Specific heat and bimodality in canonical and grand canonical versions of the thermodynamic model

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Abstract

We address two issues in the thermodynamic model for nuclear disassembly. Surprisingly large differences in results for specific heat were seen in predictions from the canonical and grand canonical ensembles when the nuclear system passes from liquid-gas co-existence to the pure gas phase. We are able to pinpoint and understand the reasons for such and other discrepancies when they appear. There is a subtle but important difference in the physics addressed in the two models. In particular if we reformulate the parameters in the canonical model to better approximate the physics addressed in the grand canonical model, calculations for observables converge. Next we turn to the issue of bimodality in the probability distribution of the largest fragment in both canonical and grand canonical ensembles. We demonstrate that this distribution is very closely related to average multiplicities. The relationship of the bimodal distribution to phase transition is discussed.

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I.   INTRODUCTION

In models of statistical disassembly of a nuclear system formed by the collision of two heavy ions at intermediate energy one assumes that because of multiple nucleon-nucleon collisions a statistical equilibrium is reached. The temperature rises. The system expands from normal density and composites are formed on the way to disassembly. As the system reaches between three to six times the normal volume, the interactions between composites become unimportant (except for the long range Coulomb interaction) and one can do a statistical equilibrium calculation to obtain the yields of composites at a volume called the freeze-out volume. The partitioning into available channels can be solved in the canonical ensemble where the number of particles in the nuclear system is constant (as it would be in experiments) or in the grand canonical ensemble where the particle number fluctuates but the average number can be constrained to a given value. Usually the grand canonical model is more easily solved. Hence it is more commonly used although in the case of nuclear physics (where particle numbers are typically ≈ 200 or less) the use of the canonical ensemble would be more appropriate.

Apart from ease of calculation, there is another reason why the grand canonical model is very useful. Known properties of nuclear interactions predict that if nuclear systems were arbitrarily large (consider a fictitious system where the Coulomb interaction is switched off) disassembly of nuclear systems would show features of liquid-gas phase transition [1]. Since the grand canonical ensemble is expected to become accurate for large systems, this would seem to be a suitable framework to describe bulk properties. The canonical model, built with a constant particle number in mind, can not be pushed to arbitrarily large particle number although it can be implemented for fairly big systems containing thousands of particles. One can then extraprolate from finite particle number systems to the infinite particle number case. When this was done, a huge difference showed up between grand canonical and canonical results for c_v (specific heat per particle at constant volume). In the grand canonical model c_v was merely discontinuous at phase transition [2] but in the canonical model c_v would go to infinity as the system particle number approached infinity [3].

This discrepancy was examined in detail for a system with 2000 particles [4]. The analysis showed that in the co-existence region, even when the average number of particles is 2000, fluctuations in the number of particles is huge if one uses the grand canonical ensemble.

The c_v with a fixed number of particles is sharply peaked at a temperature T where T is a function of the number of particles. Because in the grand canonical ensmble the particle number fluctuations are significant when the average number is 2000, the resulting c_v is smeared out. What this analysis did not answer are two significant questions: (a) under what conditions are the grand canonical results valid and (b) under what conditions can the canonical and grand canonical results agree? We answer both these questions in this work. The apparent paradox is explained.

We also address the issue of bimodality in the probability distribution of the largest fragment as a function of the mass number of the largest fragment for a finite system when the thermodynamic model is used. Clearly the canonical model is appropriate here but we also study bimodality in the grand canonical ensemble, where the average value of the number of particles is constrained to a typical value expected in heavy ion collisions. In the thermodynamic model it is easy to devise systems which may (as in the nuclear matter case) or may not (i.e., by switching off surface tension term in binding energy formula) have a phase transition (some other models may not have this versatility). Thus in this model the connection of bimodality to phase transition can be directly established. It is interesting to note (as described in detail later) that both canonical model and the approximation of a finite system with the grand canonical model show features of bimodality but quantitatively the results are quite different.

The plan of the paper is as follows. In section II we set up the the formulae for the grand canonical ensemble. In section III the methodology of the canonical ensemble is presented. We point out that, although not obvious, the two ensembles actually addressed different physics causing the difference in results for specific heat. In section IV we reformulate the canonical model to better approximate the grand canonical model. We show that results for c_v progressively converge. We then turn to the question of bimodality in the probability distribution of the largest fragment as a function of the fragment mass number. Formulae for the probability distribution are given in section V. In section VI we present results for this distribution and discuss the bimodality in both the canonical and grand canonical ensembles. The connection between the probability distribution of the largest fragment and average multiplicity is established in section VII. Summary is presented in section VIII.

As in [1, 2, 4] we use one kind of particle and no Coulomb interaction. This is adequate for the purpose of this study and offers considerable numerical simplifications. Numerous

applications of the canonical [5] and the grand canonical models [6] with two kinds of particles exist where fits experimental data are the main issues.

II. FORMULAE IN THE GRAND CANONICAL MODEL

If we have n_a particles of type a, n_b particles of type b, n_c particles of type c etc. all enclosed in a volume V and interactions between particles can be neglected, the grand partition function for this case can be written as

$$Z_{gr} = \prod_{i=a,b,c...} \exp(e^{\beta\mu_i}\omega_i) \tag{1}$$

Here the μ_i is the chemical potential and ω_i the canonical partition function of one particle of type i. The average number of particles of type i is given by $\partial(lnZ_{gr})/\partial(\beta\mu_i)$:

$$n_i = e^{\beta\mu_i}\omega_i \tag{2}$$

It is possible that one of the species can be built from two other species. In reverse, a heavier species can also break up into two lighter species. If α number of particles of type a can combine with β number of particles of type b to produce γ number of particles of type c, then chemical equilibrium implies [7] that the chemical potentials of a, b and c are related by $\alpha\mu_a + \beta\mu_b = \gamma\mu_c$.

