Simulation of statistical ensembles suitable for the description of nuclear multifragmentation

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A general statistical ensemble is defined. The statistical weights for each configuration and consequently the mean value of any global observable can be expressed analytically. Since the resulting formulas are not numerically tractable, a statistical method of simulation is proposed. The method, a generalization of Koonin and Randrup's procedure, provides an exploration of configuration space according to the detailed balance principle. This method is then applied to investigate the nuclear multifragmentation phenomenon. Charge and mass distributions calculated for reactions $^{40}Ar+^{45}Sc$ at 35–115 MeV/nucleon and $^{93}Nb+^{9}Be$ at 11.4 and 30.3 MeV/nucleon are compared with the respective experimental data. [S0556-2813(97)04303-3]

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I. INTRODUCTION

Over the last decade the phenomenon of the nuclear disassembly of hot nuclear matter produced in high-energy nuclear collisions has been intensely studied from both theoretical and experimental points of view. Several models based on different theoretical approaches have been proposed in order to describe the continuously increasing amount of data. Some of the most widely used fragmentation approaches are statistical theories [1,4–6], cold fragmentation theories [7], transport theories [8,9], percolation theories [10,11], and compound nucleus decay models. One should also mention the hybrid theories, which employ both dynamical and statistical hypotheses, and the intermittence analysis based on factorial moments.

The method presented here is based on a statistical approach. Our aim is to provide a general algorithm for simulating several statistical ensembles, some of which can be used to describe successfully nuclear multifragmentation. One defines a general statistical ensemble which is suitable for various cases, not only physical ones, which results in statistical weights and the formulas expressing the probability of any configuration to appear. Since in most cases these formulas cannot be analytically simplified or numerically evaluated, they have to be statistically simulated. The proposed simulation method is a generalization of Koonin and Randrup's procedure [1–3] and consists of generating a trajectory in configuration space which is in accordance with detailed balance. This method is applied to the case of the nuclear multifragmentation of highly excited nuclei and the results are compared with the corresponding experimental data.

The paper is organized as follows. Section II describes the general statistical ensemble. Section III offers a method for simulating any of the defined statistical ensembles. Section IV presents an application of this method to the case of nuclear multifragmentation. Section V discusses the numerical results. Finally, the conclusions are drawn in Sec. VI.

II. STATISTICAL ENSEMBLE

We consider the most general case, that of a statistical ensemble of N_C elements, $N_C \in N_{C_{\min}}\text{-}N_{C_{\max}}$, each of them being described by m parameters. Thus, the set of parameters associated with a given *element* i can be written as

$$\{X_i^1, X_i^2, \ldots, X_i^m\}. \tag{2.1}$$

Suppose now that the first d parameters are discrete variables while the last $m-d$ parameters are continuous. To distinguish between the two types of parameters a more convenient notation is introduced:

$$\{\widetilde{X}_i^1, \ldots, X_i^d, X_i^{d+1}, \ldots, X_i^m\}. \tag{2.2}$$

The set of parameters corresponding to the ith element is denoted by $\mathcal{X}_i$:

$$\mathcal{X}_i \equiv \{\widetilde{X}_i^1, \ldots, \widetilde{X}_i^d, X_i^{d+1}, \ldots, X_i^m\}. \tag{2.3}$$

The set $\{\mathcal{X}_i\}$ with $i=1,\ldots,N_C$ defines a configuration which hereafter is denoted by C:

$$C:\{\mathcal{X}_i, i=1,\ldots,N_C\}. \tag{2.4}$$

Our basic assumption is that all configurations which are compatible with a given set of constraints are equally probable.

The elementary number of possible values for the kth parameter belonging to the ith element X_i^k is denoted by ΔN_i^k. Then, the elementary number of states Δv_C of configuration C is

$$\Delta v_C = \prod_{i=1}^{N_C} \Delta N_i^1 \cdots \Delta N_i^d \Delta N_i^{d+1} \cdots \Delta N_i^m = \prod_{i=1}^{N_C} \Delta N_i^{d+1} \cdots \Delta N_i^m. \tag{2.5}$$

Obviously, since the first d variables are discrete, the relation $\Delta N_i^1 = \cdots = \Delta N_i^d = 1$ is valid. The notation can be further simplified by replacing the product of the elementary number of each parameter's states by $\Delta \mathcal{N}_i$:

$$\Delta v_C = \prod_{i=1}^{N_C} \Delta \mathcal{N}_i. \tag{2.6}$$

The total number of possible states can be expressed as follows:

$$N_{\rm tot}=\sum_{N_C=N_{C_{\min}}}^{N_{C_{\max}}}\frac{1}{N_C!}\prod_{i=1}^{N_C}\left(\sum_{\mathcal{D}_d}\int_{\mathcal{D}_c}dN_i^{d+1}\cdots dN_i^m\right)$$
$$=\sum_{N_C=N_{C_{\min}}}^{N_{C_{\max}}}\frac{1}{N_C!}\prod_{i=1}^{N_C}\left(\sum_{\mathcal{D}_d}\int_{\mathcal{D}_c}d\mathcal{N}_i\right), \tag{2.7}$$

where $\mathcal{D}_c$ and $\mathcal{D}_d$ denote the allowed domain for the discrete and continuous variables, respectively. Supposing that for each continuous variable X_n there exists a function α_i^n such that $dN_i^n=\alpha_i^n X_i^n$, one has

$$dN_i^{d+1}=\alpha_i^{d+1}dX_i^{d+1},\ \ldots,dN_i^m=\alpha_i^m dX_i^m. \tag{2.8}$$

Consequently, we can write

$$dN_i^{d+1}\cdots dN_i^m=(\alpha_i^{d+1}\cdots\alpha_i^m)(dX_i^{d+1}\cdots dX_i^m)\equiv\mathcal{A}_i d\mathcal{X}_i, \tag{2.9}$$

and formula (2.7) becomes

$$N_{\rm tot}=\sum_{N_C=N_{C_{\min}}}^{N_{C_{\max}}}\frac{1}{N_C!}\prod_{i=1}^{N_C}\left(\sum_{\mathcal{D}_d}\int_{\mathcal{D}_c}\alpha_i^{d+1}dX_i^{d+1}\ldots\alpha_i^m dX_i^m\right)$$
$$=\sum_{N_C=N_{C_{\min}}}^{N_{C_{\max}}}\frac{1}{N_C!}\prod_{i=1}^{N_C}\left(\sum_{\mathcal{D}_d}\int_{\mathcal{D}_c}\mathcal{A}_i d\mathcal{X}_i\right). \tag{2.10}$$

