Conditions for equivalence of Statistical Ensembles in Nuclear Multifragmentation

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Statistical models based on canonical and grand canonical ensembles are extensively used to study intermediate energy heavy-ion collisions. The underlying physical assumption behind canonical and grand canonical models is fundamentally different, and in principle agree only in the thermodynamical limit when the number of particles become infinite. Nevertheless, we show that these models are equivalent in the sense that they predict similar results if certain conditions are met even for finite nuclei. In particular, the results converge when nuclear multifragmentation leads to the formation of predominantly nucleons and low mass clusters. The conditions under which the equivalence holds are amenable to present day experiments.

PACS numbers: 25.70Mn, 25.70Pq

I. INTRODUCTION

In the disintegration of a nuclear system formed by the collision of two heavy-ions at intermediate energy, it is assumed that a statistical equilibrium is reached. This facilitates the use of statistical models \[ \text{in order to obtain the yields of the composites at the freeze-out volume.} \] In such models of nuclear disassembly the populations of the different channels are solely decided by their statistical weights in the available phase space. One can use different ensembles (microcanonical, canonical or grand canonical) in order to account for the fragmentation of the nucleus into different channels. The partitioning into available channels can be solved in the canonical model \[ \text{where the number of particles in the nuclear system is finite (as it would be in experiments).} \] Even when the number of particles is fixed one can replace a canonical model by a grand canonical model where the particle number fluctuates but the average number is constrained to a given value \[ 0 \text{.} \] Both canonical and grand canonical models have been extensively used to study the physics of intermediate energy heavy ion collisions \[ \text{and results for different observables have been routinely compared to experimental data} \] \[ 8-12. \]

It is well known that results from different statistical ensembles agree in the thermodynamical limit \[ \text{that is, when the number of particles become infinite.} \] For example, for one kind of particle (nucleon) and for arbitrarily large nuclear system \[ \text{(therefore approximates the thermodynamical limit)} \] \[ \text{it was observed that results agree} \] \[ \text{with each other under certain conditions. This equivalence is generally known not to be valid for nuclear systems of finite size.} \]

The main result of this work lies in showing that results from the canonical and grand canonical models can agree even for finite nuclei. This equivalence is observed when nuclear multifragmentation leads to the formation of predominantly nucleons and low mass clusters. This condition can be achieved either by increasing the temperature or freeze-out volume of the fragmenting nucleus or source size, or by decreasing the asymmetry of the source. In fact, when all the four conditions are satisfied then one can get the best agreement between the two models. We have confined our study to the observables and conditions that can be easily accessed by present day experiments.

Specifically we investigate the multiplicity of the fragments leading to charge and mass distributions from the canonical and grand canonical distributions under varying conditions and identify the underlying reasons behind the differences. This led us to identify the conditions under which results from both the models converge. For example by comparing charge distributions of fragments obtained from both models under varying temperature, freeze-out volume, fragmenting source size and asymmetry, it becomes possible to obtain the conditions under which the models give rise to similar results.

II. THEORETICAL FORMALISM

In this section we describe briefly the canonical and the grand canonical model of nuclear multifragmentation. The basic output from canonical or grand canonical model is multiplicity of the fragments. This allows one to obtain the charge or the mass distribution of the fragments. By multiplicity we mean that the average number of fragments produced for each proton number \( Z \) and neutron number \( N \). Assuming that the system with \( A_0 \) nucleons and \( Z_0 \) protons at temperature \( T \), has expanded to a volume higher than normal nuclear volume and thermodynamical (statistical) equilibrium is reached at this freeze-out condition, the partitioning into different composites can be calculated according to the rules of equilibrium statistical mechanics.