In our model we have N nucleons in a volume V (which is significantly larger than the normal nuclear volume) but these nucleons can be singles or form bound dimers, trimers etc. Chemical equilibrium implies that a composite with k bound nucleons has a chemical potential $k\mu$ where μ is the chemical potential of the monomer (nucleon). Thus our ensemble has monomers, dimers, trimers etc. upto some species with k_{max} bound nucleons. In the actual world of nuclear physics k_{max} terminates around 250 because of Coulomb interaction but in the model pursued here we may terminate it arbitrarily at 1 (monomers only), 2(monomers and dimers), 3 or any large k_{max}. It was demonstrated in [8] that liquid-gas type phase transition occurs for large $k_{max} > 2000$.

The total number of nucleons will be denoted by N. Of course, the grand canonical ensemble works best when N is very large, ideally infinite.

We now look into ω_i, the partition function of one composite of i nucleons.This factors into two parts, a traditional translation energy part and an intrinsic part: $\omega_i = z_i(tran)z_i(int)$

where

$$z_i(tran) = \frac{V}{h^3} \int \exp(-\beta p^2/2m_i) d^3p = \frac{V}{h^3}(2\pi m_i T)^{3/2} \tag{3}$$

The intrinsic part $z_i(int)$ of course contains the key to phase transition. If we regard each composite to exist only in a ground state with energy e_i^{gr}, then $z_i(int) = \exp(-\beta e_i^{gr})$. We use $e_i^{gr} = -iW + \sigma i^{2/3}$ where nuclear physics sets W=16 MeV and $\sigma = 18$ MeV. This simple model itself will lead to the main results of this paper. Because of the surface term, energy per particle drops as i grows. Let us denote by F the free energy of the N nucleons where N is the total number of nucleons; E be the energy and S, the entropy: $F = E - TS$. At finite temperature F will go to its minimum value. The key issue is how the system of N nucleons breaks up into clusters of different sizes as the temperature changes. At low temperature E and hence F minimises by forming very large clusters (liquid). But as the temperature increases S will increase by forming larger number of clusters thus breaking up the big clusters. Gaseous phase will appear. How exactly this will happen requires calculation and these show that the system goes through a first order liquid-gas phase transition [2, 8]. As is the common practice, we used here a slightly more sophisticated model for $z_i(int)$. We make the surface tension temperature dependent in conformity with usual parametrisation [9]; $\sigma(T) = \sigma_0[(T_c^2 - T^2)/(T_c^2 + T^2)]^{5/4}$. Here σ_0 =18 MeV and T_c=18 MeV. At $T = T_c$ surface tension vanishes and we have a fluid only. For us this is unimportant as our focus will be the temperature range 3 to 8 MeV. Also in z_i we include not only the ground state but also the excited states of the composite in the Fermi-gas approximation [1, 9]. The expression for $z_i(int)$ is now complete and easily tractable.

Let us now summarise the relevant equations. For $k = 1$ (the nucleon which has no excited states)

$$n_1 = \frac{V}{h^3}(2\pi m T)^{3/2} \exp(\mu/T) \tag{4}$$

and for $1 < k \leq k_{max}$

$$n_k = \frac{V}{h^3}(2\pi m T)^{3/2} k^{3/2} \exp[(\mu k + Wk + kT^2/\epsilon_0 - \sigma(T)k^{2/3})/T] \tag{5}$$

Here n_k is the average number of composites with k nucleons. In the rest of the paper, for brevity, we will omit the qualifier "average".

A useful quantity is the multiplicity defined as

$$M = \sum_{k=1}^{k_{max}} n_k \tag{6}$$

The number of nucleons bound in a composite with k nucleons is kn_k and obviously $N = \sum_{k=1}^{k_{max}} kn_k$. The pressure is given by

$$p = \sum_{k=1}^{k_{max}} \frac{n_k}{V}T \tag{7}$$

This follows from the identity $pV = TlnZ_{gr}$.

Quantities like N, V, n_k are all extensive variables. These equations can all be cast in terms of intensive variables like $N/V = \rho, n_k/N$ etc so that we can assume both N and V approach very large values and fluctuations in the number of particles can be ignored. Thus for a given temperature and density we solve for μ using

$$\rho = \frac{(2\pi mT)^{3/2}}{h^3}(\exp(\mu/T) + \sum_{k=2}^{k_{max}} k^{5/2}\exp[(\mu k + Wk + kT^2/\epsilon_0 - \sigma(T)k^{2/3})/T]) \tag{8}$$

The sum rule $N = \sum_{k=1}^{k_{max}} kn_k$ changes to $1 = \sum kn_k/N$. The energy per particle is given by

$$\frac{E}{N} = \sum_{k=1}^{k_{max}} \frac{n_k}{N}E_k \tag{9}$$

where $E_k = \frac{3}{2}T$ for k=1 and for $1 < k \le k_{max}$

$$E_k = \frac{3}{2}T + k(-W + \frac{T^2}{\epsilon_0}) + \sigma(T)k^{2/3} - T[\partial\sigma(T)/\partial T]k^{2/3} \tag{10}$$

The term $T[\partial\sigma(T)/\partial T]k^{2/3}$ arises from the temperature dependence of the surface tension. The effect of this term is small. Eqs. (9) and (10) follow from the identity $E = \mu N - \frac{\partial}{\partial\beta}lnZ_{gr}$.

