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MICROCANONICAL SIMULATION OF NUCLEAR MULTIFRAGMENTATION

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We discuss the formal basis for the theoretical treatment of nuclear multifragmentation within a microcanonical framework. The important role played by highly excited nuclear states and the interfragment forces is illustrated. The requirement of detailed balance is especially discussed and illustrated for the fission-fusion Metropolis moves in configuration space.

1. INTRODUCTION

The properties of hot nuclear matter at subsaturation densities are of general physical interest, especially within the context of the "Equation of State" of matter at high energy densities. The topic is of direct relevance to astrophysics (*e.g.* supernova processes) and is intertwined with energetic nuclear collisions: a good understanding of the nuclear equation of state over a wide range of energies and densities is a prerequisite for making reliable predictions about the outcome of nuclear collisions and, conversely, nuclear collisions present a unique tool for probing the properties of nuclear matter away from its normal state. Because of its strong link to nuclear collision dynamics, the study of subsaturation matter is often performed in the guise of multifragmentation, in the sense that one considers an assembly of interacting nuclear fragments within a finite ("freezeout") volume Ω.

The theoretical interest in nuclear multifragmentation has increased in concert with the substantial improvements in accelerator capability through the past decade. The emergence of the field was originally stimulated by the Bevalac and it has gained further momentum in recent years through the construction and planning of several modern intermediate-energy heavy-ion accelerators throughout the world, especially CERN CS (Europe), GANIL (France), CELCIUS (Sweden), and SIS-18 (Germany). This latter facility will provide beams of nuclei over the entire mass range at energies up to $\approx$1 GeV/N and with intensities exceeding those of the present Bevalac by 2-3 orders of magnitude. It is noteworthy that these developments have occurred outside of this country, and it appears that a drastic modernization of the US accelerator capabilities would be required for this country to maintain a significant role in the expanding field of medium-energy nuclear collisions.

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In this note, we discuss some central aspects of the microcanonical simulation of nuclear multifragmentation. Much of the material is based on recent work reported elsewhere.[1]

The first formulation of a model for nuclear multifragmentation processes was made within the framework of a grand canonical model.[2] In that model, an assembly of non-interacting, excitable nuclear fragments was considered and the general expressions for the one-fragment observables were derived. Only particle-stable nuclear levels were included for simplicity, although it is clear that there is abundant production of unbound fragments that subsequently deexcite on a time scale long compared with that characterizing the primary disassembly. The inclusion of such unstable nuclei, and their sequential decay by evaporation of light particles, was made later.[3]

The development of powerful multifragment detection systems have demanded more detailed models and established the need for addressing complete fragmentation events. For this task an approximate microcanonical procedure was developed and tested [4]; it is based on the recursive use of the grand canonical model for an ever smaller source. This convenient method was then exploited to formulate a microcanonical model for generating complete multifragment events in nuclear collisions at medium energies.[5] This model divides the colliding system into a number (≈ 3) of sources which independently disassemble into metastable nuclear fragments. Interfragment forces can not be incorporated in this approach, although the Coulomb energy can be included at the one-particle level (such as the Wigner-Seitz approximation) and the nuclear incompressibility can be approximated through the use of a reduced, effective volume $\chi\Omega$. In conjunction with this work, a computer code, named *FREESCO*, was developed [6]; it has been employed in numerous theoretical and experimental studies.

Nuclear multifragmentation has also been studied by other groups. Most relevant to our present discussion is the work of Gross *et al.* and Bondorf *et al.*: Gross *et al.* started by addressing the deexcitation process following a high-energy proton-nucleus reaction. The focus was on the fragment mass distribution and it was found that the interfragment Coulomb repulsion is instrumental in enhancing the production of heavy fragments (leading to a U-shaped yield curve), at the relatively low excitations involved.[7] After these grand-canonical studies, Monte Carlo simulations were made within the canonical approximation.[8] Most recently, an approximate microcanonical simulation model has been developed.[9] It differs from ours in many important respects, both as regards the physical assumptions and in the numerical implementation. For example, metastable fragments are not included. The descriptions in the literature are not sufficiently complete to let us ascertain the validity of the particular simulation procedure adopted.

Bondorf *et al.* have formulated a model for statistical multifragmentation of nuclei.[10] Their focus is on the mass partition and so a canonical approach is taken. The model does not incorporate any fragment interactions, although the Coulomb energy is included in the Wigner-Seitz approximation. Furthermore, there is no suppression of the level density for highly excited fragments. The numerical sampling procedure chooses evenly between all possible mass partitions and subsequently performs a weighted average of the partition-dependent observables, employing the canonical weights for the different partitions selected. While tecnically correct, this method is probably less efficient than sampling the partitions according to their (strongly varying) weights, as is done in [1].

2. CLASSES OF MULTIFRAGMENT STATES

In the current literature on multifragmentation problems, the distinction between various conceptually different classes of multifragment states is often blurred. In the following we shall define some classes of multifragment states that are frequently of interest, in the hope that this may contribute to establishing common terms and help avoid confusion in discussions of multifragmentation processes.

It is convenient to define a *fragmentation* F as a set of elementary multifragment states that all have the same fragment masses, positions, momenta, and internal excitations. Thus a given fragmentation F contains the following specific information,

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

Here the number of fragments is denoted by N_F, they are labeled by the index $n, n = 1, ..., N_F$, and they have the mass numbers A_n. Furthermore, their internal excitation energies are ϵ_n, and their positions and momenta are $\mathbf{r}_n$ and $\mathbf{p}_n$, respectively. We find it convenient to consider only fragments with a mass number in a specified range, $A_{\min} \leq A_n \leq A_{\max}$. Although we do not distinguish between neutrons and protons in the present discussion, it would be formally simple to incorporate the isospin degree of freedom by simply interpreting the nucleon number A_n as a two-dimensional quantity $\mathbf{A}_n$ whose components are the respective neutron and proton numbers, N_n and Z_n.