When we deal with global restrictions [let us denote them by $\mathcal{R}(\mathcal{X}_1,\ldots,\mathcal{X}_{N_C})$], the total number of states can be written as

$$N_{\rm tot}=\sum_{N_C=N_{C_{\min}}}^{N_{C_{\max}}}\frac{1}{N_C!}\prod_{i=1}^{N_C}\left(\sum_{\mathcal{D}_d}\int_{\mathcal{D}_c}\mathcal{A}_i d\mathcal{X}_i\right)\mathcal{R}(\mathcal{X}_1,\ldots,\mathcal{X}_{N_C})$$
$$=\sum_C W_C, \tag{2.11}$$

where W_C represents the statistical weight of a given configuration,

$$W_C=\frac{1}{N_C!}\prod_{i=1}^{N_C}\mathcal{A}_i\mathcal{R}(\mathcal{X}_1,\ldots,\mathcal{X}_{N_C}), \tag{2.12}$$

and

$$\sum_C(\cdot)=\sum_{N_C=N_{C_{\min}}}^{N_{C_{\max}}}\prod_{i=1}^{N_C}\left(\sum_{\mathcal{D}_d}\int_{\mathcal{D}_c}d\mathcal{X}_i\right)(\cdot). \tag{2.13}$$

The multiplicity of a given configuration is then given as

$$P(C)=\frac{W_C}{\Sigma_C W_C}. \tag{2.14}$$

Before closing this section we would like to say a few words about the global restrictions $\mathcal{R}(\mathcal{X}_1,\ldots,\mathcal{X}_{N_C})$. Generally, these restrictions are required by some conservation laws. In what follows we enumerate three kinds of restrictions which are usually imposed in physical systems. This results in a classification for the system parameters.

(a) Global conservation laws of the type

$$\sum_{i=1}^{N_C}X_i^{aj}=\mathcal{C}_j^a\quad\text{for any configuration } C,\quad j=1,\ldots,N_a, \tag{2.15}$$

where X_i^{aj} denotes both the discrete and continuous parameters of the system that obey restrictions of the type (a) and N_a the total number of restrictions. We denote the factor accounting for this kind of conservation law by

$$\mathcal{R}_a(X_i^{aj},i=1,\ldots,N_C)=\prod_{j=1}^{N_a}\delta\left(\sum_{i=1}^{N_C}X_i^{aj}-\mathcal{C}_j^a\right). \tag{2.16}$$

(b) Global conservation laws of the type

$$\sum_{i=1}^{N_C}F_j(X_i^{bk_j})=\mathcal{C}_j^b\quad\text{for any configuration } C,$$
$$j=1,\ldots,N_b,$$
$$k_j=1,\ldots,N_b^j, \tag{2.17}$$

where N_b represents the number of possible functions F_j, N_b^j is the number of variables corresponding to the jth restriction, and $X_i^{bk_j}$ denotes both integer and continuous parameters of the system (2.2). This kind of conservation law is represented by the factor

$$\mathcal{R}_b(X_i^{bk_j},i=1,\ldots,N_C)=\prod_{j=1}^{N_b}\delta\left(\sum_{i=1}^{N_C}F_j(X_i^{bk_j})-\mathcal{C}_j^b\right). \tag{2.18}$$

(c) No global conservation laws. Obviously, the corresponding restrictions are

$$\mathcal{R}_c(X_i^{cj},i=1,\ldots,N_C)=1, \tag{2.19}$$

where X_i^{cj} $(j=1,\ldots,N_c)$ corresponds to the parameters belonging to the ith element that does not obey any conservation law.

Once this classification is adopted, one may say that the global restriction mentioned in Eq. (2.11) is a product of the above-defined restrictions.

III. GENERAL SIMULATION ALGORITHM

Since the number of contributing configurations is very large in all but very small systems, formulas like those given by Eqs. (2.11) and (2.14) cannot be numerically evaluated. Because of this fact, we shall simulate the statistical ensemble and then gather the information we need. The method we propose generates a *correct* exploration of the configuration space. This means that the exploration must generate configuration C with its *real* probability of appearance, $P(C)$, given by Eq. (2.14). The method is based on the principle that any trajectory in configuration space is *correct* if each movement from a point C_k to the next point on the trajectory, C_{k+1}, obeys the detailed balance principle.

Ordinarily, this principle states that when a system is in

statistical equilibrium, the rate of transition from a given configuration C to another one C' is equal to the rate of the reverse motion. For the ensemble under consideration, this fact can be expressed in the form

$$\frac{P(C\rightarrow\widetilde{C}')}{P(\widetilde{C}\leftarrow C')}=\frac{W_{C'}\Delta C' N_{C'}!}{W_C \Delta C N_C!}, \tag{3.1}$$

where $\widetilde{C}$ denotes $N_C!$ identical systems obtained by permutating the elements label while ΔC stands for the elementary interval of configuration C ($\Delta C=\Pi_{i=1}^{N_C}\Delta\mathcal{X}_i$).

The method of generating a *correct* trajectory in the configuration space, which we put forth, consists of two steps.

(1) Generate a trajectory which is able to scan all the configuration space.

(2) Correct this trajectory so that it obeys the detailed balance principle. This correction is achieved by adjusting the primary generation with a statistical factor which is a solution of the detailed balance equation. This factor influences the probability of transition from a given configuration C_k to the next configuration C_{k+1}. Thus, if $P(C_k\rightarrow\widetilde{C}_{k+1})$ is the probability of passing from the configuration C_k to the configuration C_{k+1} according to the initial way of generating the trajectory, after correction, the probability of passing from the configuration C_k to the configuration C_{k+1} will be $P(C_k\rightarrow\widetilde{C}_{k+1})[\alpha]$, where $[\alpha]$ is the factor mentioned above. Let us now describe these two steps.

A. Generation of the primary trajectory

In principle any trajectory capable of scanning *the entire* configuration space can be used. However, it is particularly important to explore configuration space in *small* moves, namely, to pass from a given configuration C_k only to those configurations C_{k+1} which differ from C_k by a single element. To be more specific, if configuration C_k has N_C elements, configuration C_{k+1} should have either N_C+1 or N_C-1 elements.