From what we have described so far it would appear that V in eqs.(3) to (9) is the freeze-out volume V, the volume to which the system has expanded. Actually if the freeze-out volume is V then in these equations we use $\tilde{V}$ which is close to V but less. The reason for this is the following. To a good approximation a composite of k nucleons is an incompressible sphere with volume k/ρ_0 where the value of ρ_0 is $\simeq 0.16$ fm^{-3}. The volume available for translational motion (eq.(3)) is then $\tilde{V} = V - V_{excluded}$ where we approximate $V_{excluded} \simeq N/\rho_0 = V_0$ the normal volume of a nucleus with N nucleons. Similar corrections are implicit in Van der Waals equation of state. This is meant to take care of hard sphere

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interactions between different particles. This answer is approximate. The correct answer is multiplicity dependent. The approximation of non-interacting composites in a volume gets to be worse as the volume decreases. We restrict our calculation to volumes V greater than $2V_0$. This is how the calculations reported proceed. We choose a value of $V_0/V = \rho/\rho_0$ from which $V_0/\tilde{V} = \tilde{\rho}/\rho_0 = \rho/(\rho_0 - \rho)$ is deduced. This value of $\tilde{\rho}$ is used in eq.(8) to calculate μ and all other quantities. We plot results as function of ρ/ρ_0. If we plotted them as function of $\tilde{\rho}/\rho_0$ the plot would shift to the right.

III. THE CANONICAL MODEL SOLUTION

The statistical equilibrium model as described above can be solved for a given fixed number of particles when the number of particles N is finite. No spread in the number of particles, which is inherent in the grand canonical ensemble, needs to be made. Extensive use of the canonical model has been made to fit experimental data [5] so just an outline will be presented for completeness. Among other applications, the canonical model can be used to study finite particle number effects on phase transition characteristics.

Consider again N identical particles in an enclosure V and temperature T. These N nucleons will combine into monomers, dimers, trimers etc. The partition function of the system in the canonical ensemble can be written as

$$Q_N = \sum \prod_i \frac{(\omega_i)^{n_i}}{n_i!} \tag{11}$$

Here ω_i is the one particle partition function of a composite which has i nucleons. We already encountered ω_i in section II: $\omega_i = z_i(tran)z_i(int)$ with $z_i(tran)$ and $z_i(int)$ given in detail. Other forms for ω_i can be used in the method outlined here. The summation in eq.(11) is over all partitions which satisfy $N = \sum i n_i$. The summation is non-trivial as the number of partitions which satisfy the sum is enormous. We can define a given allowed partition to be a channel. The probablity of the occurrence of a given channel $P(\vec{n}) \equiv P(n_1, n_2, n_3....)$ is

$$P(\vec{n}) = \frac{1}{Q_N} \prod \frac{(\omega_i)^{n_i}}{n_i!}. \tag{12}$$

The average number of composites of i nucleons is easily seen from the above equation to be

$$n_i = \omega_i \frac{Q_{N-i}}{Q_N} \tag{13}$$

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Since $\sum i n_i = N$, one readily arrives at a recursion relation [10]

$$Q_N = \frac{1}{N} \sum_{k=1}^{N} k\omega_k Q_{N-k} \qquad (14)$$

For one kind of particle, Q_N above is easily evaluated on a computer for N as large as 3000 in matter of seconds. It is this recursion relation that makes the computation so easy in the model. Of course, once one has the partition function all relevant thermodynamic quantities can be computed. For example, eq. (7) still gives the expression for pressure although one could correct for the center of mass motion by reducing the multiplicity by 1: $p = T(M-1)/\tilde{V}$. The chemical potential can be calculated from $\mu = F(N) - F(N-1)$ where the free energy is $F(N) = -T \ ln \ Q_N$ which is readily available from the calculation.

IV. GENERATING GRAND CANONICAL RESULTS FROM THE CANONICAL ENSEMBLE

We first consider pressure (eq.(7)) in the grand canonical ensemble. The V in eq.(7) cancels out the V in eqs. (4)and (5) and thus pressure is given in terms of intensive variables directly. We may assume that this is truly the pressure in infinite systems (V and n_k arbitrarily large in which case fluctuations in the grand canonical ensemble can be ignored). However the grand canonical answer does depend upon the value of k_{max}. In Fig.1 we have used k_{max}=2000, a value large enough so that liquid-gas transition type features emerge (the flatness of pressure against ρ). For k_{max} significantly lower, the flatness disappears (see details in [8]). In Fig.1 we also show several canonical model results all with the same k_{max}=2000 but different values of N. For N=2000, the canonical results are quite different from the grand canonical results except for very low densities. In particular a region of mechanical instability is seen which can give rise to a region of negative c_p, the specific heat per particle at constant pressure (see [5] for detailed discussion). In the same figure, we have also shown prssures in the canonical model when N=100,000 and 500,000. We see that the pressure approaches the grand canonical value as N increases (the periodicity obvious in the curve for N= 100,000 arises from the fact the largest composite has k =2000 but we will not get into a detailed analysis here). The conclusion here is that the grand canonical value of pressure in Fig.1 refers to a system which has $N = \infty$ where the largest cluster has $k = 2000$. This is quite different from the usual canonical model result which would have

$N = k_{max} = 2000$. To address the physics of the grand canonical model we keep k_{max} still at 2000 but need to keep on increasing the value of N. Then the canonical results converge towards the grand canonical values.

For this given problem we have approached the grand canonical result from a canonical ensemble. One can consider the reverse problem: getting the canonical result starting from the grand canonical model. It is of course obvious that the correspondence would be exact provided one uses the appropriate V in the grand canonical ensemble and then projects from it the part which has an exact N. This is because the grand canonical ensemble is a particular weighted sum of canonical ensembles with different N's.

Let us now turn to Fig.2 which deals with c_v, the specific heat per particle at constant volume. We again keep $k_{max} = 2000$. One finds that the c_v in a canonical calculation for $N = k_{max} = 2000$ produces a very sharp peak. The grand canonical expression for energy per particle (eq.(9)) is an intensive quanity and so is its derivative c_v. We expect this grand canonical result for c_v is valid for N very large. Comparison shows that the grand canonical result differs drastically from the canonical N=2000 result in a very narrow window when the system passes from the co-existence to a pure gas phase. Can we make the results converge by successively increasing the value of N in the canonical model? The answer is "yes" as Fig.2 demonstrates. We see that the canonical result with k_{max}=2000 approaches the grand canonical result with k_{max}=2000 as the number of particles N in the canonical calculations is progressively increased beyond N=2000.