An "interval" ΔF in the space of fragmentations is generated by the tolerances $\Delta\mathbf{r}_n$, $\Delta\mathbf{p}_n$, and $\Delta\epsilon_n$ for position, momentum, and excitation, respectively. The number of elementary multifragment states in the interval ΔF is then

$$\Delta\nu_F = \prod_{n=1}^{N_F} \rho_n(\epsilon_n)\Delta\epsilon_n \; \frac{\Delta\mathbf{r}_n \; \Delta\mathbf{p}_n}{h^3} \; . \tag{2}$$

Here h is Planck's constant and $\rho_n(\epsilon_n)$ is the density of states in the fragment n at the excitation energy ϵ_n. [We have here chosen to consider ϵ_n as a continuous variable, even though is strictly quantized. This is convenient because of the large level density. In a discrete formulation the excitation energy ϵ_n should be replaced by the level index i_n and the state density $\rho_n(\epsilon_n)$ by the level degeneracy g_{i_n}, as was done in ref. [3].]

Multifragment states that differ only by a permutation of the fragment labels n are physically identical. Nevertheless, it is formally convenient to distinguish between such states. Consequently, the fragmentations F form some sort of hyperspace, with the redundant dimensions corresponding to label permutations, and observable features are obtained by projecting onto the space of physical fragmentations where label permutations have no effect. The summation over all possible multifragment states can then be expressed in terms of a sum over fragmentations, with each fragmentation weighted according to the measure (2): .

$$\sum_F (\cdot) \; = \; \sum_{N_F=1}^{\infty} \frac{1}{N_F!} \prod_{n=1}^{N_F} \left[\sum_{A_n=A_{\min}}^{A_{\max}} \int \rho_n(\epsilon_n) d\epsilon_n \int \frac{d\mathbf{r}_n d\mathbf{p}_n}{h^3} \right] (\cdot) \tag{3}$$

The factor $1/N_F!$ appears because label permutations are taken to be significant. It is convenient to define the *family* $\tilde{F}$ of fragmentations as the set of $N_F!$ fragmentations obtained by performing all possible permutations of the fragment labels in a particular fragmentation F.

A fragmentation represents the most complete information available. Most often this degree of detail is not required and it is convenient to integrate over some of the variables. For example, in an ordinary collision experiment, only asymptotic variables are observable and so it is of interest to eliminate the fragment positions $\mathbf{r}_n$ from the characterization of the multifragment states. This has been done in ref. [5] where the concept of an *event* was defined as

$$f \ : \ \{A_n, \epsilon_n, \mathbf{p}_n, n = 1, ..., N_f\} \ . \tag{4}$$

[Actually, for notational convenience, in ([5]) the notation f was used for the entire event family $\tilde{f}$ containing all states obtained by permuting the fragment labels in f.] In [5] the algebraic properties of the event set $\mathcal{F} = \{f\}$ were discussed and the associated notation was developed. In particular, it was shown that it is possible to introduce a partial ordering in $\mathcal{F}$, that $\mathcal{F}$ is an Abelian semi-group with respect to event addition, and that $\mathcal{F}$ is a complete lattice with respect to event intersection and union.

In the present study, we find it convenient to eliminate the fragment momenta $\mathbf{p}_n$ and define a *configuration* C as a set of fragmentations that differ only by the values of the fragment momenta,

$$C \ : \ \{A_n, \epsilon_n, \ \mathbf{r}_n, n = 1, ..., N_C\} \ . \tag{5}$$

If both positions and momenta are eliminated we obtain a *channel*,

$$\mathcal{C} \ : \ \{A_n, \epsilon_n, \ n = 1, ..., N_C\} \ . \tag{6}$$

Thus a channel is characterized by the mass numbers of its fragments and their intrinsic state of excitation, as in ordinary reaction theory.

Finally, it is convenient to define a *partition* as a set of channels that differ only with respect to the internal excitation of the fragments. A partition is then characterized by the sequence of the mass numbers of its fragments,

$$\mathcal{P} \ : \ \{A_n, n = 1, ...N_F\} \ . \tag{7}$$

In the work of Bondorf *et al.*the interest is focussed on the statistical distribution of multifragment partitions.

The are of course still other classes of possible interest. In particular, one may wish to eliminate the information about the internal excitations ϵ_n and focus the attention on $\{A_n, \mathbf{r}_n, \mathbf{p}_n\}$, as is done by Gross *et al.*, or possibly eliminate the momenta $\mathbf{p}_n$ as well, leaving $\{A_n, \mathbf{r}_n\}$. No names have yet been proposed for these multifragment classes.

It should be recalled that throughout our discussion the particular order of fragment labeling is taken to be significant, as a matter of convenience. It is of course straightforward to abandon this purely formal distinction. In that permutation-invariant case the various classes of multifragment states introduced above are enlarged by a factor of $N_F!$, the number of possible permutations of N_F elements.

3. GENERAL DESCRIPTION OF THE MODEL

We consider an ensemble of systems which each consists of a number of spherical nuclear fragments that are individually excitable and mutually interacting.