At this stage, we would like to comment on the optimal way of passing from one configuration,

$$C:\{\mathcal{X}_i, i=1,\ldots,N_C\}, \tag{3.2}$$

to another. Certainly, these ways depend on the particular global restriction $\mathcal{R}(\mathcal{X}_1,\ldots,\mathcal{X}_{N_C})$. There exist two kinds of systems with specific suitable generating methods.

(i) *Systems that obey at least one of the global conservation laws* mentioned in the previous section [which means (a) or (b)]. We consider the most general case, namely, that involving parameters which satisfy all three kinds of restrictions.

In this case the optimal way in which one can pass from configuration C into a next configuration is to ''split'' a randomly chosen element into two elements (a ''fission'' move) or to ''combine'' two randomly chosen elements into a final one (a ''fusion'' move). The significance of the terms ''split'' or ''combine'' is explained in the following example. The two kinds of movements will be generated with equal probability.

1. ''Fission'' move

Consider the starting configuration C given by Eq. (2.14). We randomly choose a ''fissioning'' element i from the N_C elements. The probability of this movement is

$$p_1=\frac{1}{N_C}. \tag{3.3}$$

At the next step we randomly choose as ''fission'' products two elements denoted by i' and j'. The parameters of these two elements are fixed as follows.

The parameters of the ''fission'' products i' and j', which are not of the type (a), will be randomly chosen in their maximum domains; the (a)-type parameters will be randomly chosen such that $X_{i'}^{ak}+X_{j'}^{ak}=X_i^{ak}$. The probability for making this move is

$$p_2=\frac{\Pi_{k=1}^{N_a}\Delta X_{i'}^{ak}}{\Pi_{k=1}^{N_a}X_i^{ak}}\frac{\Pi_{k=1}^{m-N_a}\Delta X_{i'}^{bck}\Delta X_{j'}^{bck}}{\Pi_{k=1}^{m-N_a}L(\mathcal{D}_{i'}^{bck})L(\mathcal{D}_{j'}^{bck})}, \tag{3.4}$$

where $\mathcal{D}_i^{bck}$ represents the allowed domain of the kth parameter of the element i and $L(\cdot)$ the length of the domain under brackets. Of course, the parameters chosen in this way may not satisfy the restrictions (a) and/or (b). Thus, if one of the restrictions $\mathcal{R}_a$ and $\mathcal{R}_b$ is violated, one must reject the move and consider the starting configuration C as the next configuration. The probability of choosing a good configuration C' can then be written as

$$P'(C\rightarrow\widetilde{C}')=2\frac{1}{N_C}\frac{\Pi_{k=1}^{N_a}\Delta X_{i'}^{ak}}{\Pi_{k=1}^{N_a}X_i^{ak}}\frac{\Pi_{k=1}^{m-N_a}\Delta X_{i'}^{bck}\Delta X_{j'}^{bck}}{\Pi_{k=1}^{m-N_a}L(\mathcal{D}_{i'}^{bck})L(\mathcal{D}_{j'}^{bck})}\prod_{k=1}^{m}H(X_i^k-\inf(\mathcal{D}_i^k))H(\sup(\mathcal{D}_i^k)-X_i^k)H(X_{i'}^k-\inf(\mathcal{D}_{i'}^k))$$
$$\times H(\sup(\mathcal{D}_{i'}^k)-X_{i'}^k)H(X_{j'}^k-\inf(\mathcal{D}_{j'}^k))H(\sup(\mathcal{D}_{j'}^k)-X_{j'}^k)\mathcal{R}_a\mathcal{R}_b, \tag{3.5}$$

where we have denoted by $\mathcal{D}_i^k$ the allowed domain of the kth parameter of the ith element and by H the Heaveside function. The correction to the fission movement will be made by accepting this resulting configuration with the probability $[\alpha]$. Thus, the probability for the corrected movement can be written as

$$P(C\rightarrow\widetilde{C}')=[\alpha]P'(C\rightarrow\widetilde{C}'). \tag{3.6}$$

2. ''Fusion'' move

We now consider C' as a starting configuration having N_C+1 elements. We first choose the two ''fusing'' elements i' and j'. This move has the probability

$$p_1'=\frac{1}{N_C(N_C+1)}. \tag{3.7}$$

The parameters of the ''fusion'' product will be fixed as follows. Obviously, the parameters of type (a) will have the values $X_i^{ak}=X_{i'}^{ak}+X_{j'}^{ak}$ $k=1,\ldots,N_a$; the remaining parameters will be randomly chosen in their domains. The probability for this move is

$$p_2'=\frac{\Pi_{k=1}^{m-N_a}\Delta X_i^{bck}}{\Pi_{k=1}^{m-N_a}L(\mathcal{D}_i^{bck})}. \tag{3.8}$$

If the chosen parameters do not obey the restrictions $\mathcal{R}_a$ and $\mathcal{R}_b$, the move is aborted and C' is used again. Thus, the probability for obtaining this new, good configuration C' is

$$P'(\widetilde{C}\leftarrow C')=2\frac{1}{N_C(N_C+1)}\frac{\Pi_{k=1}^{m-N_a}\Delta X_i^{bck}}{\Pi_{k=1}^{m-N_a}L(\mathcal{D}_i^{bck})}\prod_{k=1}^{m}H(X_i^k-\inf(\mathcal{D}_i^k))H(\sup(\mathcal{D}_i^k)-X_i^k)H(X_{i'}^k-\inf(\mathcal{D}_{i'}^k))H(\sup(\mathcal{D}_{i'}^k)-X_{i'}^k)$$
$$\times H(X_{j'}^k-\inf(\mathcal{D}_{j'}^k))H(\sup(\mathcal{D}_{j'}^k)-X_{j'}^k)\mathcal{R}_a\mathcal{R}_b. \tag{3.9}$$

The correction to the ''fusion'' movement will be made by accepting the resulting configuration with the probability $[1/\alpha]$. Then, the corrected probability can be written as

$$P(\widetilde{C}\leftarrow C')=\left[\frac{1}{\alpha}\right]P'(\widetilde{C}\leftarrow C'). \tag{3.10}$$

(ii) *Systems obeying only restrictions of type (c)* (in other words, systems which do not obey any global conservation law). In this case, the optimal way (of generating ''small moves'') in which one can pass from a configuration C to a next configuration C' is to add an element to the system (''adding move'') or to remove an element from the system (''removing move''). These two kinds of movements are generated with equal probabilities.