To summarise: the grand canonical model is applicable when $N \gg k_{max}$. The limit $N \gg k_{max}; k_{max} \to \infty$ is robust (as shown in [8]) and produces a first order phase transition. This model is distinct from the canonical model $N = k_{max}; k_{max} \to \infty$. There is no scaling in this latter model:$N = k_{max}$, both N and k_{max} very large is not equivalent within a factor of scaling to a system with $2N = 2k_{max}$. We are unable to provide a robust limit for the canonical model of $N = k_{max}; N \to \infty$. Fig. 3 shows the progression of the E/N and pressure curves as $N = k_{max}$ increases from 2000 to 50,000.

V. BIMODALITY: THE BASIC FORMULAE IN GRAND CANONICAL AND CANONICAL ENSEMBLE

In event by event analysis in experiments, one can in principle ascertain the largest mass (or the largest charge) emerging in each event from multifragmentation. The probability distribution of this largest mass can be plotted as a function of the value of mass of this largest fragment. It is shown that a bimodality in this distribution at a certain temperature is a signature of a first order phase transition: that is, if the system were infinitely large it would have a first order phase transition [12, 13]. Thus from a finite system one can have a signal for phase transition. We will now see how the probability distribution of the largest fragment as a function of the mass of the largest fragment can be computed in the thermodynamic model in the two ensembles. First the grand canonical ensemble.

The grand canonical ensemble works best for a large system and we have already seen in the previous section that application of this model to multifragmentation of finite nuclei can lead to serious errors in some temperature (equivalently energy) window. Nonetheless, let us proceed to see how results can be derived. We fix a value for ρ/ρ_0 (in figs. (4) and (5) we have kept this at 0.25) and choose the appropriate value of the volume so that the average number $N = \sum_1^{k_{max}} k n_k$ is 150, the system whose results we show. The heaviest composite allowed in the model k_{max} is also 150.

From eqs. (1) and (2) one can derive that the probability that a particular composite with k nucleons does not occur at all is

$\frac{1}{e^{n_k}}$

and the probability that it occurs at least once or more is

$\frac{e^{n_k} - 1}{e^{n_k}}$.

Note that our n_k here is the same as n_k's of eqs. (4) and (5), the average values in the grand canonical ensemble. The probability that k is the highest mass fragment in an event is then given by $(k < k_{max})$

$$P_m(k) = \frac{e^{n_k} - 1}{e^{n_k}} e^{-(n_{k+1} + n_{k+2} + \dots n_{kmax})} \tag{15}$$

From the above eq. one readily derives

$$\frac{P_m(k+1)}{P_m(k)} = \frac{e^{n_{k+1}} - 1}{e^{n_k} - 1} e^{n_k} = \frac{e^{n_{k+1}} - 1}{1 - e^{-n_k}} \tag{16}$$

If $n_{k+1} > n_k$ then $P_m(k+1) > P_m(k)$. If further both n_{k+1} and n_k are small compared to 1 then

$$\frac{P_m(k+1)}{P_m(k)} = \frac{n_{k+1}}{n_k} \tag{17}$$

Let us turn to the calculation of the probability disribution of the largest fragment as a function of the mass of the largest fragment in the canonical model. A detailed formulation when two kinds of particles are present was given in a recent paper [11] but for competeness, we review the development.There is an enormous number of channels in Eq.(11). Different channels will have different values for the largest fragment. For example there is a term $\frac{\omega_1^N}{N!}$ in the sum of Eq.(11). In this channel all the fragments and hence also the largest fragment has mass 1. The probability of this channel occurring is (from Eq.(12)) $P_m(1) = \frac{1}{Q_N}\frac{\omega_1^N}{N!}$. The full partition function can be written as $Q_N = Q_{(\omega_1, \omega_2, \omega_3, ...\omega_{kmax})}$. If we construct a Q_N where we set all ω's except ω_1 to be zero then this $Q_N(\omega_1, 0, 0, 0..............) = \frac{\omega_1^N}{N!}$ and this has the largest mass 1. Consider now constructing a Q_N with only two ω's : $Q_N(\omega_1, \omega_2, 0, 0, 0, ...)$. This will have the largest mass sometimes 1 (as $\frac{\omega_1^N}{N!}$ is still there) and sometimes 2 (as, for example, in the term $\frac{\omega_2^3}{3!}\frac{\omega_1^{N-6}}{(N-6)!}$). It then follows that

$$P_m(k) = \frac{Q_N(\omega_1, \omega_2, ...\omega_k, 0, 0, 0..) - Q_N(\omega_1, \omega_2, ...\omega_{k-1}, 0, 0, 0...)}{Q_N} \tag{18}$$

In the above the first term in the numerator takes care of the occurrence of all partitions where the largest fragment is between 1 and k and the second term takes care of all the partitions where the largest fragment is between 1 and $k-1$. The difference, divided by Q_N is the desired answer.

Since one has the general formula for the probability $P_m(k)$, one can compute the average value of the mass of the largest fragment as well as the root mean square deviation. In fact, these have been measured in some experiments [14] and have recently been calculated [11]. But we will not need this for this paper.

VI. REPRESENTATIVE RESULTS

The probability distribution $P_m(k)$ of the largest fragment as a function of k where k is the largest fragment in an event is shown in Fig.(4) where the freeze-out density ρ/ρ_0 is 0.25 and the dissociating system has N=150 (for the grand canonical ensemble the average

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value is 150). The canonical and grand canonical results are quite different but both display bimodality (there are two maxima with similar heights), the grand canonical at temperature ≈ 5.9 MeV and the canonical at temperature ≈ 6.2 MeV. In Fig.(5) we have compared the n_k's of the two models. Near the end value 150 the differences are very substantial at all temparatures. At lower values of k they agree very well at $T = 6.8$ MeV, quite well at T=6.2 MeV but gets worse at lower temperatures becoming quite different at T=5.0 MeV. These differences have been noted and discussed before [15].