Our fundamental statistical hypothesis is that all multifragment states consistent with specified values of the total nucleon number A and energy E are equally probable. The properties of the system can then be expressed in terms of the density of states, $\rho(\Omega, A, E)$, which is obtained by performing the above summation using the appropriate weight of a given fragmentation,

$$\rho_{\text{microcan}}(\Omega, A, E) = \sum_F \delta(A_F - A)\delta(E_F - E) \ . \tag{8}$$

Here $A_F = \sum_n A_n$ is the total number of nucleons in F and E_F is its total energy, to be specified later (see eq. (11)). It should be noted that conservation of linear and angular momentum is *not* demanded, nor is conservation of the center-of-mass position. These simplifying omissions have been made for convenience, since they are not expected to be of great importance. Conservation of the total linear momentum $\mathbf{P}$ can be included without difficulty by attaching the factor $\delta(\mathbf{P}_F - \mathbf{P})$ and the further formal developments are not made more complicated by that (see eq. (14)). However, it would be more cumbersome to incorporate conservation of angular momentum and center of mass.

In order to develop a well-defined model, it is necessary to impose constraints on the fragment positions. This is most conveniently done by requiring their centers to be confined within a (usually spherical) volume Ω. The mean nuclear density is then $\rho \approx A/\Omega$ in the bulk of the system and falls off rapidly near the surface of Ω. This particular prescription is the natural one when one is simulating a translationally invariant system by way of imposing periodic boundary conditions, as is of relevance in astrophysical systems and for the general discussion of matter at subsaturation densities. In [8] a different prescription is used: the boundary of Ω are considered to be an infinite potential wall causing the entire fragment (not merely its center) to be within Ω. For the same Ω, this of course leads to a slightly more compact (and correspondingly denser) system, but by adjusting Ω appropriately the two prescriptions can be made nearly identical. [Contrary to the above two prescriptions, Bondorf *et al.* adopt a freezeout volume depending on the fragment multiplicity N, based on the intuitive expectation that the freezeout happens at a certain gap with so that a many-fragment partition of the system will have a alrger spatial extent than one consisting of only a few fragments.]

Our microcanonical formulation should be contrasted with the canonical or grand canonical approaches [2,3], where the density of states (8) is replaced by the partition functions

$$Z_{\text{canonical}}(\Omega, A, \tau) = \sum_F \delta(A_F - A)e^{-E_F/\tau} \ , \tag{9}$$

or

$$Z_{\text{grand can}}(\Omega, \mu, \tau) = \sum_F e^{(\mu A_F - E_F)/\tau} \ . \tag{10}$$

In the latter, the chemical potential μ and the temperature τ are specified and $\bar{E}$ and $\bar{A}$ follow from the appropriate derivatives of Z, whereas $\bar{\mu}$ and $\bar{\tau}$ follow from E and A

in the microcanonical formulation. While the two formulations are equivalent for large (thermodynamic) systems, there may well be differences between the two approaches for the finite systems formed in heavy-ion collisions. It is a particularly appealing feature of the microcanonical formulation that inter-fragment forces are readily incorporated, as these are expected to be important. [An analytical grand canonical treatment is impractical when the fragments interact and only when there are no forces between the fragments can sufficient simplification be achieved [2].]

In our studies, the total energy of a given fragmentation is taken to be of the form

$$E_F = \sum_{n=1}^{N_F} \left[\frac{p_n^2}{2mA_n} - B_n + \epsilon_n + \frac{1}{2} \sum_{n \neq n'} V_{nn'} \right] . \tag{11}$$

Here the first term represents the the kinetic energy of the moving fragments. The second term is the binding energy of a given fragment species. In the present study, this quantity is approximated by the semi-empirical mass formula $B_n = a_V A_n - a_S A_n^{\frac{2}{3}} - a_C Z_n^2 \, A_n^{-\frac{1}{3}}$. The coefficients are taken to be $a_V = 16$ MeV, $a_S = 16$ MeV, $a_C = 0.70$ MeV, and, since only one generic type of nucleon is considered and we wish to be fairly schematic, we assume that $Z_n = A_n/2$. In more realistic studies, it is quantitatively important to employ more accurate values for the binding energies of the lighter fragments which are the most abundant.

The last term in (11) represents the potential energy of the configuration arising from pairwise interactions between the fragments. This quantity has both Coulomb and nuclear components:

$$V_{nn'} = \frac{e^2 Z_n Z_{n'}}{|\mathbf{r}_n - \mathbf{r}_{n'}|} + V_{\text{nuc}}(|\mathbf{r}_n - \mathbf{r}_{n'}|) . \tag{12}$$

We have here used the asymptotic form of the electrostatic interaction potential, since the fragments rarely overlap in realistic situations, due to the high incompressibility of nuclear matter reflected in the nuclear interaction potential. For fairly dilute systems, in which the nuclear surfaces are well separated, the proximity potential can be conveniently used for V_{nuc}. However, it may be relatively inaccurate for the ordinarily rather small nuclear fragments occuring and for denser configurations a more refined calculation is required, in order to avoid pathological results. In particular, the strong minimum in the proximity potential between two small fragments as a function of their separation leads to the formation of an ordered, "crystalline" state in our simulations, which we regard as unphysical. In the present study we therefore disregard the attractive nuclear contribution to the inter-fragment potential and sometimes model the repulsive contribtuion as a hard-sphere potential. How to best treat this important physical ingredient is currently under study.

The significance of the interfragment forces is illustrated in figure 1, which shows the resulting values for the maen fragment mass number and the energy per nucleon for in various physical scenarios.