3. ''Adding'' move

Consider now the starting configuration C, with N_C elements. At this point, we check first whether $N_C+1\leqslant N_{C_{\max}}$. If this is satisfied, one performs the next step; otherwise, one considers C as the next configuration by adding an element to the system and keeping the parameters of the former system C the same. Let C' be the resulting system. The parameters of the (N_C+1)th element are randomly chosen in the allowed domains. Since there are no global restrictions, one can say that the new configuration C' was generated with the probability

$$P'(C\rightarrow\widetilde{C}')=p'=\frac{\Delta\mathcal{X}_{i'}}{L(\mathcal{D}_{i'})}. \tag{3.11}$$

The correction for the ''adding'' movement is performed by accepting this resulting configuration with the probability $[\alpha]$. The probability of the corrected movement is

$$P(C\rightarrow\widetilde{C}')=[\alpha]P'(C\rightarrow\widetilde{C}'). \tag{3.12}$$

4. ''Removing'' move

Let C' be the starting configuration, having N_C+1 elements. At this point we check first if $N_C\geqslant N_{C_{\min}}$. If this relation holds, one passes to the next step; otherwise, we count C' as the next configuration by removing an element from the system and keeping the remaining ones as they are. The next configuration C is obtained by removing one of the N_C+1 elements from the C' configuration. Since there are no global restrictions, one may say that a new configuration C' has been generated with the probability

$$P'(\widetilde{C}\leftarrow C')=\frac{1}{N_C+1}. \tag{3.13}$$

The ''removing'' movement correction will be made by accepting the configuration C with the probability $[1/\alpha]$. The probability of the corrected movement is

$$P(\widetilde{C}\leftarrow C')=\left[\frac{1}{\alpha}\right]P'(\widetilde{C}\leftarrow C'). \tag{3.14}$$

The factors $[\alpha]$ and $[1/\alpha]$ are defined as follows:

$$[\alpha]=\begin{cases}\alpha, & \alpha<1,\\ 1, & \alpha\geqslant 1,\end{cases}\qquad \left[\frac{1}{\alpha}\right]=\begin{cases}\frac{1}{\alpha}, & \alpha\geqslant 1,\\ 1, & \alpha<1.\end{cases} \tag{3.15}$$

It is worth noticing that $[\alpha]/[1/\alpha]=\alpha$ for any α.

B. Evaluation of the correction factor

(i) Using the formulas (2.12) and (2.32), the right-hand side (RHS) of the detailed balance equation becomes:

$$\frac{W_{C'}\Delta C' N_{C'}!}{W_C\Delta C N_C!}=\frac{\mathcal{A}_{i'}\cdot\mathcal{A}_{j'}}{\mathcal{A}_i}\frac{\Delta\mathcal{X}_{i'}\Delta\mathcal{X}_{j'}}{\Delta\mathcal{X}_i}. \tag{3.16}$$

On the other hand, the LHS of the detailed balance equation is written as

$$\frac{P(C\rightarrow\widetilde{C}')}{P(\widetilde{C}\leftarrow C')}=\alpha(N_C+1)\frac{L(\mathcal{D}_i^{bc})}{L(\mathcal{D}_{i'}^{bc})L(\mathcal{D}_{j'}^{bc})}\frac{\Delta\mathcal{X}_{i'}\Delta\mathcal{X}_{j'}}{\Delta\mathcal{X}_i}. \tag{3.17}$$

From Eqs. (3.16) and (3.17) one derives the following expression for α:

$$\alpha=\frac{1}{N_C+1}\frac{\mathcal{A}_{i'}\cdot\mathcal{A}_{j'}}{\mathcal{A}_i}\frac{L(\mathcal{D}_{i'}^{bc})L(\mathcal{D}_{j'}^{bc})}{L(\mathcal{D}_i^{bc})}. \tag{3.18}$$

(ii) By means of Eqs. (2.12) and (2.31), the RHS of the detailed balance equation is written as

$$\frac{W_{C'}\Delta C' N_{C'}!}{W_C\Delta C N_C!}=\mathcal{A}_{i'}\cdot\Delta\mathcal{X}_{i'}, \tag{3.19}$$

while the LHS acquires the form

$$\frac{P(C\rightarrow\widetilde{C}')}{P(\widetilde{C}\leftarrow C')}=\alpha(N_C+1)\frac{\Delta\mathcal{X}_{i'}}{L(\mathcal{D}_{i'})}. \tag{3.20}$$

From Eqs. (3.19) and (3.20) the following expression for α is obtained:

$$\alpha=\frac{1}{N_C+1}\mathcal{A}_{i'}L(\mathcal{D}_{i'}). \tag{3.21}$$

At this stage, we are able to generate a correct trajectory in configuration space in both cases (i) and (ii). Having the value of α in any point of the trajectory, we can calculate the factors $[\alpha]$ and $[1/\alpha]$ by means of Eq. (3.15) and then adjust the movement. The resulting trajectory obeys the detailed balance principle and consequently each configuration C is generated with a probability given by the formula (2.14).

IV. APPLICATION TO THE NUCLEAR DISASSEMBLY

Let us first analyze the case of a hot nucleus breaking up into primary fragments. We shall name this event an ''explosion.'' The result of this ''explosion'' will be a collection of nuclear fragments (A_n,Z_n), each of them having different excitation energies in the interval 0-$B(A_n,Z_n)$. Obviously, these nuclei can further decay exactly in the same manner and create a new generation of fragments. In turn this generation can also create another new generation and so on. The decrease of the excitation energies of the fragments from one generation to another is a well-known fact. Theoretically, this process could continue until the excitation energies of fragments become smaller than the corresponding nucleon binding energy $[B(A_n,Z_n)/A_n]$. Thus, one may say that the multifragmentation phenomenon consists of successive ''explosions.'' Many authors treat the primary and the next order explosions in distinct ways. For these secondary decays the name ''evaporation'' is often used. Of course, because of the small values of the excitation energies for all descendent generations, the dominant phenomenon is the ''explosion'' into a main large fragment and some small fragments. However, one should not forget that in some cases the fragments of the first generation can also produce intermediate-mass fragments. In principle a complete statistical description of an ''explosion'' event offers the ingredients for a complete statistical description of the entire decay process. Consequently, we shall focus our attention on studying the ''explosion'' events. With this aim we shall apply the formalism described in the previous sections to the ''explosion'' of a nuclear system with a fixed number of protons and neutrons.