VII. CONNECTION BETWEEN PROBABILITY DISTRIBUTION OF THE LARGEST FRAGMENT AND AVERAGE MULTIPLICITY

The very first experiments in heavy ion collisions measured n_k, the average multiplicity against k. One of the earliest postulates was the following. At low energy n_k first falls with k but after reaching a minimum rises again. This is the so-called "U" shape. This shape at lower temperature is an indication that the system will undergo a liquid-gas type phase transition. As the energy of collision increases, the height of the maximum on the heavier side will decrease, will then disappear (this marks the phase transition temperature). At higher energy, n_k decreases monotonically with k. This is discussed in many places including [1, 3]. Basically then one looks at the behaviour of n_k as a function of k and energy as one signature of phase transition. Since bimodality in the probability distribution is also a signature of phase transition, we hope to get a connection between $P_m(k)$ and n_k.

For bimodality one requires that after the minimum following the first maximum, $P_m(k)$ will rise again witk k. Similarly in conjectures involving the multiplicity, n_k, after reaching a minimum must rise again with k. These two features are intimately related. In the grand canonical model this is very simple to prove. Equation (16) shows that if $n_{k+1} > n_k$ then $P_m(k+1) > P_m(k)$ and bimodality can happen. The reverse is not true; $n_{k+1} < n_k$ does not imply that $P_m(k + 1)$ is less than $P_m(k)$.

There is similar connection in the canonical model. Here it can be proven that on the heavier side $k > N/2$, a rise of n_k with k guarantees that $P_m(k)$ will rise with k. In fact it is even more direct than that. For $k > N/2$, we have an equality; $P_m(k) = n_k$. This can be proven from eq. (18) but there is a an easier proof. We can rewrite $P_m(k)$ as a sum of

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terms:

$$P_m(k) = P_m^1(k) + P_m^2(k) + P_m^3(k) + \ldots\ldots \tag{19}$$

where in each of the terms in the right hand side k is the highest mass that occurs but in $P_m^1(k)$ the composite k occurs only once, in $P_m^2(k)$ it occurs twice, in $P_m^3(k)$ it occurs three times and so on. Specifically,

$$P_m^1(k) = \frac{1}{Q_N}\omega_k \prod_{i<k} \frac{(\omega_i)^{n_i}}{n_i!}; \qquad N - k = \sum_{i=1}^{k-1} i n_i$$

$$P_m^2(k) = \frac{1}{Q_N}\frac{(\omega_k)^2}{2!} \prod_{i<k} \frac{(\omega_i)^{n_i}}{n_i!}; \qquad N - 2k = \sum_{i}^{k-1} i n_i$$

It is clear what the structures for higher terms in the series will be. It is then also obvious that

$$n_k = P_m^1(k) + 2P_m^2(k) + 3P_m^3(k) + \ldots\ldots + O.C. \tag{20}$$

In the above, $O.C.$ stands for other channels where mass k occurs but it is not the highest mass in the channel. If $k > N/2$ then only $P_m^1(k)$ exists. Thus for $k > N/2$ we have $P_m(k) = n_k$. If n_k rises with k in this region then so does $P_m(k)$. For $k \leq N/2$, the relationship is $n_k \geq P_m(k)$, with n_k usually significantly larger than $P_m(k)$. For bimodality to exist we need to have n_k rising with k in some region $k > N/2$.

The relation $P_m(k) = n_k$ for $k > N/2$ is not limited to the thermodynamic model only. It is true in any number conserving model.

VIII. SUMMARY

This paper had two goals. One, to resolve and understand the difference between grand canonical and canonical values of specific heat and pressure in thermodynamic models as applied to heavy ion collisions. This issue we believe is resolved. Second, to understand the link between bimodality in the distribution of the heaviest fragment and the average multiplicity of fragments (which has also been linked with aspects of phase transition). We think we have gained an understanding. In a later publication we expect to show more results for bimodal distributions for realistic cases with two kinds of particles and the Coulomb interactions included. Calculations for a particular case have already appeared [11].

IX. ACKNOWLEDGEMENT

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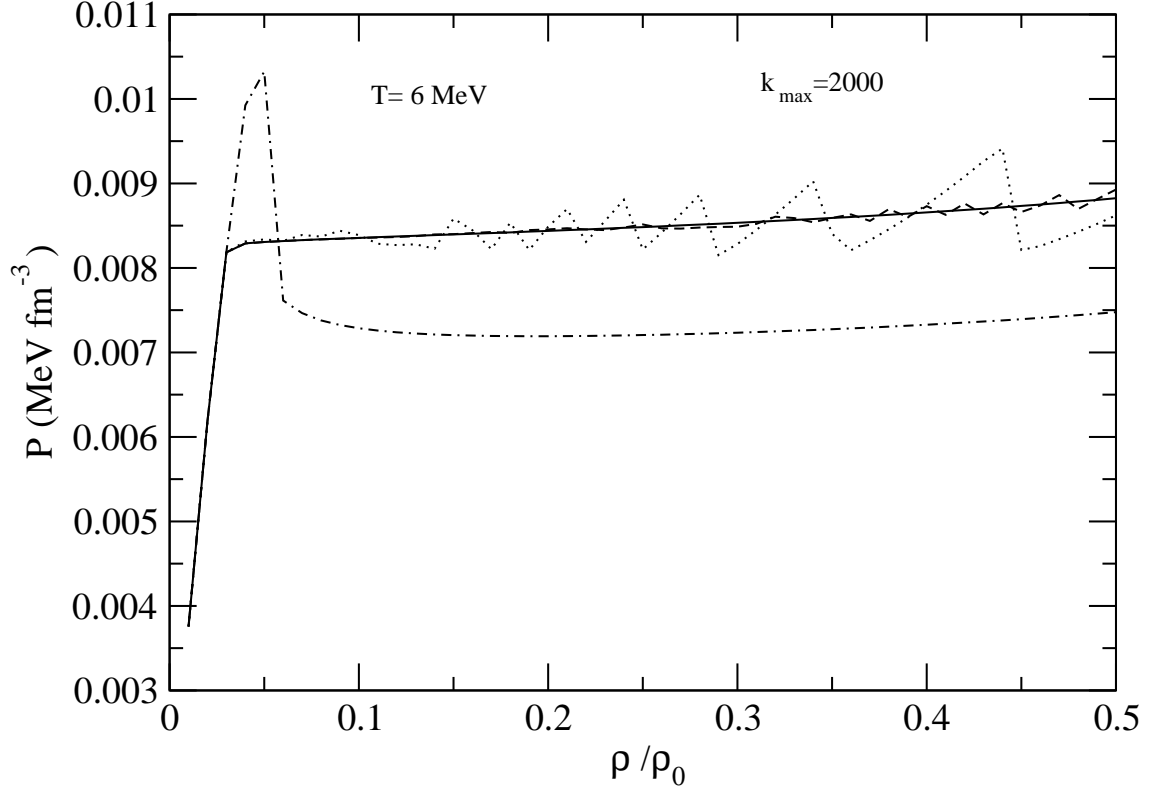[15] C. B. Das, S. Das Gupta, and B. K. Jennings, Phys. Rev. C**70**,044611(2004)