In a canonical model \[ \text{the partitioning is done such that all partitions have the correct} \] \[ A_0, Z_0 \] (equivalently \( N_0, Z_0 \). The canonical partition function is given by

\[
Q_{N_0,Z_0} = \sum \prod \frac{\omega_{N_0,Z}^{n_{N,Z}}}{n_{N,Z}!} \tag{1}
\]

where the sum is over all possible channels of break-
up (the number of such channels is enormous) satisfying
\(N_0 = \sum N \times n_{N,Z}\) and \(Z_0 = \sum Z \times n_{N,Z}\); \(\omega_{N,Z}\) is
the partition function of the composite with \(N\) neutrons
and \(Z\) protons and \(n_{N,Z}\) is its multiplicity. The partition
function \(Q_{N_0,Z_0}\) is calculated using a recursion relation
[1]. From Eq. (1) and the recursion relation, the average
number of composites is given by [1]

\[
\langle n_{N,Z} \rangle_c = \omega_{N,Z} \frac{Q_{N_0-Z, Z_0-Z}}{Q_{N_0, Z_0}} \tag{2}
\]

It is necessary to specify which nuclei are included in
computing \(Q_{N_0,Z_0}\). For \(N, Z\) we include a ridge along the
line of stability. The liquid-drop formula gives neutron
and proton drip lines and the results shown here include
all nuclei within the boundaries.

In the grand canonical model [4], if the neutron chemical
potential is \(\mu_n\) and the proton chemical potential is
\(\mu_p\), then statistical equilibrium implies [5] that the
chemical potential of a composite with \(N\) neutrons and \(Z\) pro-
tons is \(\mu = \mu_n N + \mu_p Z\). The average number of composites
with \(N\) neutrons and \(Z\) protons is given by [4]

\[
\langle n_{N,Z} \rangle_{gc} = e^{\beta(\mu_n N + \mu_p Z)} \omega_{N,Z} \tag{3}
\]

The chemical potentials \(\mu_n\) and \(\mu_p\) are determined by
solving two equations \(N_0 = \sum N e^{\beta \mu_n N + \beta \mu_p Z} \omega_{N,Z}\) and
\(Z_0 = \sum Z e^{\beta \mu_n N + \beta \mu_p Z} \omega_{N,Z}\). This amounts to solving
for an infinite system but we emphasize that this infinite
system can break-up into only certain kinds of species as
are included in the above two equations. We can look
upon the sum on \(N\) and \(Z\) as a sum over \(A\) and a sum
over \(Z\). In principle \(A\) goes from 1 to \(\infty\) and for a given
\(A, Z\) can go from 0 to \(A\). Here for a given \(A\) we restrict
\(Z\) by the same drip lines used for canonical model.

In both the models, the partition function of a com-
posite having \(N\) neutrons and \(Z\) protons is a product of two
parts: one is due to the translational motion and the
other is the intrinsic partition function of the composite:

\[
\omega_{N,Z} = \frac{V}{h^3(2\pi m T)^{3/2}} A^{3/2} \times z_{N,Z}(\text{int}) \tag{4}
\]

where \(A = N + Z\) is the mass number of the composite
and \(V\) is the volume available for translational motion.
Note that \(V\) will be less than \(V_f\), the volume to which the
system has expanded at break up. In general, we take
\(V_f\) to be equal to three to six times the normal nuclear
volume. We use \(V = V_f - V_0\), where \(V_0\) is the normal
volume of nucleus with \(Z_0\) protons and \(N_0\) neutrons.
For nuclei in isolation, the internal partition function is
given by \(z_{N,Z}(\text{int}) = \exp[-\beta F(N, Z)]\) where \(F = E - TS\).

For mass number \(A = 5\) and greater we use the
liquid-drop formula for calculating the binding energy
and the contribution for excited states is taken from the
Fermi-gas model. The properties of the composites used
in this work are listed in details in [14].

III. RESULTS AND DISCUSSIONS

![FIG. 1: (Color online) Total charge distribution of \(A_0 = 60,\)
\(Z_0 = 25\) system from canonical (red solid lines) and grand
canonical model (black dotted lines) at same freeze-out vol-
ume \(V_f = 3V_0\) but three different temperatures (a) 3.8 MeV
, (b) 5 MeV and (c) 8 MeV.

