (dashed line) and without (solid line) Coulomb. The inclusion of Coulomb reduces the amount of energy needed for fragmentation. Whereas canonical calculations yield a sharp peak in the correlation coefficient, microcanonical calculations reveal a broad maximum. Even when Coulomb is neglected, the IMF multiplicity distributions remain sub-Poissonian at all excitations.

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References

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