FIG. 1: Pressures calculated in the canonical model compared with pressure calculated in the grand canonical model. For all of these the largest composite allowed has 2000 nucleons ($k_{max} = 2000$) and the temperature is 6 MeV. The grand canonical calculation is the solid curve. The canonical calculations are done with N=2000 (dash-dot), N=100,000 (dots) and N=500,000(dash). As N increases, agreement with the grand canonical result becomes better and better.
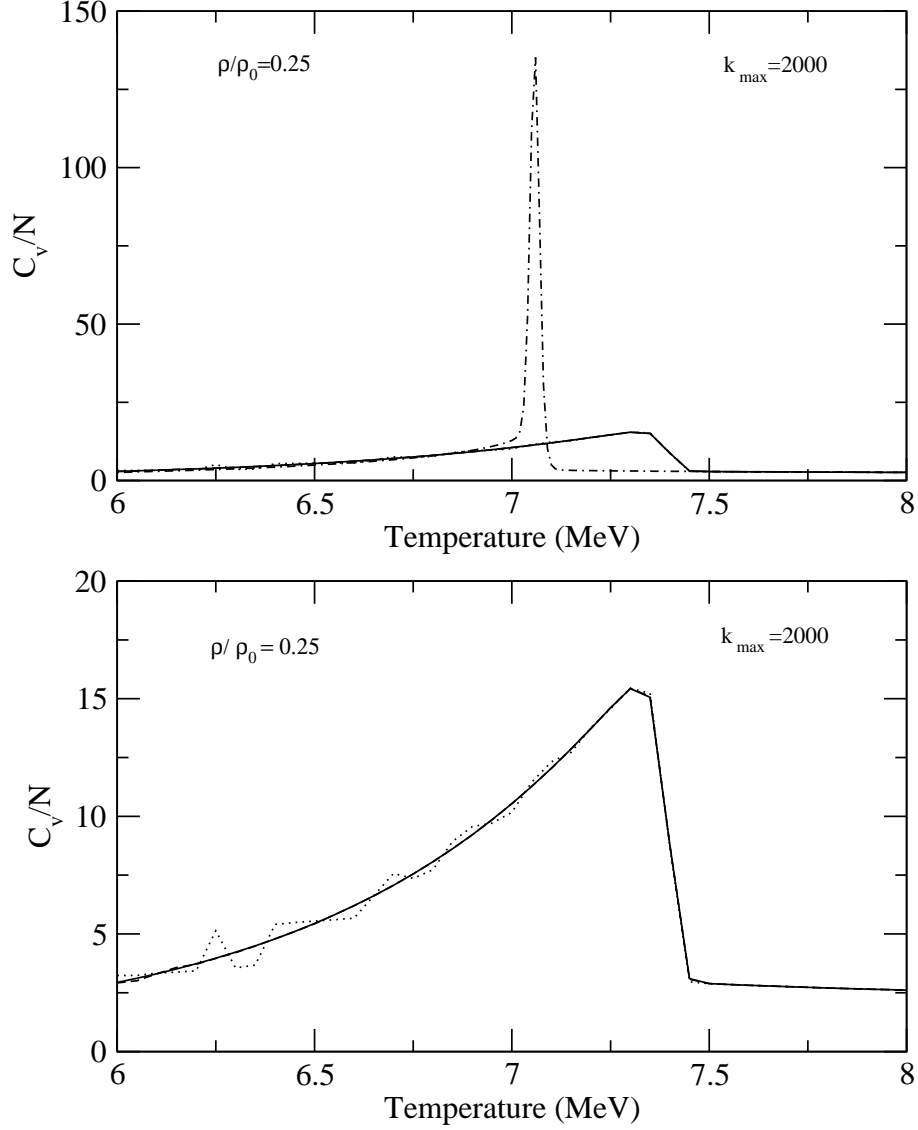
FIG. 2: Specific heat at constant volume in grand canonical and canonical models. Two different scales are needed to highlight differences in values. Again the canonical calculations are done with N=2000 (dash-dot), N=100,000 (dots) and N=500,000 (dash). The difference