Let us denote by A the total number of nucleons and by Z the total number of protons. The system depends on a set of parameters which defines a configuration $C_1:\{A_n,Z_n,\vec{p}_n,\epsilon_n,\vec{r}_n,n=1,\ldots,N_{C_1}\}$, where A_n, Z_n, $\vec{p}_n$, ϵ_n, and $\vec{r}_n$ represent the mass number, the atomic number, the momentum, the excitation energy, and the position of the nth fragment, respectively. The number of fragments corresponding to the configuration C_1 is denoted by N_{C_1}. The collection of all possible configurations defines a statistical ensemble. To keep closely to the language used in Sec. III, we notice that A_n and Z_n stand for discrete variables while $\vec{p}_n$, ϵ_n, and $\vec{r}_n$ stand for continuous variables.

According to Eqs. (2.5)–(2.9), the elementary number of states for configuration C_1 can be written as

$$dv_{C_1}=\prod_{n=1}^{N_{C_1}}dN(\vec{p}_n)dN(\epsilon_n)dN(\vec{r}_n)=\prod_{n=1}^{N_{C_1}}d\mathcal{N}_i=\prod_{n=1}^{N_{C_1}}\mathcal{A}_n d\mathcal{X}_n, \tag{4.1}$$

where

$$dN(\vec{p}_n)dN(\vec{r}_n)=\frac{d\vec{r}_n\vec{p}_n}{h^3},\quad dN(\epsilon_n)=\rho_n(\epsilon_n)d\epsilon_n \tag{4.2}$$

and

$$d\mathcal{X}_n=d\vec{r}_n d\vec{p}_n d\epsilon_n,\quad \mathcal{A}_n=\rho_n(\epsilon_n)\frac{1}{h^3}, \tag{4.3}$$

with $\rho_n(\epsilon_n)$ denoting the nuclear level density of the nth fragment.

We are working under the assumption that all possible configurations are equally probable.

Let us enumerate the restrictions appearing in this application.

Restrictions of type (a): This kind of restriction is reflected in the conservation of mass, charge, and momentum of the system:

$$R_a=\prod_{j=1}^{N_a}\left(\sum_{n=1}^{N_{C_1}}X_n^{aj}-C_j^a\right)=\delta\left(\sum_{n=1}^{N_{C_1}}A_n-A\right)\delta\left(\sum_{n=1}^{N_{C_1}}Z_n-Z\right)\delta\left(\sum_{n=1}^{N_{C_1}}\vec{p}_n\right). \tag{4.4}$$

Restrictions of type (b): The conservation of the total energy is the only restriction of type (b):

$$R_b=\prod_{j=1}^{N_b} F_j^b(X_n^{bk})=\delta(E_{\rm tot}-E_{C_1})=\delta\left(K-\sum_{n=1}^{N_{C_1}}\frac{p_n^2}{2m_n}\right)H(K), \tag{4.5}$$

where E_{C_1} represents the total energy of the system,

$$E_{C_1}=\sum_{n=1}^{N_{C_1}}\left[\frac{p_n^2}{2m_n}-B(A_n,Z_n)+\epsilon_n+\frac{1}{2}\sum_{n\neq n'}V_{nn'}\right], \tag{4.6}$$

and K the kinetic energy:

$$K=E-\sum_{n=1}^{N_{C_1}}\left[-B(A_n,Z_n)+\epsilon_n+\frac{1}{2}\sum_{n\neq n'}V_{nn'}\right]. \tag{4.7}$$

In Eqs. (4.6) and (4.7), $B(A_n,Z_n)$ denotes the binding energy of fragment n and $V_{nn'}$ the interaction energy between fragment n and the fragment n'. In the present simulation $V_{nn'}$ is taken to have both a Coulomb interaction part and a hard sphere nuclear repulsive potential which prevents the fragments from overlapping.

According to Eq. (2.11) one can express the total number of distinct possible C_1 configurations when the restrictions mentioned above are considered, using Eqs. (4.4) and (4.5), as

$$N_{\rm tot}=\sum_{N_{C_1}=1}^{A}\frac{1}{N_{C_1}!}\prod_{n=1}^{N_{C_1}}\left(\sum_{A_n=1}^{A}\sum_{Z_n=Z_{\min}(A_n)}^{Z_{\max}(A_n)}\int_0^{\epsilon_{n\max}}d\epsilon_n\int d\vec{p}_n\times\int_\Omega d\vec{r}_n\frac{\rho_n(\epsilon_n)}{h^3}\right)\delta\left(\sum_{n=1}^{N_{C_1}}A_n-A\right)\delta\left(\sum_{n=1}^{N_{C_1}}Z_n-Z\right)\times\delta\left(\sum_{n=1}^{N_{C_1}}\vec{p}_n\right)\delta\left(K-\sum_{n=1}^{N_{C_1}}\frac{p_n^2}{2m_n}\right)H(K). \tag{4.8}$$

If we integrate over the fragments momenta, one can identify a new type of configuration $C:\{A_n, Z_n,\epsilon_n,\vec{r}_n,n=1,\ldots,N_C\}$, whose statistical weight W_C (i.e., the total number of states in the configuration C) can be easily evaluated:

