Comparison of Statistical Multifragmentation Model simulations with Canonical Thermodynamic Model results: a few representative cases

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Abstract

The statistical multifragmentation model (SMM) has been widely used to explain experimental data of intermediate energy heavy ion collisions. A later entrant in the field is the canonical thermodynamic model (CTM) which is also being used to fit experimental data. The basic physics of both the models is the same, namely that fragments are produced according to their statistical weights in the available phase space. However, they are based on different statistical ensembles, and the methods of calculation are different: while the SMM uses Monte-Carlo simulations, the CTM solves recursion relations. In this paper we compare the predictions of the two models for a few representative cases.

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I. INTRODUCTION

The statistical multifragmentation model (SMM) has had wide applications in the field of intermediate energy heavy ion collisions. The basic assumption is that when two heavy ions collide, after pre-equilibrium emission, they form a compound system with given mass number $A_0$, charge number $Z_0$ and given energy $E_0$. This system will expand and break up into different composites. In this expanded volume the nuclear interaction between different composites can be neglected and Coulomb interaction can be included in an approximate way. Assuming that the populations of different channels are solely given by statistical weights in the available phase space, the average yield of given species with a neutron number $N$ and proton number $Z$ can be computed by Monte-Carlo simulation. Details may be found in [1]. Many versions of the Monte-Carlo simulations are possible. For example, one can choose the freeze-out volume to be dependent on the multiplicity of a channel. For reactions where equilibrated sources are formed, the SMM gives very good description of experimental data [1, 2, 3, 4].

The canonical thermodynamic model (CTM) characterises the disintegrating system by a temperature $T$, the mass number $A_0$, charge number $Z_0$ and a fixed freeze-out volume. With these simplifications, computations of average yields of composites are straightforward and do not need Monte-Carlo simulations. Details can be found in [5]. This model has also been used successfully to fit experimental data [5, 6]. It is expected that results will be similar to those obtained from the SMM. Here we embark on more quantitative comparison of the results generated in the two frameworks for a few representative cases. Such a comparison is long overdue.

II. PARAMETERS OF THE CTM AND SMM USED IN THE PRESENT WORK

First, we give description of the CTM. For the SMM more than one approach was used which will be described below. Details of the computational procedures for the canonical model can be found elsewhere [5, 7] hence we provide here only the bare minimal.

The fragmenting system has $N_0$ neutrons and $Z_0$ neutrons. We consider all break-up channels (partitions) $\{p\}$, and define $n_{i,j}$ as the number of fragments with neutron number $i$ and the number of protons $j$. As is well known, the number of partitions of medium and
heavy systems \((N_0 \sim Z_0 \sim 100)\) is enormous (see e.g. [8]). The canonical partition function for non-interacting fragments is given by

\[
Q_{N_0,Z_0} = \sum_{\{p\}} \prod_{i,j} \frac{\omega_{i,j}^{n_{i,j}}}{n_{i,j}!}
\tag{1}
\]

Here the sum is over all possible partitions, which satisfy the conditions \(N_0 = \sum i \cdot n_{i,j}\) and \(Z_0 = \sum j \cdot n_{i,j}\); \(\omega_{i,j}\) is the partition function of one composite with neutron number \(i\) and proton number \(j\), respectively. The one-body partition function \(\omega_{i,j}\) is a product of two parts: one arising from the translational motion of the composite and another from the intrinsic partition function of the composite:

\[
\omega_{i,j} = \frac{V_f}{k^3} (2\pi m_N aT)^{3/2} \cdot z_{i,j}(\text{int})
\tag{2}
\]

where \(m_N \approx 939\) MeV is the average nucleon mass, and \(a = i + j\) is the mass number of the composite \((i, j)\). Here \(V_f\) is the volume available for translational motion; \(V_f\) will be less than \(V\), the volume to which the system has expanded at break up. We use \(V_f = V - V_0\), where \(V_0\) is the normal volume of nucleus with \(Z_0\) protons and \(N_0\) neutrons.

The probability of a given channel \(P(\vec{n}_{i,j}) \equiv P(n_{0,1}, n_{1,0}, n_{1,1}, \ldots, n_{i,j}, \ldots)\) is given by

\[
P(\vec{n}_{i,j}) = \frac{1}{Q_{N_0,Z_0}} \prod_{i,j} \frac{\omega_{i,j}^{n_{i,j}}}{n_{i,j}!}
\tag{3}
\]

The average number of composites with \(i\) neutrons and \(j\) protons is seen easily from the above equation to be

\[
\langle n_{i,j} \rangle = \omega_{i,j} \frac{Q_{N_0-i,Z_0-j}}{Q_{N_0,Z_0}}
\tag{4}
\]

The constraints \(N_0 = \sum i \cdot n_{i,j}\) and \(Z_0 = \sum j \cdot n_{i,j}\) can be used to obtain different looking but equivalent recursion relations for partition functions. For example

\[
Q_{N_0,Z_0} = \frac{1}{N_0} \sum_{i,j} i \omega_{i,j} Q_{N_0-i,Z_0-j}
\tag{5}
\]

These recursion relations allow one to calculate \(Q_{N_0,Z_0}\).