between the grand canonical result (solid) and the N=2,000 calculation is huge around 7 MeV (upper panel) but for N=100,000 and N=500,000 the results are so close to the grand canonical values that they are nearly indistinguishable in the scale of the upper panel. In the lower panel results for N=100,000 and N=500,000 are compared with grand canonical values. Even in this expanded scale the N=500,000 canonical results are indistinguishable in the curve from the grand canonical results.
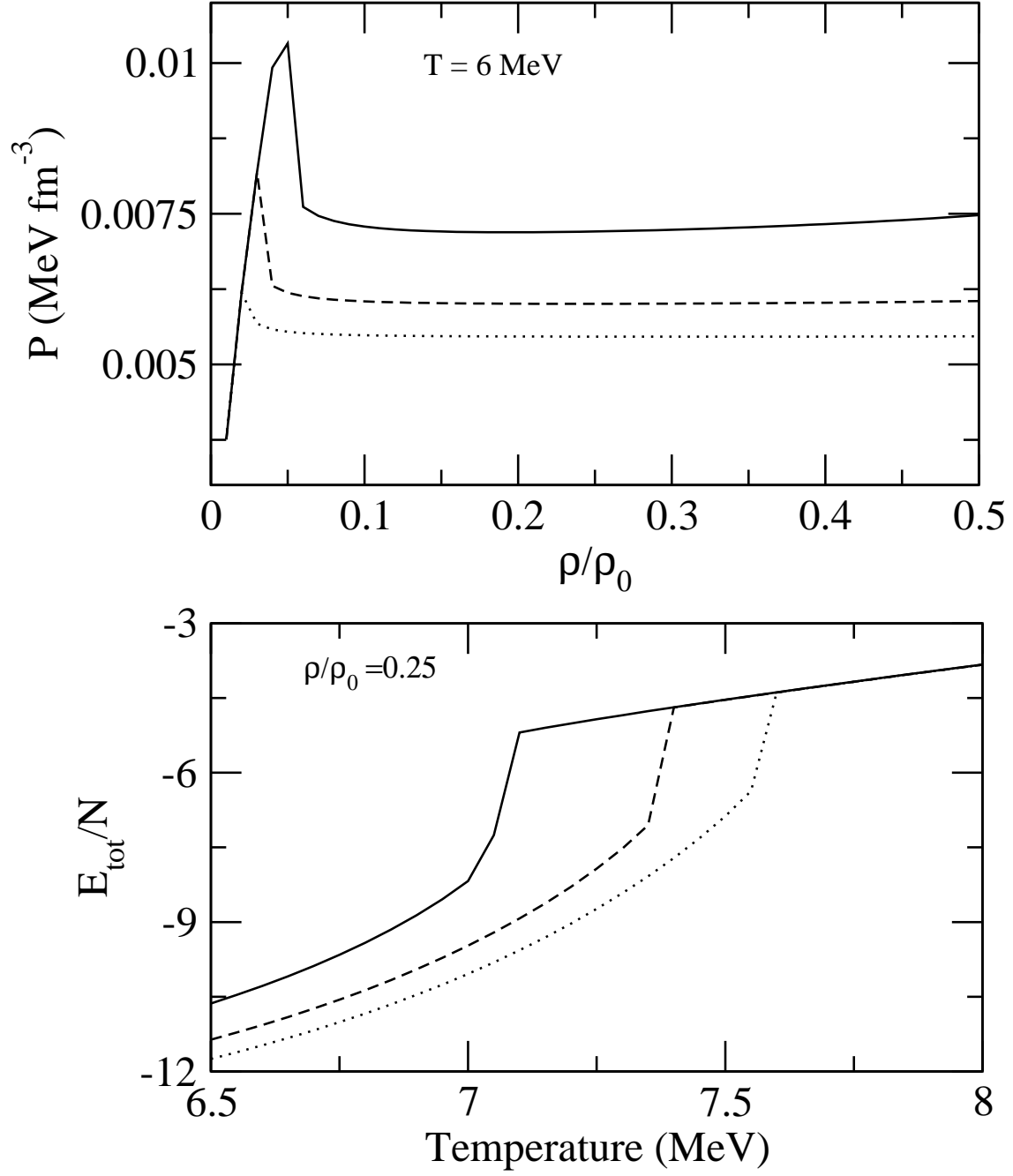
FIG. 3: Pressure and energy per particle for the canonical model of $N = k_{max}$ for N=2000 (solid), N=10,000 (dash) and N=50,000 (dot).
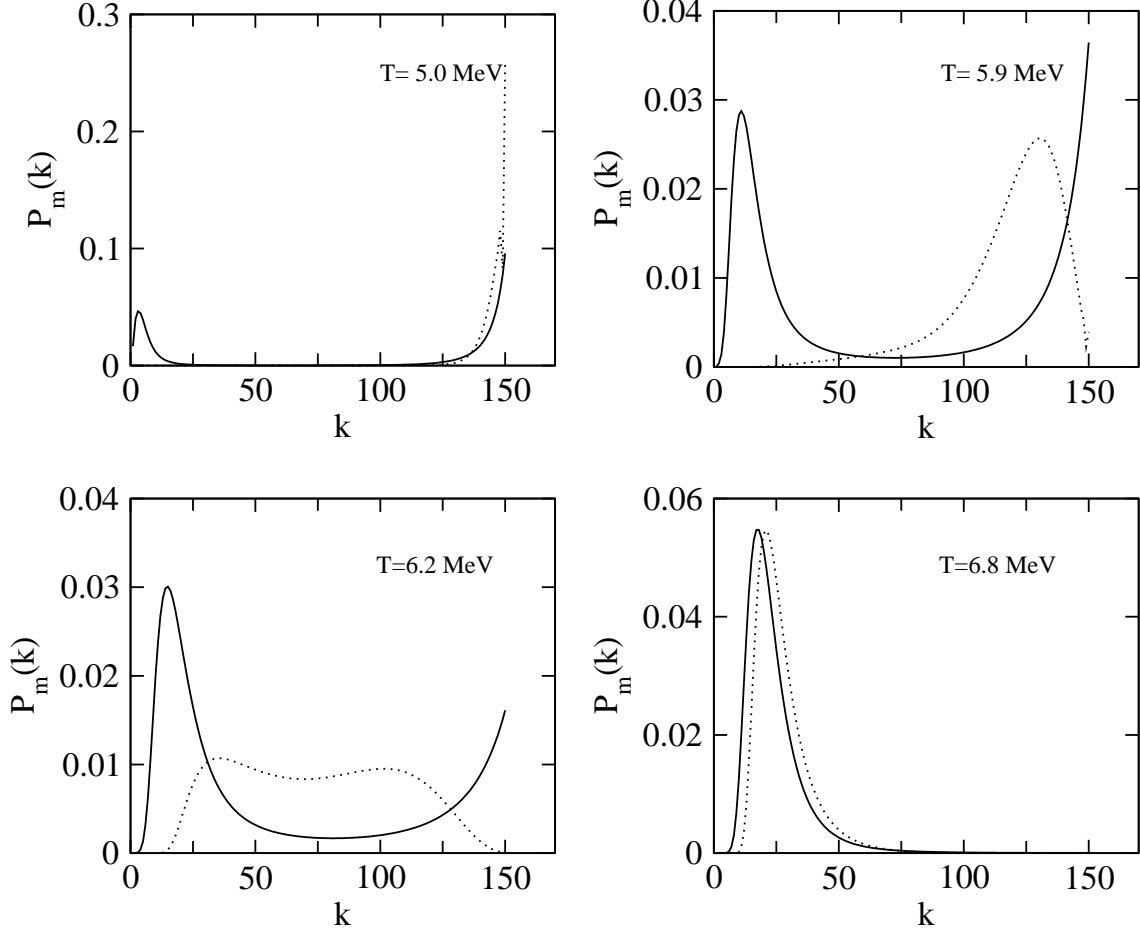