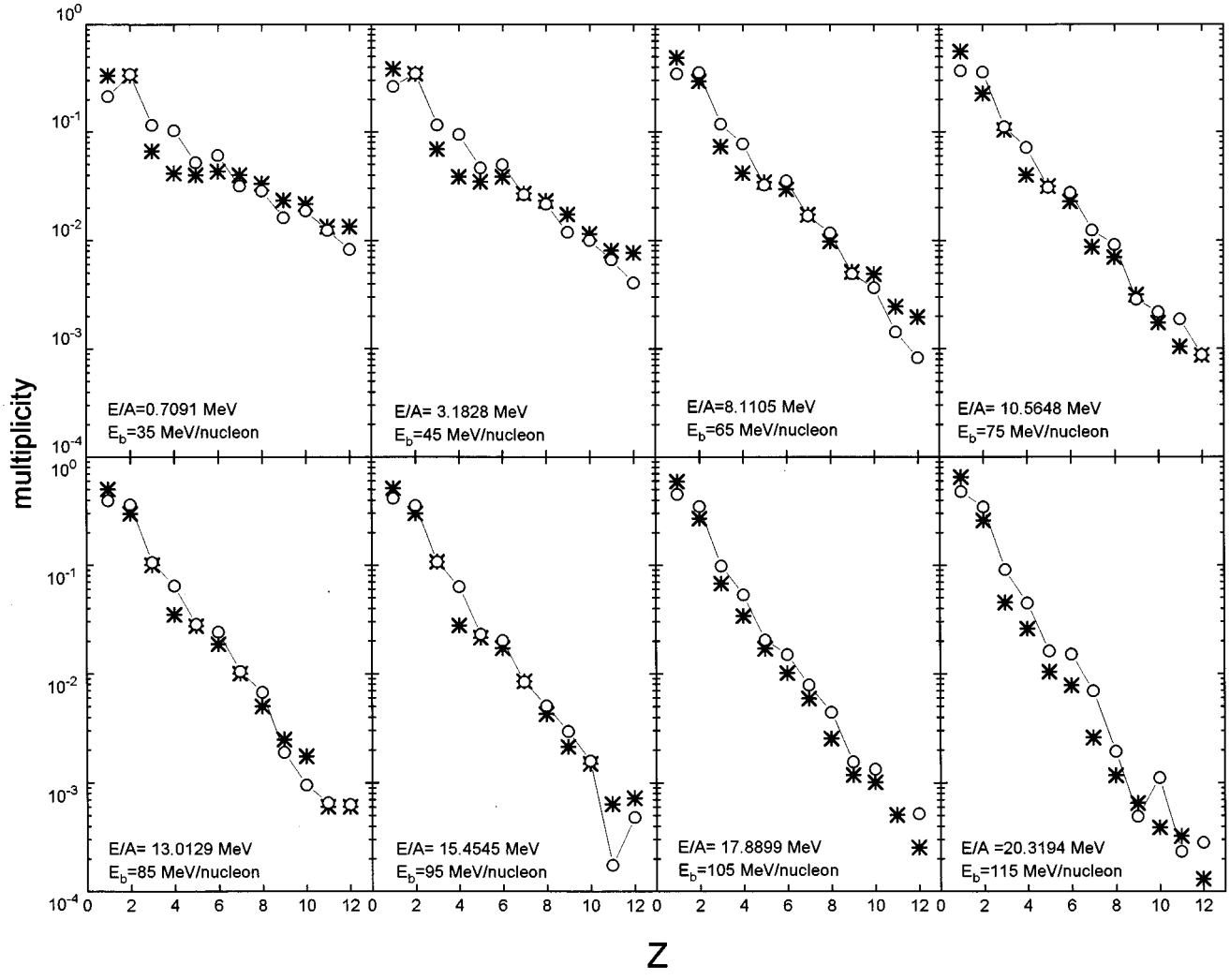

FIG. 1. Charge distribution for central collision for the reaction ^{40}Ar+^{45}Sc at different bombarding energies (E_b). The open circles represent the predictions of the present simulation while the stars represent the experimental data taken from Ref. [17].

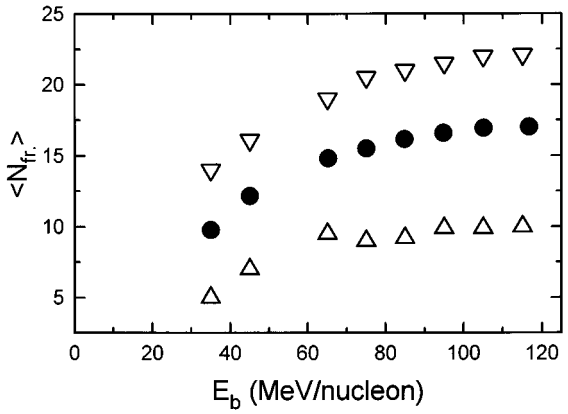

FIG. 2. The average number of charged particles ($Z=1-12$) versus bombarding energy E_b. The solid circles represent the predictions of the present simulation; the open down and up triangles represent the corrected and uncorrected data, respectively (from Ref. [17]).

$$W_C=\frac{1}{N_C!}\prod_{n=1}^{N_C}\left(\Omega\frac{\rho_n(\epsilon_n)}{h^3}(mA_n)^{3/2}\right)\times\frac{2\pi}{\Gamma(3/2(N_C-1))}\frac{(2\pi K)^{3/2N_C-5/2}}{(mA)^{3/2}}\times\delta\left(\sum_{n=1}^{N_C}A_n-A\right)\delta\left(\sum_{n=1}^{N_C}Z_n-Z\right)\delta\left(\sum_{n=1}^{N_C}\vec{p}_n\right)H(K). \tag{4.9}$$

In the fission move we just have to choose a ''fissioning'' element i and from this one to generate two ''fission products'' i' and j'. That means that we have to choose randomly a fissioning element (A_i,Z_i) and then to choose randomly the number of nucleons and the atomic number of the first product $(A_{i'},Z_{i'})$ in the domains $1\text{-}A_i-1$, $0\text{-}Z_i$. For the second fission product $(A_{j'},Z_{j'})$, we have $A_{j'}=A-A_{i'}$ and $Z_{j'}=Z-Z_{i'}$. If at least one of the chosen fragments is unstable, the move is aborted and configuration C is used for the next step. Otherwise, we generate the excitation energies $\epsilon_{i'},\epsilon_{j'}$ in the allowed domains (having the binding energy of the fragment as an upper limit) and the positions $\vec{r}_{i'}$ and $\vec{r}_{j'}$ in the considered volume Ω. At this point one can calculate the kinetic energy K. If $K<0$, the move is aborted and C is counted again. Otherwise, C' is a ''good'' configuration and could be a next new configuration for the system. C' is used as a next configuration with the probability $[\alpha]$.

In the fusion move we have to choose randomly two ''fusing'' elements i' and j' and to generate a ''fission product'' i. Thus, we choose randomly two fusing elements $(A_{i'},Z_{i'})$ and $(A_{j'},Z_{j'})$ and form a product (A_i,Z_i). If the product is unstable, the move is aborted and C' is counted again. Otherwise, the move is continued and the excitation energy ϵ_i and the position $\vec{r}_i$ are randomly generated in their domains. As we proceeded before, one calculates K, and if $K<0$, the move is aborted and the old configuration is used again. If $K\geqslant 0$, C is accepted as the next configuration with probability $[1/\alpha]$.