We list now the properties of the composites used in this work. The proton and the neutron are fundamental building blocks thus \(z_{1,0}(\text{int}) = z_{0,1}(\text{int}) = 2\) where 2 takes care of the spin degeneracy. For deuteron, triton, \(^3\)He and \(^4\)He we use \(z_{i,j}(\text{int}) = (2s_{i,j} + 1) \exp(-\beta e_{i,j}(\text{gr}))\) where \(\beta = 1/T\), \(e_{i,j}(\text{gr})\) is the ground state energy of the composite and \((2s_{i,j} + 1)\) is the experimental spin degeneracy of the ground state. Excited states
for these very low mass nuclei are not included. For mass number \( a = 5 \) and greater we use the liquid-drop formula. For nuclei in isolation, this reads

\[
  z_{i,j}(\text{int}) = \exp\left[-\frac{F_{i,j}}{T}\right] 
\]

(6)

Here \( F_{i,j} \) is the internal free energy of species \((i, j)\):

\[
  F_{i,j} = -W_0 a + \sigma(T)a^{2/3} + \kappa \frac{j^2}{a^{1/3}} + s \frac{(i - j)^2}{a} - \frac{T^2 a}{\epsilon_0}.
\]

(7)

The expression includes the volume energy, the temperature dependent surface energy, the Coulomb energy and the symmetry energy. The term \( \frac{T^2 a}{\epsilon_0} \) represents contribution from excited states since the composites are at a non-zero temperature. For nuclei with \( A=5 \) we include \( Z=2 \) and 3 and for \( A=6 \) we include \( Z=2,3 \) and 4. For higher masses we compute the drip lines using the liquid-drop formula above and include all isotopes within these boundaries.

In the grand canonical formulation for the SMM [1], after integrating out translational degrees of freedom, one can write the mean multiplicity of nuclear fragments with \( i \) and \( j \) as

\[
  \langle n_{i,j} \rangle = (2s_{i,j} + 1) \frac{V}{\lambda_T^3} a^{3/2} \exp \left[ -\frac{1}{T} (F_{i,j}(T, V) - \mu a - \nu j) \right].
\]

Here \( \lambda_T = \left( \frac{2\pi \hbar^2}{m_N T} \right)^{1/2} \) is the nucleon thermal wavelength. The chemical potentials \( \mu \) and \( \nu \) are found from the mass and charge constraints:

\[
  \sum_{i,j} \langle n_{i,j} \rangle a = A_0, \quad \sum_{i,j} \langle n_{i,j} \rangle j = Z_0.
\]

(8)

We use the same treatment of the lightest particles with \( A < 5 \) as in the canonical case, i.e., the free energy is just their binding energy. However, for large fragments we take into account all possible charges starting from \( Z = 2 \) up to \( Z = A - 2 \). We have checked that this extension beyond the drip line has a very small influence on final results in the range of nuclei covered by experiments. The grand canonical occupations are used for Monte-Carlo fragment generation in the SMM.

At small excitation energies the standard SMM code [1] uses a microcanonical treatment, however, taking into account a limited number of disintegration channels: as a rule, only partitions with total fragment multiplicity \( M \leq 3 \) are considered. This is a very reasonable
approximation at low temperature, when the compound nucleus and low-multiplicity channels dominate. Recently, a full microcanonical version of the SMM using the Markov Chain method was introduced [8, 9]. It can be used for exploring all partitions without limitation. However, it is a more time consuming approach, and it is used in special cases only [9].

Within the microcanonical ensemble the statistical weight of a partition \( p \) is calculated as

\[
W_p \propto \exp S_p, \tag{9}
\]

where \( S_p \) is the corresponding entropy, which depends on fragments in this partition, as well as on the excitation energy \( E_0 \), mass number \( A_0 \), charge \( Z_0 \) and volume \( V \) of the system. In the present work we follow a description which corresponds to approximate microcanonical ensemble. Namely, we introduce a temperature \( T_p \) characterising all final states in each partition \( p \). It is determined from the energy balance equation taking into account the total excitation energy \( E_0 \) [1]. In the following we determine \( S_p \) for the found \( T_p \) by using conventional thermodynamical relations. For instance, in this work, it can be written as

\[
S_p = \ln\left(\prod_{i,j} (2s_{i,j} + 1)\right) + \ln\left(\prod_{i,j} a^{3/2}_i\right) - \ln(A_0^{3/2}) - \ln\left(\prod_{i,j} n_{i,j}\right) +
(M - 1)\ln(V_f/\lambda_p^3) + 1.5(M - 1) + \sum_{i,j} \left(\frac{2T_p a}{\epsilon_0} - \frac{\partial \sigma(T_p)}{\partial T_p} a^{2/3}\right), \tag{10}
\]

where summations are performed over all fragments of the partition \( p \). We enumerate all considered partitions and select one of them according to its statistical weight by the Monte-Carlo method.