FIG. 4: Probability that the largest cluster has k nucleons plotted as a function of k in the grand canonical(solid) and the canonical model(dot). Here $N=150$ in the canonical model and in the grand canonical model the average value is set at $N=150$. The value of k_{max} is also 150. The density is fixed at $\rho/\rho_0 = 0.25$. In the grand canonical model bimodality is seen at about 5.9 MeV and in the canonical model this appears at about 6.2 MeV.
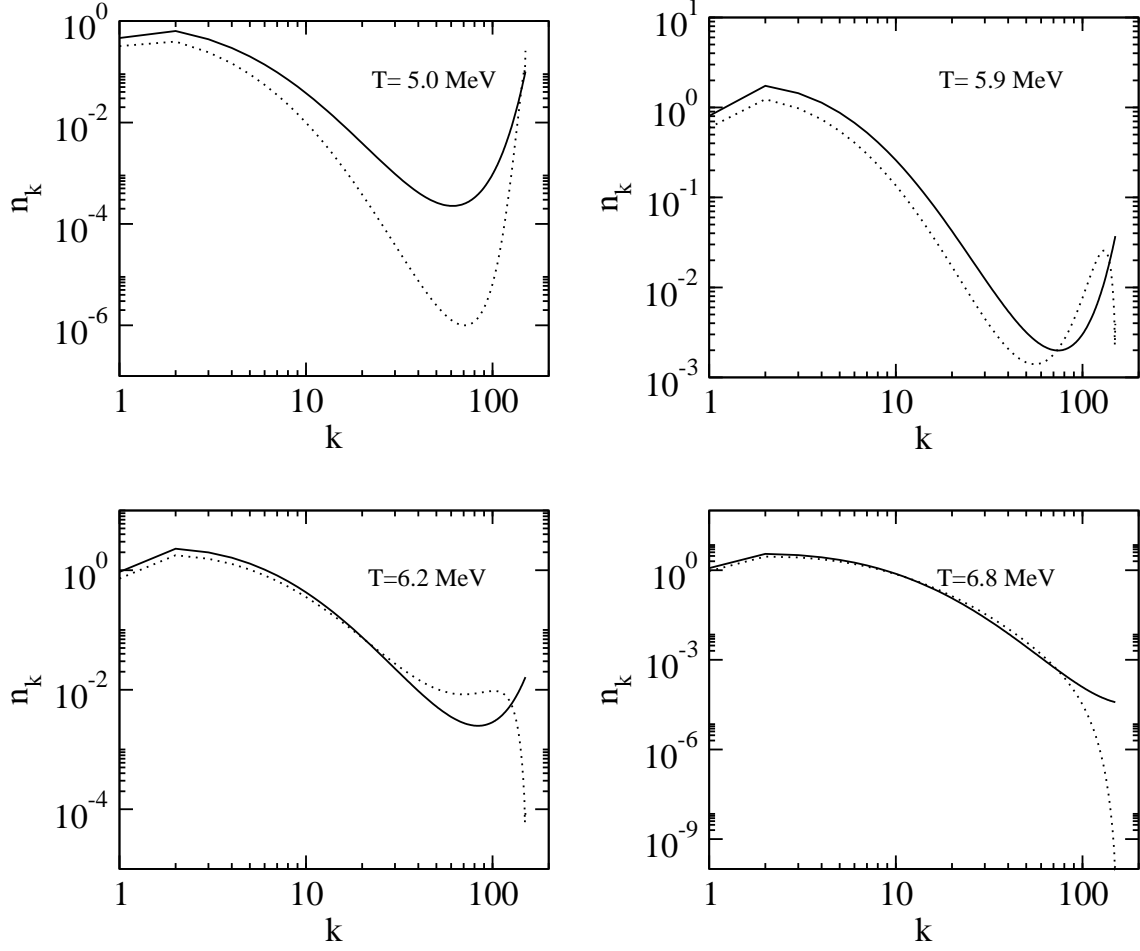
FIG. 5: For the same cases as above, the average multiplicity of each composite plotted as a function of mass number k. Note that the grand canonical results (solid) approximate the canonical results (dots) quite well at the highest temperature (except at very high mass numbers) but the agreement worsens as the temperature is lowered.