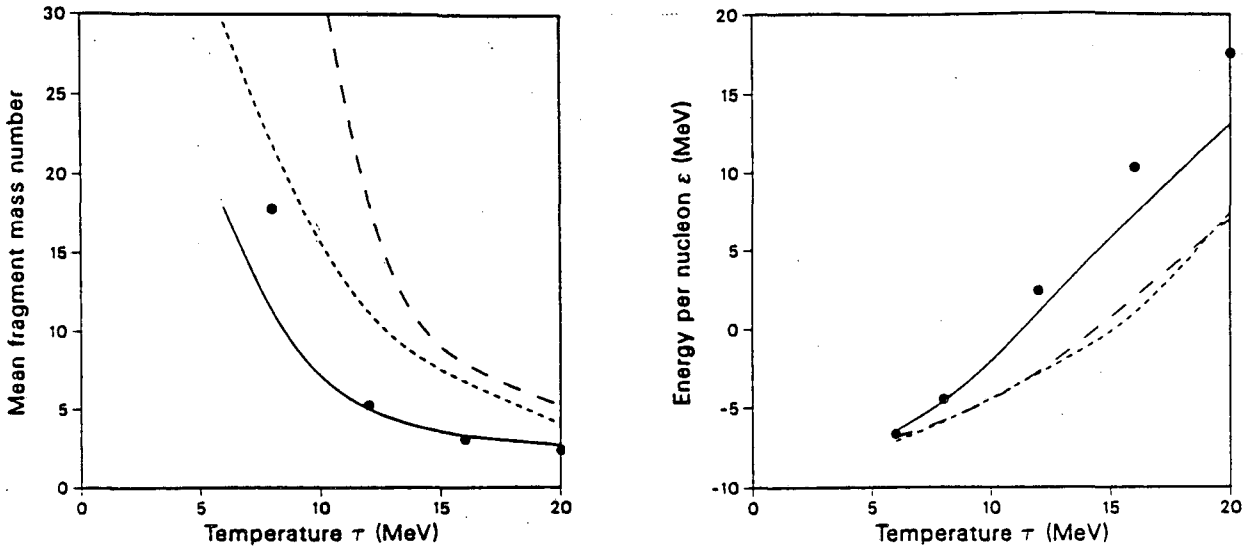

FIGURE 1.

The mean fragment mass number $\bar{A}$ (left) and the mean energy per nucleon ϵ (right), as functions of the temperature τ specified in a canonical treatment of a source with $A = 100$ nucleons at a mean density of ρ=0.08 fm^{-3}. The solid curve shows the results for non-interacting fragments, using the adopted standard value τ_0=12 MeV, while the short-dashed curve corresponds to surrounding each fragment with a spherical hard repulsive potential, and the long-dashed curve arises when the mutual Coulomb repulsion between fragments are also included. The solid dots indicate the results when this latter system is expanded to ρ=0.04 fm^{-3}. (Taken fron ref. [1].)

Because E_F depends quadratically on the fragment momenta, the integrals over $\mathbf{p}_n$ in (8) can be expressed analytically:

$$\int d\mathbf{p}_1 ... d\mathbf{p}_N \; \delta\Big(\sum_{n=1}^{N} \frac{p_n^2}{2m_n} - K\Big) \; = \frac{2\pi}{\Gamma(\frac{3}{2}N)} (m_1 ... m_N)^{\frac{3}{2}} \; (2\pi K)^{\frac{3}{2}N-1} \; . \tag{13}$$

If conservation of the total momentum were also demanded, the result would be modified to:

$$\int d\mathbf{p}_1 ... d\mathbf{p}_N \; \delta\Big(\sum_{n=1}^{N} \frac{p_n^2}{2m_n} - K\Big) \; \delta\Big(\sum_{n=1}^{N} \mathbf{p}_n\Big) \; = \frac{2\pi}{\Gamma(\frac{3}{2}(N-1))} \Big(\frac{m_1 ... m_N}{m_1 + ... + m_N}\Big)^{\frac{3}{2}} \; (2\pi K)^{\frac{3}{2}N-\frac{5}{2}} \; . \tag{14}$$

The essential difference is that the quantity N is replaced by $N-1$, both in the power of K and in the Γ-function; this change can readily be made in the expression (16) for the statistical weights. While such a refinement is not expected to be important in the present simplified model, it should be included in more realistic treatments. Furthermore, the quantitative importance of conserving the overall angular momentum and the center-of-mass position also ought to be examined.

In our current studies, we are not interested in observables depending on the individual fragment momenta and so the above analytical result may be employed to eliminate the

explicit appearance of the momentum variables. The density of states can then be written in the form

$$\rho(\Omega, A, E) = \sum_{N=1}^{\infty} \prod_{n=1}^{N} \left[\sum_{A_n=A_{\min}}^{A_{\max}} \int_0^{\infty} d\epsilon_n \int \frac{d\mathbf{r}_n}{\Omega} \right] W \equiv \sum_C W(C) \,, \tag{15}$$

where C denotes multifragment configurations, as defined in eq. (5). The statistical weight of a particular configuration is

$$W(C) = \frac{1}{N!} \frac{1}{\Gamma(\frac{3}{2}N)} \prod_{n=1}^{N} \left[\Omega \left(\frac{mA_n}{2\pi\hbar^2} \right)^{\frac{3}{2}} \rho_n(\epsilon_n) \right] \delta(\sum_{n=1}^{N} A_n - A) \; K^{\frac{3}{2}N-1} \,, \tag{16}$$

where

$$K = E - \sum_{n=1}^{N} [-B_n + \epsilon_n] + \frac{1}{2} \sum_{nn'} V_{nn'} \tag{17}$$

is the total kinetic energy of the N fragments. Note that in (15) the integration over fragment positions has been changed into an average by dividing by the volume Ω; this change, which is made merely for dimensional convenience, introduces an explicit factor of Ω^N into the statistical weight (16).