Thus, we have described the generation of the primary trajectory. The correction to this trajectory will be achieved by the adjustment with the correction factor α [see Eq. (3.21)]:

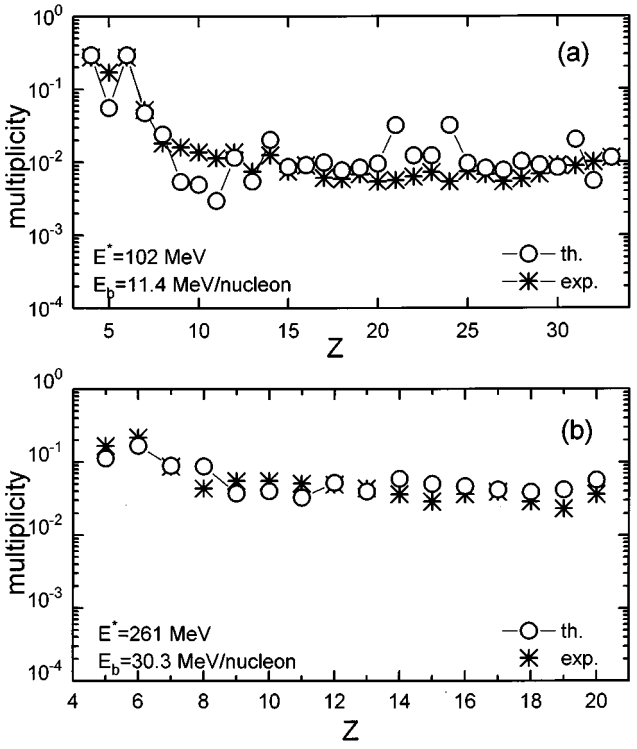

FIG. 3. Charge distribution for the reaction $^{93}Nb+^{9}Be$ at the bombarding energies 11.4 MeV/nucleon (a) and 30.3 MeV/nucleon (b). The stars represent experimental data, taken from [13], while the open circles stand for the predictions of the present simulation.

$$\alpha=\frac{(A_i-1)(Z_i+1)}{N_C+1}\Omega\frac{\epsilon_{i'\max}\epsilon_{j'\max}}{\epsilon_{i\max}}\frac{\Gamma(\frac{3}{2}(N_C-1))}{\Gamma(\frac{3}{2}N_C)}\times\frac{\rho_{i'}(\epsilon_{i'})\rho_{i'}(\epsilon_{i'})}{\rho_i(\epsilon_i)}\left(\frac{A_{i'}A_{j'}}{A_i}\right)^{3/2}\left(\frac{mK}{2\pi\hbar^2}\right)^{3/2}\left(\frac{K'}{K}\right)^{(3N_C/2)-1}. \tag{4.10}$$

At this stage, the method of simulating an ''explosion'' event is well formulated. As we said before, for a complete description of the multifragmentation process we should account for all ''explosions.'' *Obviously, the same method is applicable to the ''explosions'' of any order*. But a simulation that considers all secondary decays requires an unreasonably long computing time. However, we have found a way to overcome these difficulties and applications are in progress.

In order to evaluate to what extent the contribution of the primary decay to the mass and charge multiplicities and average number of charged particles describes the physical phenomenon, we compare the model predictions with experimental data [13,17].

V. RESULTS

To emphasize the virtues of the present model, we describe some theoretical predictions and compare them with the corresponding data. Our applications refer to the reac-

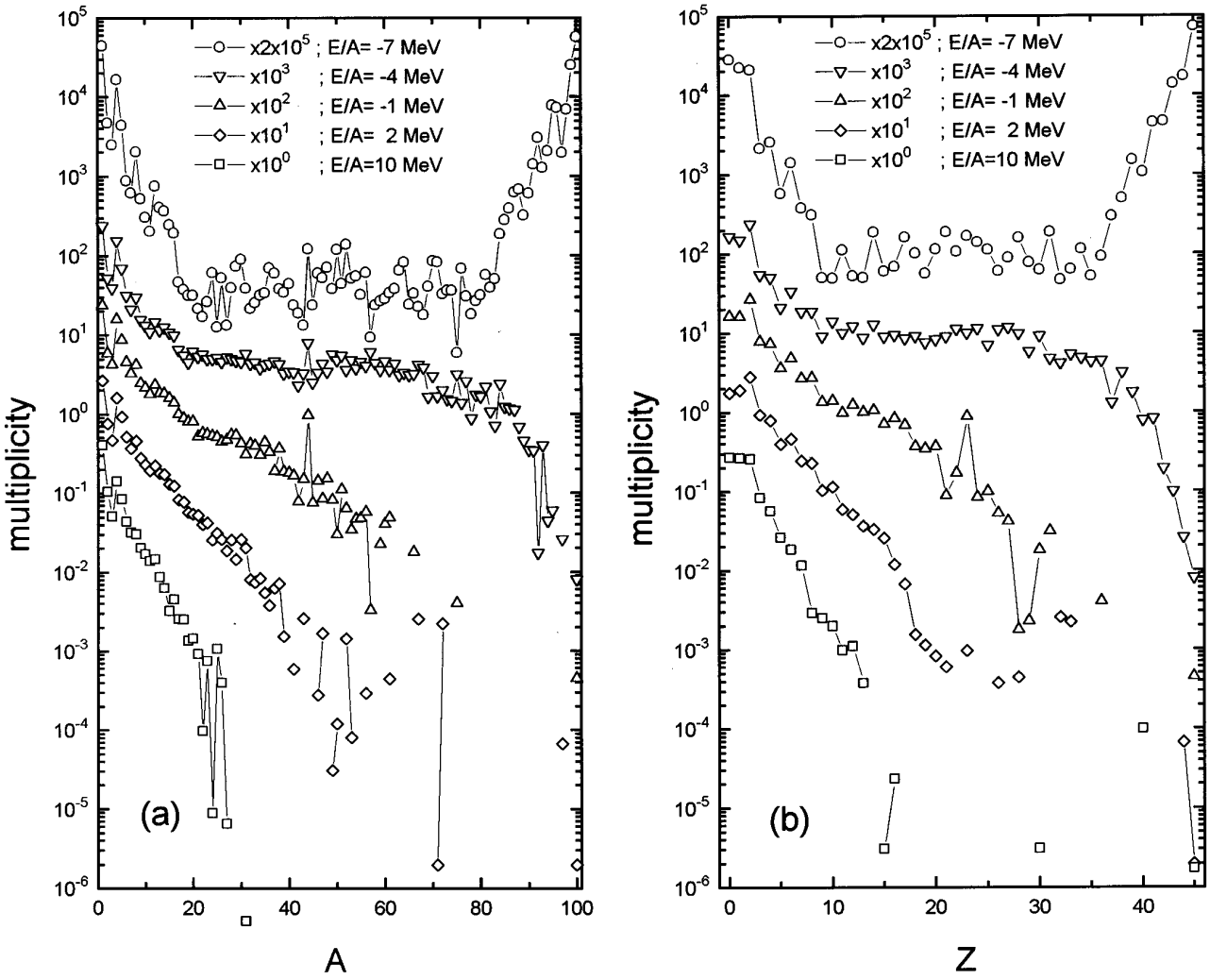

FIG. 4. (a) Mass and (b) charge distributions for various total energies (E/A) obtained for a fireball having $A=100$ and $Z=45$.

tions ^{40}Ar+ ^{45}Sc with an incident energy varying from 35 MeV/nucleon to 115 MeV/nucleon [16], and ^{93}Nb+ ^{9}Be at the incident energies 11.4 MeV/nucleon and 30.3 MeV/nucleon [13]. Also, for a more complete conception of the model we present some global characteristics like mass and charge distributions for a wide range of energies.