We compare the total charge distribution \(\langle n_Z \rangle = \sum N \langle n_{N,Z} \rangle\) obtained from both the ensembles at differ-
ent temperatures (3.8 MeV, 5 MeV and 8 MeV) from
disassembly of a particular source \((Z_0 = 25, A_0 = 60)\)
at a fixed freeze-out volume \(3V_0\) (Fig. 1). The differ-

![FIG. 2: (Color online) Total charge distribution of \(A_0 = 60,\)
\(Z_0 = 25\) system at \(T = 5.0\ MeV\) by using canonical (red solid lines)
and grand canonical model (black dotted lines) for three
different freeze-out volumes (a) \(V_f = 3V_0\), (b) \(V_f = 4V_0\)
and (c) \(V_f = 5V_0\).]
ence in result is maximum at the lowest temperature 3.8 MeV where fragmentation is less and the disassembly of the nucleus results in more of ‘liquid-like’ fragments or higher mass fragments. As one increases the temperature, fragmentation increases, the number of such higher mass fragments decrease (at the expense of the lower mass ones) and the results from the canonical and grand canonical ensembles begin to converge. This is easily seen at the two higher temperatures. At 8 MeV the results from both the ensembles are very close to each other since fragmentation is maximum at this temperature, the nucleons and the lower mass fragments dominating the distribution.

The effect of increasing the freeze-out volume (decreasing the density) is equivalent to that of increasing the temperature and this is seen in Fig. 2. Here we have repeated the same calculation for the same source at $T = 5$ MeV for three different freeze-out volumes. It is seen that results from both the ensembles agree with each other as one increases the freeze-out volume when the nucleus fragments more into smaller pieces. Similar effect is also seen if we vary the source asymmetry $y = (N_0 - Z_0)/(N_0 + Z_0)$ keeping the temperature fixed 5 MeV, freeze-out volume at $3V_0$ and source size at $A_0 = 60$. Fig 3 shows the charge distribution for three nuclei having $y = 0.33, 0.17$ and 0 respectively. We observe that the difference in results between both the ensembles is maximum when the asymmetry is more (Fig 3(a)) and the difference is least for the symmetric nucleus (Fig 3(c)).

The reason behind the differences is the same as that in the case of temperature variation. When the nucleus is more asymmetric, fragmentation (breaking of the nucleus) is less and the fraction of higher mass fragments is more as compared to the more symmetric case which will be shown later. This effect is also seen if we keep both temperature, freeze-out volume and the asymmetry parameter fixed but increase the source size(mass) as shown in Fig. 4. The difference in result between both the ensembles is maximum when the source size is minimum as expected and the results become close to each other for a large nucleus. We can say that the nucleus fragments more and more as one increases the source size (keeping other parameters fixed) and the effect is similar to that of increasing the temperature keeping the source size fixed.

In order to investigate the effect more, we have calculated the ratio (normalized) of higher mass fragments formed to that of the total number of fragments (total multiplicity). The fragment whose size is more than 0.8 times $A_0$ (more than 80% of the source in size) are considered as higher mass fragments i.e. the ratio is defined as

$$\eta = \frac{\sum_{A>0.8A_0} \langle n_{N,Z} \rangle}{\sum_{A=1}^{A_0} \langle n_{N,Z} \rangle}$$  \hspace{1cm} (5)$$

This criteria of choosing the higher mass fragments is not very rigid and can be relaxed. We have checked that even if we make it 0.75 or 0.85 instead of 0.8 the trend of the results remain same. We have done this calculation in both canonical and grand canonical models and the results are similar. We have shown the results in Fig 5 from the grand canonical model. In Fig 5.a we show the variation of this ratio as a function of temperature (keeping source size, freeze-out volume and asymmetry

![FIG. 3: (Color online) Total charge distribution at $T = 5.0$ MeV and $V_f = 3V_0$ from canonical (red solid lines) and grand canonical model (black dotted lines) for three different source sizes $A_0 = (a) 60$, (b) 96 and (c) 144 each having same isospin asymmetry $y = 0.17$.](image)