Similar expressions can be derived for the canonical and grand canonical partition functions, eqs. (9-10). In particular, the canonical partition function (9) takes precisely the form (15) with

$$W_{\text{canonical}}(C) = \frac{1}{N!} \prod_{n=1}^{N} \left[\Omega \left(\frac{mA_n\tau}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{B_n/\tau} \rho_n(\epsilon_n) e^{-\epsilon_n/\tau} \right] \delta \left(\sum_{n=1}^{N} A_n - A \right) e^{-V/\tau} \,, \tag{18}$$

while the grand-canonical partition function (10) corresponds to

$$W_{\text{grand can}}(C) = \frac{1}{N!} \prod_{n=1}^{N} \left[\Omega \left(\frac{mA_n\tau}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{B_n/\tau} e^{\mu A_n/\tau} \rho_n(\epsilon_n) e^{-\epsilon_n/\tau} \right] e^{-V/\tau} \,. \tag{19}$$

In these expressions, V is the total potential energy of the system, as given by the last term in (11).

Observables can be evaluated as averages over a representative sample of configurations, $\{C\}$. For example, as shown in ref. [1], the mean values of the inverse temperature β and the fragment multiplicity N are obtained as

$$\bar{\beta} \approx \frac{\sum_C W(C) \left[\left(\frac{3}{2}N - 1 \right) / K \right]}{\sum_C W(C)} \,, \quad \bar{N} \approx \frac{\sum_C W(C) N_C}{\sum_C W(C)} \,. \tag{20}$$

4. UNBOUND FRAGMENTS

In the first, grand-canonical, treatment of disassembly of nuclear matter [2], only particle-stable fragment levels were considered. Subsequently, the production (and sequential decay) of particle-unstable fragments was incorporated [3], an extension that requires the inclusion of highly excited nuclear levels. Since the density of these levels increases strongly with energy, the results are sensitive to this quantity. Morevover, the fact that the surface tends to reduce the level density makes a highly excited system prefer to coalesce into a single large fragment, rather than break up into many small ones, as physical intuition would suggest. Some caution must therefore be exercised, as we now discuss.

The density of highly excited nuclear levels is given approximately by the Fermi-gas formula so that $\rho_a(\epsilon) \approx \rho_A^{TF}(\epsilon) \sim \exp(2\sqrt{a_A \epsilon})$. The general very strong increase of ρ with ϵ implies that at high energies the configuration space will be dominated by the intrinsic level density. It has been argued previously on physical grounds that only sufficiently long-lived excited levels should be included in the partition function.[3] With the assumption that the stability of excited levels generally descreases with energy, this criterion can be implemented through a modulation factor expressing the probability that levels at a given excitation are sufficiently long-lived to be counted as possible final states.[3] As the modulation factor, we use a simple exponential, $e^{-\epsilon/\tau_0}$, which is formally convenient, and thus introduce an effective state density, $\rho_A^{\rm eff}(\epsilon) = \rho_A(\epsilon)e^{-\epsilon/\tau_0}$.[1] By considering the corresponding effective intrinsic partition function,

$$\begin{aligned} \zeta_A^{\rm eff}(\tau) &= \int \rho_A^{\rm eff}(\epsilon)\, e^{-\epsilon/\tau} d\epsilon \qquad (21) \\ &= \int \rho_A(\epsilon)\, e^{-\epsilon/\tau_0}\, e^{-\epsilon/\tau} d\epsilon = \zeta_A(\tau_{\rm eff}) \ , \end{aligned}$$

it can be seen that the introduction of the exponential suppression factor formally is equivalent to describing the intrinsic nuclear excitation in terms of an effective temperature $\tau_{\rm eff}$ given by

$$\tau_{\rm eff}^{-1} = \tau^{-1} + \tau_0^{-1} \ . \qquad (22)$$

This effective temperature is always smaller than τ and approaches τ_0 when $\tau \gg \tau_0$. Thus, τ_0 can be interpreted as the maximum temperature attainable by nuclear fragments. The existence of such a limiting temperature has been suggested on theoretical grounds and values in the range of 10-12 MeV have been calculated.[11] In our calculations we have used the value $\tau_0 = 12$ MeV. [Moreover, it has been pointed out [12] that Levinson's theorem, which relates bound-state properties and scattering phase shifts, implies that the nuclear level density will in general decrease and ultimately vanish at high excitation. The suggested limiting value for the excitation energy in ^{208}Pb of around 8 MeV/N corresponds to a limiting temperature of ≈ 8 MeV.]

The importance of reducing the intrinsic level density is illustrated in figure 2. It is seen that there is a large sensitivity to this physical ingredient. Our present approach should only be regarded as a temporary prescription will have to suffice until this problem has been better understood.