At high excitation energy the standard SMM code makes a transition to the grand-canonical ensemble, and generate partitions by Monte-Carlo sampling from the grand-canonical distribution [1]. In all ensembles the long range Coulomb interaction between different composites is included in the Wigner-Seitz approximation. For details of this incorporation see references [1, 5]. In all calculations later on we use the fixed break-up volume \( V = 6V_0 \) independently of fragment multiplicity.

### III. FRAGMENT MASS DISTRIBUTIONS

One major goal of this work is to compare the average yields \( \langle n_{i,j} \rangle \) of a composite with neutron number \( i \) and proton number \( j \), when systems with different temperatures dissociate.
In the canonical model this is simply given by eq.(4). For brevity we will display most often \( \langle n_a \rangle \equiv \sum_{a=i+j} \langle n_{i,j} \rangle \). While for the CTM one needs to specify which composites are allowed in channels, this is not needed for SMM simulations. We consider a medium-mass nucleus with \( A_0=73 \) and \( Z_0=32 \) at low excitation energy. Such a compound system can be formed by \(^{64}\text{Ni}\) projectile on \(^9\text{Be}\) and has actually been studied experimentally \([10]\). In order to demonstrate the mass effect on the fragmentation picture we take also two-times larger sources.

First, we start from low excitation energies, and consider \( E_0 = 1 \text{ MeV/nucleon} \) to perform calculations with the microcanonical version of the SMM described above. At such low excitation energy the multiplicity should be low and for simplicity we restrict the microcanonical ensemble to multiplicities \( M = 1, 2 \) and \( 3 \). The average \( T_p \) (see section II) for the excitation energy of \( 1 \text{ MeV/nucleon} \) is \( 3.13 \text{ MeV} \). We perform the CTM calculations for this temperature. We will get an exact answer for the canonical model, but only an approximate one for the SMM because of restriction of multiplicity. Another reason for disagreement between the two models is that in the SMM some channels, even at low multiplicity, will be just prohibited because of high Coulomb barrier. We can therefore hope that when the yield \( \langle n_{i,j} \rangle \) is significant the agreement between the two models can emerge but for very small yields there will be deviations. Fig. 1 shows that for important yields, the agreement between the two models is very good. This also shows that, at least in the present example, the average yields are about the same whether excitation energy per particle is kept constant or an appropriate temperature is kept fixed. In real physical processes, as we know, the compound nucleus channel \( (M = 1) \) dominates at low excitations. Both models describe correctly a transition to this low-energy limit.

Now we turn to medium and high excitation energies, which lead to real multifragmentation. In Fig. 2 we compare the CTM and SMM models at intermediate temperatures of 5 and 8 MeV for three systems. One system is the same as before \((A_0 = 73, Z_0 = 32)\), another system is twice of this size \((A_0 = 146, Z_0 = 64)\), and the third one is more neutron rich \((A_0 = 146, Z_0 = 56)\). The canonical model calculations are the same as before, but the SMM simulations are dictated by convenience and simplicity, and are performed with the grand canonical version, as discussed. Instead of excitation energy per nucleon, we consider fixed temperature and the starting point of Monte-Carlo simulations is grand canonical population of composites. Remarkable agreement is obtained between the two
models except when $\langle n_a \rangle$ is very small. We will comment upon the discrepancies for very small populations shortly. However, as is clear from the comparison, both models can be used in multifragmentation region.

**IV. ISOTOPE YIELDS**

Further important details about characteristics of produced fragments are given in Figs. 3 and 4. For selected isotopes we compare the yields in the two models as the neutron number changes. Now we are directly comparing individual values of $\langle n_{i,j} \rangle$ rather than the sum of all isobars. We see once again, unless the multiplicities are really small, the yields are very close. Given the choice of composites allowed in any channel, the CTM results are exact. In the grand canonical SMM calculations we get broader isotope distributions, especially for big fragments. This feature explains the increased yield of big fragments seen in SMM results in Fig. 2.

The reason is that the grand-canonical ensemble increases the phase space, since it takes into account many more partitions which include exotic nuclei, and conserves the mass number and charge conservation laws on the average only. Since the number of exotic nuclei is greater for large nuclei we obtain more deviation at large $A$ and $Z$. We can make a quite general statement: any restriction of the partition phase space lead to more narrow isotope distributions. We expect narrow distributions also for the microcanonical ensemble, since it imposes the exact energy conservation in the partitions additionally.