![FIG. 4: (Color online) Total charge distribution at $T = 5.0$ MeV and $V_f = 3V_0$ by using canonical (red solid lines) and grand canonical model (black dotted lines) for three different source sizes $A_0 = (a) 60$, (b) 96 and (c) 144 each having same isospin asymmetry $y = 0.17$.](image)
fixed) and it is seen that the ratio decreases with increase in \( T \). This shows that for a source with lower values of \( T \), the fraction of higher mass fragments formed as a result of fragmentation is more as compared to those with higher \( T \) values. We emphasize that the difference in the charge distributions from the canonical and grand canonical ensembles is mainly caused by the presence of the higher mass fragments in the distribution. The lesser is the fraction of the higher mass fragments, the deviation in results between both the ensembles will be less and this is exactly what we saw in Fig. 1. Similar effect is seen when one plots this ratio (Fig 5.b) as a function of \( V_f/V_0 \) keeping other parameters fixed. It is clearly seen that with increase in the freeze-out volume, the fraction of higher mass fragments decrease and this causes the results between both the ensembles to be very close when \( V_f \) is maximum as shown in Fig. 2. We also plot \( \eta \) as a function of the asymmetry parameter \( y \) of the source, the source size (\( A_0 = 60 \)), temperature (5 MeV) and freeze-out volume (\( 3V_0 \)) being kept fixed and it is seen that the ratio increases with \( y \) (Fig 5(c)). So here we observe that the less is the asymmetry of the source, less is the number of large fragments and hence fragmentation of the nucleus is more. In this scenario, when the nucleus is more symmetric the results from the two ensembles agree to a very good extent than when the nucleus is less symmetric as seen in Fig 3. The same effect is seen (Fig 5(d)) if one increases the source size keeping the other parameters fixed and we assert that the effect of increasing the source size is similar to that of increasing the temperature or freeze-out volume or decreasing the asymmetry of the source as far as convergence between both the ensembles is considered. What we wish to convey is that the differences in results between the canonical and the grand canonical ensemble is mainly because of the presence of the higher mass fragments in the fragmentation of a nucleus. If the conditions are such that the fragmentation is more and there are only lower mass clusters, then the results from both the ensembles agree to a much better extent. The same condition is also valid for convergence between microcanonical and canonical ensembles where energy plays the role of the extensive variable instead of the total number of particles. The more the nucleus disintegrates, the less will be the fluctuation in energy and better will be the convergence between the microcanonical and the canonical ensembles.

**IV. SUMMARY AND CONCLUSION**

This Letter analyzes the charge distributions of fragments formed in nuclear multifragmentation in both canonical and grand canonical versions of the multifragmentation model. Both models are typically used to study experimental data from heavy-ion collisions at intermediate energies. We have shown that results from both models are in agreement for finite nuclei provided the nucleus fragments predominantly into nucleons and low mass clusters. We have seen that this condition is achieved under certain conditions of temperature, freeze-out volume, source size and source asymmetry. The main message that we wish to convey in this work is that while canonical and grand canonical models have very different underlying physical assumption, the results from both models can be in agreement with each other provided the contribution of higher mass fragments in nuclear disassembly is insignificant. This condition can be achieved either by increasing the the temperature or freeze-out volume of the fragmenting nucleus or by increasing the source size, or by decreasing the asymmetry of the source. In fact when all these four conditions are satisfied then one obtains the best convergence between the two models. On the other hand, when the temperature and freeze-out volume are low, nucleus is small and more asymmetric then fragmentation of the nucleus is least; in these cases higher mass fragments dominate the distribution and the results from both the ensembles will be very different. We would like to add that the convergence between the microcanonical and the canonical ensemble will also be achieved under the similar conditions as those between the canonical and the grand canonical ensembles.

**V. ACKNOWLEDGEMENT**

We would like to thank Prof. S. Das Gupta (Mcgill University) for introducing us to this subject.
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