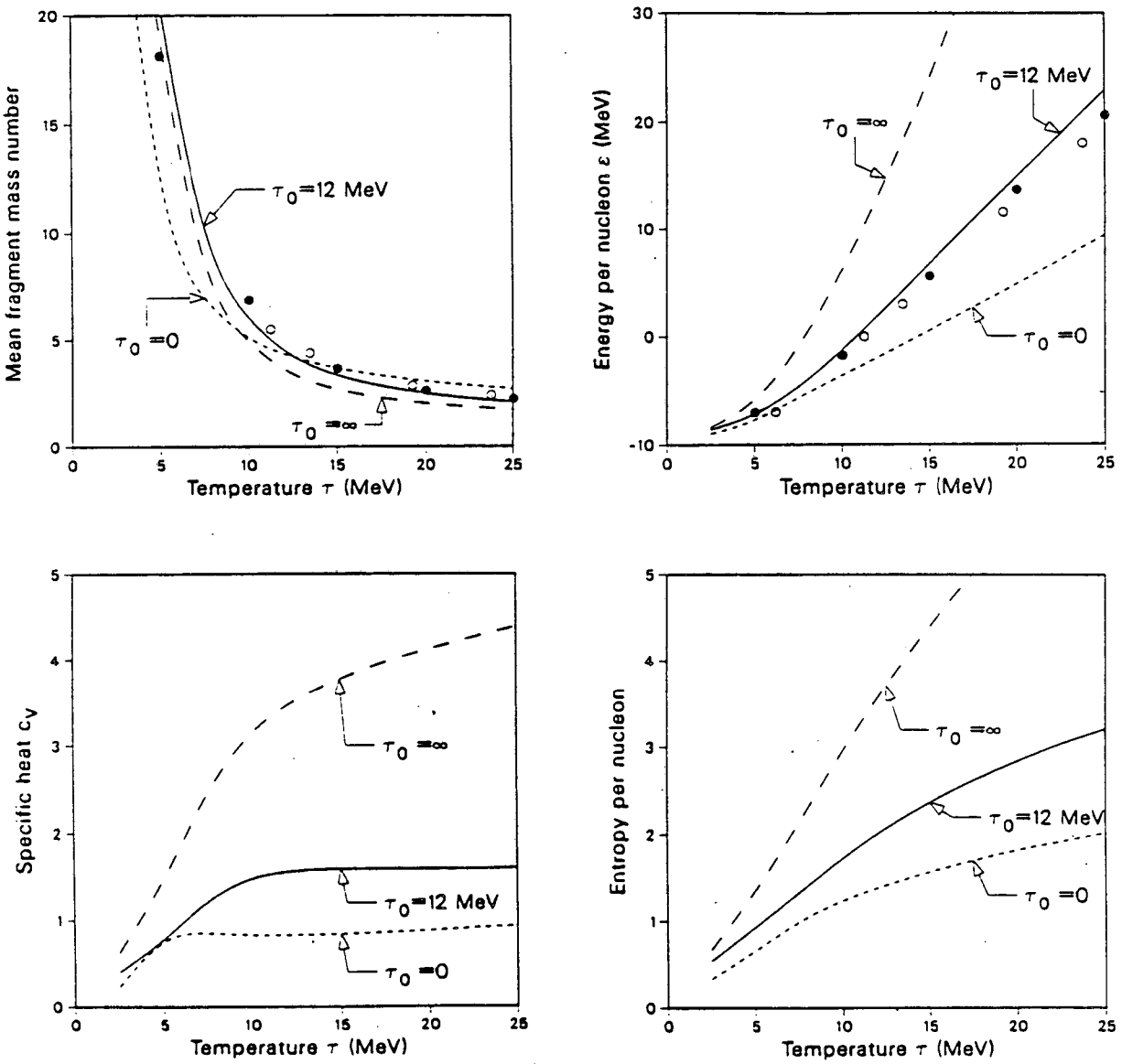

FIGURE 2.

Grand canonical calculation of a) the mean fragment mass number, $\bar{A}$, b) the energy per nucleon, ϵ, c) the specific heat, C_V, and d) the entropy per nucleon, σ, as functions of the temperature τ, for the values τ_0 = 0, 12 MeV, 1000 MeV. Also shown are results of canonical (solid dots) and microcanonical (open dots) calculations, for the standard value τ_0 = 12 MeV. The system considered has 40 nucleons and a mean bulk density of $\rho = 0.5\rho_0$ =0.08 fm^{-3}, the values $A_{\min} = 1$ and $A_{\max} = 40$ were used, and there is no interaction between the fragments. (Taken form ref. [1].)

5. THE NUMERICAL METHOD

While the large of the number of contributing configurations precludes an exact evaluation in all but the smallest systems, it does invite to employ statistical methods. We therefore evaluate observables as averages over a representative sample of configurations, generated by application of the method first proposed by Metropolis *et al.*,[13] which provides a Markovian sequence of configurations $\{C_k, k = 1, ...\}$. In the present case, the method is implemented as follows. Given any configuration C_k, we form a trial configuration, C', by making any one of several small "moves" in configuration space. These moves consist of changing the location or excitation energy of a fragment, exchanging nucleons and excitation energy between two fragments (a "reaction"), dividing a fragment into two ("fission"), or combining two fragments ("fusion"). These moves suffice to make any configuration reachable. (In fact, there is some redundancy: the reaction moves are not strictly necessary, but they are calculationally convenient since they produce a faster exploration of partition space.)

The trial configuration C' is accepted as the next member of the sequence, C_{k+1}, with the probability $[\rho]$; if C' is unsuccessful the C_k is used again: $C_{k+1} = C_k$. Here $[\rho] = \rho$ if $\rho \leq 1]$ and $\rho] = 1$ otherwise. The quantity ρ is proportional to the ratio of the statistical weigths, $\rho \sim W(C')/W(C)$. However, careful account must be taken of the fact that the probability $T(C \rightarrow C')$ for forming the trial configuration C' form C is in general different from the probability $T(C \leftarrow C')$ for forming C form C'. Indeed, certain elementary moves in configuration space have no reverse moves, as is the case with the fusion moves (see later).

The Metropolis algorithm produces a diffusive exploration of the configuration space in a physically appealing way, and, if the sample of configurations, $\{C_s\}$, is drawn from the sequence $\{C_k\}$ at intervals of such size that correlations between successive configurations are unimportant, the required average can be evaluated directly. It is important to note the flexibility and generality of this method; as we need only be able to compute W for given configurations, it is possible to use realistic mass formulas and level densities and, in particular, inter-fragment forces are easily included.

While there is a large degree of freedom with respect to choosing the specific types of elementary moves in configuration space, it is mandatory that the particular procedure devised conforms with the principle of detailed balance, in order to ensure that the configuration sequence C_k be sampled in accordance with the probability measure provided by the statistical weigth $W(C)$.