In order to obtain a realistic simulation, we have used real binding energies of all the elements with A lying between 1 and 266. For level densities we have used the following formula [14]:

$$\rho(\epsilon)=\frac{1}{\sqrt{48}\epsilon}e^{\sqrt{4a\epsilon}},\quad a=\frac{A}{\alpha},\quad \alpha=8\left(1+\frac{\epsilon}{B(A,Z)}\right), \tag{5.1}$$

where the factor $[1+\epsilon/B(A,Z)]$ was included so as to describe the dependence of the factor entering the Fermi-gas formula on the excitation energy ϵ for the (A,Z) system with the binding energy $B(A,Z)$. It is worth stressing that the nuclear matter freeze-out density is the only fitting parameter of simulation. For high excitation energies and light fragments this formula produces similar results as that used in Ref. [15].

For the case of the ^{40}Ar+ ^{45}Sc reaction we compared the predicted charge distributions with the corresponding experimental data at eight bombarding energies 35, 45, 65, 75, 95, 105, and 115 MeV/nucleon. These correspond to the center-of-mass total energies (which include the binding energy) of 0.7091, 3.1828, 8.1105, 10.5648, 13.0129, 15.4545, 17.8899, and 20.3194 MeV/nucleon, respectively [16]. The calculations are performed considering a fireball with $A=80$ and $Z=36$ [16]. Since the experimental data lie between $Z=1$ and 12, we normalized our results in these limits. Also, we have normalized the experimental data in order to express them in terms of multiplicities.

As one can see from Fig. 1, the agreement with the experimental data is very good for all the energies considered. This fit was obtained considering the freeze-out density to be $0.249\rho_0$ (ρ_0 represents the normal nuclear density and is taken to be 0.17 fm^{-3}). Figure 2 shows the average number of charged particles with $Z=1-12$ as a function of the bombarding energy in comparison with the corrected and uncorrected experimental data [16,17]. For the central collision ^{93}Nb+ ^{9}Be we have considered a fireball with $A=102$ and $Z=45$ [13]. The considered energies correspond to the excitation energies 102 and 261 MeV, respectively. The comparison of the predictions and experimental data for charge distributions (Fig. 3) shows good agreement. The fit was obtained with a freeze-out density of $0.263\rho_0$. From the above analysis one may conclude that (a) the agreement for

multiplicities suggests that the possible contribution coming from secondary decays might be negligible and (b) these corrective events improve the agreement for the average number of charged particles (see Fig. 2). Indeed, these added decays contribute to the increase in the number of fragments.

Finally, we present some global characteristics like mass and charge distributions obtained with our code for a large range of the total energy. Figures 4(a) and 4(b) show the mass and charge distributions for $A=100$, $Z=45$ for various total energies, E/A. It is worth noting that general characteristics of the nuclear disassembly charge and mass distribution, such as the U shape, the shoulderlike shape, and the exponentially falling shape, are well reproduced.

In conclusion we may assert that, in first order, the model describes very well charge distributions for a wide range of energies, which suggests small contributions due to the higher orders. As shown in Fig. 2 the predicted average numbers of fragments lie below the corrected experimental data. This supports the model assumptions since the higher order decays cause an increase in the number of fragments and, consequently, the theoretical curve will approach the experimental one. Another virtue of this model is that, even in this first order approach, it can describe charge distributions for decays of highly excited nuclei in energy ranges where many authors [13,16,18–20] suggest different decay mechanisms. For example, in the case of the $^{40}\mathrm{Ar}+^{45}\mathrm{Sc}$ reaction two decay mechanisms are suggested [16]: For bombarding energies below $\simeq$60 MeV/nucleon the decay is supposed to be sequential, while for upper energies the disassembly is supposed to be simultaneous.

VI. CONCLUSIONS

Summarizing, we have formulated a general statistical ensemble for the case of a system composed of N ''elements'' with $N\in[N_{\min},N_{\max}]$, each element being described by a set of parameters. A set of constraints, usually met in physical systems, has been defined. The statistical weights and the probability for obtaining a certain configuration C have been analytically expressed. In most cases the resulting formulas are not numerically tractable due to the large number of possible configurations. Thus, a statistical method for simulating this ensemble is employed. The method is a generalization of the adapted Monte Carlo Metropolis algorithm [12] proposed by Koonin and Randrup [3] and consists of generating a trajectory in configuration space obeying the detailed balance principle. We discuss both the most general case in which the system can have any type of restriction and the case in which the system is not subject to global restrictions. A suitable generation scheme is described for each of these cases.

This method is applied to the case of nuclear multifragmentation which is realistically treated taking into account the total charge, mass, momentum, and energy conservation laws. Also, real binding energies for all the elements with $A=1-266$ have been employed in the resulting computer code. The numerical results are compared with experimental data and very good agreement is obtained over a large domain of energies. In fact, this result supports the theoretical assumption of our model. It is worth mentioning that the energy domains for which calculations have been performed are supposed by many authors to present two decay mechanisms: sequential decay (for bombarding energies below $\simeq$60 MeV/nucleon) and simultaneous multifragmentation (for bombarding energies higher than $\simeq$60 MeV/nucleon). Various distribution shapes usually found in multifragmentation experimental data are also reproduced.

Before closing, we would like to mention that a method for accounting for the effects of higher order ''explosions'' has been developed and its application to the study of nuclear multifragmentation is in progress. Also more sensitive tests for the model assumptions, like the relative ratios of multifragmentation, fission, and evaporation events, are being pursued. All these improvements will be addressed in a subsequent paper.

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