**V. CALORIC CURVES**

The caloric curves, temperature $T$ against excitation energy $E^*/A_0$ agree very well in the two models. This dependence is very important for statistical systems, and it can be in many cases extracted experimentally via calorimetry. Examples of the caloric curves are shown in Fig.5. We conclude that small differences in fragments yields do not influence global thermodynamicical characteristics of the system.

We have calculated the caloric curves for all three sources under consideration, and they look practically identical. The experimental identification of the difference $\Delta T \sim 0.1$ MeV is probably impossible. However, we would like to draw attention to the interesting mass
and isospin effects which can be seen by comparing different sources, and which may be
important in big and neutron rich astrophysical systems. This can be seen in fig.6 showing
differences in excitation energies $E^*/A_0(A_0 = 146, Z_0 = 64) - E^*/A_0(A_0 = 146, Z_0 = 56)$ and
$E^*/A_0(A_0 = 146, Z_0 = 64) - E^*/A_0(A_0 = 73, Z_0 = 32)$ versus temperature. In the region
of multifragmentation ($T > 4$ MeV) a bigger system has a slightly larger excitation energy
per nucleon. This is a result of stronger Coulomb effect in big systems. An isospin effect
can also be seen at the transition from the channels with big (compound-like) fragments to
the full multifragmentation region, i.e., at temperatures $T \approx 3.5 - 5$ MeV: The neutron rich
system has a slightly lower excitation energy.

VI. SUMMARY

We have compared the yields of composites, as well as the caloric curves, in two different
model prescriptions corresponding to different ensembles. Generally they agree well. The
SMM is more versatile: one can use either the excitation energy or the temperature as
the fixed parameter. It also allows for other modifications such as multiplicity dependence
of the freeze-out volume. The disadvantage is that it is computationally quite involved.
The canonical model is more restrictive but extremely easy to use. We have found some
differences in results of different models, in particular, concerning isotope distributions. This
may cause different interpretation of some experimental observables, e.g., the isoscaling
characteristics. We should remark that in this paper we analyse the yields of primary hot
fragments. The subsequent de-excitation of these excited fragments must be taken into
account in interpretation of experimental data [1, 5]. This may lead to additional deviations
between predictions of microcanonical and canonical/grandcanonical ensembles, since the
microcanonical SMM treatment allows for temperature fluctuations in different partitions.

In this respect, the important question is what statistical ensemble would be preferable for
analysis of experimental characteristics sensitive to the kind of ensemble. The answer can be
provided by experimental information only. If the data have clear evidences of production
of a thermal source with well determined $A_0$, $Z_0$ and $E_0$ the microcanonical ensemble is
justified. If one can speak only about exact $A_0$ and $Z_0$ conservations, the canonical ensemble
is the best. If experiment can give only average values for parameters of the thermal source,
the grand canonical model can be applied. Moreover, as is well known, the preequilibrium
dynamical stage can provide a very broad distribution in parameters of the thermal sources. Including all this distribution may have a greater impact on the results, than selection of a particular ensemble. In the case of an experimental uncertainty with parameters of the thermal source, we believe, the evaluation of experimental data should include fitting the data within one of the statistical models, and addressing physical characteristics which are universal for all ensembles, like break-up volume and internal properties of hot primary fragments.

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FIG. 1: Mass distributions of fragments as predicted by the CTM (solid lines) and the SMM (dashed lines). The SMM calculations are for restricted microcanonical ensemble with excitation energy of 1 MeV/nucleon, corresponding to the temperature of 3.13 MeV taken as input in the CTM. The dissociating system is $A_0 = 73, Z_0 = 32$. 
FIG. 2: Fragment mass distributions $n_a$ predicted by the CTM (solid lines) and the SMM (dashed lines) at temperatures 5 and 8 MeV, for three dissociating systems indicated in the figure. The SMM calculations are based on the grand canonical ensemble.
FIG. 3: Yields of individual isotopes (indicated in the figure) as predicted by the CTM (solid lines) and the SMM (dotted lines). Results are presented for the dissociating system $A_0 = 73, Z_0 = 32$ and temperature 5 MeV.
FIG. 4: The same as in Fig. 3 except that the dissociating system is $A_0 = 146, Z_0 = 56$. 
FIG. 5: The caloric curves ($T$ against $E^*/A_0$) predicted by the CTM (solid line) and SMM (dotted line) for three dissociating systems.
FIG. 6: In the left panel we plot $E^*(146, 64)/_{146} - E^*(146, 56)/_{146}$ against $T$. In the right panel we plot $E^*(146, 64)/_{146} - E^*(73, 32)/_{73}$ against $T$. See section V for a discussion. Only results using CTM are shown; SMM gives very similar results.