Ordinarily, this principle states that when the system is in statistical equilibrium then the rate of transition from a given configuration C to another one C' is equal to the rate of the reverse move. This can be expressed in the form

$$W(C)\ \Delta C\ P(C \rightarrow C') = W(C')\ \Delta C'\ P(C \leftarrow C')\ , \tag{23}$$

where $P(C \rightarrow C')$ is the probability that the random walk moves to C' when it is at C and $P(C \leftarrow C')$ is the probability that the next configuration is chosen as C when the current one is C'. Furthermore,

$$\Delta C = \prod_{n=1}^{N} \left[\frac{\Delta \mathbf{r}_n}{\Omega} \Delta \epsilon_n\right] \tag{24}$$

denotes the interval in configuration space.

In our present formulation only the configuration *families* are physically significant, and the condition of detailed balance yields the weaker requirement

$$\sum_{C\in\tilde{C}} W(C)\,\Delta C\; P(C \to \tilde{C}') = \sum_{C'\in\tilde{C}'} W(C')\,\Delta C'\; P(\tilde{C} \leftarrow C')\,. \tag{25}$$

Here $P(C \to \tilde{C}')$ is the probability that the system moves to any member of the family $\tilde{C}'$ when it is currently at the configuration C, and $P(\tilde{C} \leftarrow C')$ is similarly the probability that the system moves to any member of $\tilde{C}$ when currently at C'. Since the statistical weight $W(C)$ is the same for all members of the family $\tilde{C}$, the above condition may be rewritten as

$$W(C)\,\Delta C \sum_{C\in\tilde{C}} P(C \to \tilde{C}') = W(C')\,\Delta C' \sum_{C'\in\tilde{C}'} P(\tilde{C} \leftarrow C')\,. \tag{26}$$

Furthermore, for the moves considered in the present study the transition probability $P(C \to \tilde{C}')$ is the same for all initial configurations belonging to the family $\tilde{C}$ and correspondingly for $P(\tilde{C} \leftarrow C')$. Since the family $\tilde{C}$ has $N_C!$ members, we find that detailed balance dictates that the relation

$$\frac{P(C \to \tilde{C}')}{P(\tilde{C} \leftarrow C')} = \frac{N_{C'}!}{N_C!}\,\frac{W(C')\,\Delta C'}{W(C)\,\Delta C}\,. \tag{27}$$

be satisfied for all family pairs $\tilde{C}$ and $\tilde{C}'$ that are connected by elementary moves.

6. EXAMPLE: FISSION $\leftrightarrow$ FUSION

Here we shall discuss in some detail the fission and fusion moves in configuration space. These moves are the most complicated ones considered because they change the number of fragments in the configuration.

6.1 Fission

Assume that we are at a given configuration C having N fragments and we attempt to make a fission move. The fissioning fragment i is picked randomly from the N fragments in C; if $A_i < 2A_{\min}$ or if $A_i > 2A_{\max}$ there are no open fission channels for that fragment and the move is aborted. It is also checked that the excitation energy ϵ_i lies within an interval of width ϵ_{i0} centered around $\epsilon = \epsilon_{i0}$. Usually, we take $\epsilon_{i0} = a(A_i)\tilde{\tau}^2$, *i.e.* the mean excitation energy in fragment i at a definite "temperature" $\tilde{\tau}$ prescribed ahead of time and employed throughout the entire sampling process.[1]

Provided these tests are passed, the fragment is then split in two, $A_i \to A_{i'} + A_{j'}$, selecting randomly between all the distinct binary partitions p. If $A_{\max} \geq A_i - A_{\min}$ then $p = 1 + A_i - 2A_{\min}$ and otherwise $p = 1 - A_i + 2A_{\max}$.

After the partition has been picked, the excitation energies of the two fission products are chosen, so that the fianl channel is determined. These are chosen randomly from the

intervals $[\frac{1}{2}\epsilon'_{i0}, \frac{3}{2}\epsilon'_{i0}]$ and $[\frac{1}{2}\epsilon'_{j0}, \frac{3}{2}\epsilon'_{j0}]$, where ϵ'_{i0} and ϵ'_{j0} are defined similarly to ϵ_{i0}. Thus the fission move only goes from a fragment with an excitation energy in the prescribed interval to fragments with the similar property.

Finally, the positions of the fission products are chosen. They are picked randomly within the confining volume Ω. Once they are determined, it is possible to invoke (17) to calculate the amount of energy available for kinetic energy of the fragments, K'. If this quantity comes out negative, the move is aborted. Otherwise, the thus determined configuration C' is a possible next configuration and it is accepted on the basis of the quantity ρ given below by

$$\begin{aligned} \rho &= \frac{W(C')}{W(C)} \frac{\epsilon'_{i0}\epsilon'_{j0}}{\epsilon_{i0}} \qquad (28) \\ &= \frac{1}{N+1} \frac{\Gamma(\frac{3}{2}N)}{\Gamma(\frac{3}{2}(N+1))} \Omega \left(\frac{mA'_j K'}{2\pi\hbar^2}\right)^{\frac{3}{2}} \left(\frac{A'_i}{A_i}\right)^{\frac{3}{2}} \frac{\rho'_i(\epsilon'_i)\rho'_j(\epsilon'_j)}{\rho_i(\epsilon_i)} \frac{\epsilon'_{i0}\epsilon'_{j0}}{\epsilon_{i0}} \left(\frac{K'}{K}\right)^{\frac{3}{2}N-1} . \end{aligned}$$

The new configuration C' is identical to C except that the first fission product i' has taken the place of the mother fragment i and the second fission product j' has been added as fragment number $N+1$. It is elementary to verify that there is always two different moves leading from C into the family $\tilde{C}'$. This is because the two fission products always have different positions $\{A'_i\ \epsilon'_i \mathbf{r}'_i\ \}$ and $\{A'_i\ \epsilon'_j \mathbf{r}'_j\ \}$ in the reduced one-fragment space, so that an interchange of their labels yields a different member of the configuration family $\tilde{C}'$ which is equally likely to be reached in the given step.

The probability for making a move into the specific family $\tilde{C}'$ is thus

$$P(C \to \tilde{C}') = 2 \cdot \frac{1}{N} \cdot \frac{1}{p} \cdot \frac{\Delta\epsilon'_i}{\epsilon'_{i0}} \frac{\Delta\epsilon'_j}{\epsilon'_{j0}} \cdot \frac{\Delta\mathbf{r}'_i}{\Omega} \frac{\Delta\mathbf{r}'_j}{\Omega} \cdot [\rho] \qquad (29)$$

Here the factor 2 accounts for the just discussed fact the two different moves corresponding to permuting the fission products i' and j' lead into the same family $\tilde{C}'$. The factor $1/N$ is the probability for picking the fragment i and $1/\nu$ is the probability for partitioning A_i correctly. The next factors are the probabilities for picking the excitation energies and fragment positions within the specified tolerances. The final factor $[\rho]$ is the acceptance probability; it is equal to ρ when $\rho \leq 1$ and is unity otherwise.

6.2 Fusion

Now consider the reverse process: starting at a configuration $C' \in \tilde{C}'$ we attempt to make a fusion move. First the two fusing fragments i' and j' are chosen at random from all fragment pairs in C' (*i.e.* i' is chosen randomly from the $N+1$ fragments and j' is chosen subsequently from among the remaining N fragments) and it is checked that $A'_i + A'_j \leq A_{\max}$. If so the move is allowed to proceed with the probability $1/p$, where p is as defined above using $A_i = A'_i + A'_j$. If this hurdle is overcome, the excitation energy ϵ_i in the compound fragment A_i and its position $\mathbf{r}_i$ are picked as above and it is checked that

the available kinetic energy K is positive. If so, a possible final configuration has been constructed and the move is accepted on the basis of the quantity $1/\rho$.

The probability for making a move from C' into the family $\tilde{C}$ is then

$$P(\tilde{C} \leftarrow C') = 2 \cdot \frac{1}{(N+1)N} \cdot \frac{1}{p} \cdot \frac{\Delta\epsilon_i}{\epsilon_{i0}} \cdot \frac{\Delta \mathbf{r}_i}{\Omega} \cdot [\frac{1}{\rho}] \,. \tag{30}$$

Here the factor 2 accounts for the fact that an interchange of the labels of the two fusing fragments yields an equally likely process leading into $\tilde{C}$. The hurdle $1/p$ appears to compensate for the calculational fact that only one out of the p fission partitions is being pursued; as will be clear below, it is essential to include this factor to ensure detailed balance. The acceptance probability is defined as in (15). Note that the ratio of acceptance probabilities is $[\rho]/[1/\rho] = \rho$, irrespective of the value of ρ. Moreover, we see that

$$\frac{P(C \rightarrow \tilde{C}')}{P(\tilde{C} \leftarrow C')} = (N+1)\frac{\Delta C'}{\Delta C}\frac{\epsilon_{i0}}{\epsilon'_{i0}\epsilon'_{j0}}\rho \tag{31}$$

since

$$\frac{\Delta C'}{\Delta C} = \frac{\Delta\epsilon'_i \Delta\epsilon'_j}{\Delta\epsilon_i}\,\frac{\Delta \mathbf{r}'_i \Delta \mathbf{r}'_j}{\Omega \Delta \mathbf{r}_i} \,. \tag{32}$$

6.3 Detailed balance

We finally demonstrate that the procedure described above satisfies detailed balance. In the present case, the general relation (27) becomes

$$\frac{P(C \rightarrow \tilde{C}')}{P(\tilde{C} \leftarrow C')} = (N_C+1)\frac{W(C')\,\Delta C'}{W(C)\,\Delta C} \,. \tag{33}$$

A comparison with (31) immediately gives the expression (15), which is the the quantity first given in ref.[1]. The present discussion constitutes a more formal proof of the strict validity of the sampling procedure developed in [1] and, in particular, it explicitely brings out the fact that detailed balance is satisfied. Therefore, it is ensured that the particular sampling procedure devised does indeed sample the configurations in accordance with the proper weights $W(C)$.

The fact that the proper expressions sometimes appear somewhat counterintuitive (*e.g.* the factor $1/p$ in the fusion move) should be cause for a word of warning: It is essential to demonstrate that any particular sampling scheme does in fact satisfy detailed balance! If that is not shown, there is no reason to expect that the produced sample is statistically unbiased. Indeed, if some of the elementary moves violate detailed balance the calculated "equilibrium" distribution represents a false stationary solution corrresponding to the introduction of an additional, spurious bias into the problem.

7. CONCLUDING REMARKS

Recently, we have formulated a practical and well-founded method for an exact description of the statistical mechanics of the type of finite, interacting system of nucleons and nuclei likely to be formed in an energetic nuclear collision.[1] In the present note, we have discussed some important theoretical aspects of any microcanonical model for nuclear multifragmentation. In particular, we have defined a precise nomenclature for various classes of multifragments states of frequent interest, outlined the general formulation of a microcanonical description, and discussed the importance of satisfying detailed balance in a simulation approach. Furthermore, the significance of interfragment forces and unbound fragment states has been illustrated. Both of these aspects need further study before a realistic model is in hand. In [1] a tentative extension was made to incorporate a nucleon vapor, in order to facilitate studies of liquid-gas phase transition phenomena. This part also need further development.

There are many interesting applications of the type of model discussed here, especially in astrophysics and nuclear collision dynamics. However, and this is particularly true of simulation studies which often lack the transparency of more analytical studies, the utility of massive calculations depend entirely on the soundness of the physical assumptions and the formal basis of the model. Therefore, it is essential to demonstrate that any particular simulation scheme conforms with the general physical requirements, such as conservation laws and detailed balance.

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