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Specific heat at constant volume in the thermodynamic model

C. B. Das,[1] S. Das Gupta,[1] and A. Z. Mekjian[2]
[1]*Physics Department, McGill University, Montréal, Canada H3A 2T8*
[2]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855, USA*
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A thermodynamic model for multifragmentation which is frequently used appears to give very different values for specific heat at constant volume depending upon whether canonical or grand canonical ensemble is used. The cause for this discrepancy is analyzed.

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The motivation for this work is just one puzzle. A thermodynamic model, often used for fitting data, appears to give very different answers for specific heat at constant volume depending upon whether the canonical or the grand canonical ensemble is used. We wish to resolve this issue. The relevant papers are Refs. [1] and [2]. Although for practical applications a much more sophisticated two component version of the model is used [3–5], here, as in [1,2] we use one kind of particle as in the original formulation [1]. If a system has A nucleons in a volume V at temperature T the system can break up into various composites which have a binding energy consisting of volume and surface energies. Excited states of the composite can also be included. Assuming that the break up takes place only according to the availability of phase space, it was shown in Ref. [1] that this problem for A nucleons can be solved numerically with arbitrary accuracy very easily. One can also solve the problem in a grand canonical ensemble [2,6]. We do not give any details here as they are given in many places including Refs. [1,2].

By specific heat we will always mean specific heat per particle. It was shown in the original paper [1] that for a fixed A, the total number of particles, and a fixed V, the specific heat as a function of temperature went through a maximum at a certain temperature which was labeled the boiling temperature. A numerical calculation which is rather easy and can be made sufficiently accurate showed that for a fixed $\rho\equiv A/V$ if we increase the number of particles the height of the peak rises and the width decreases. Since one sees no reason why this behavior should change at certain high value of A, it was concluded that the specific heat behaves like a δ function in the limit $A\rightarrow\infty$. There is a physics picture one can associate with this. Below the boiling temperature there is a blob of liquid. Just above the boiling temperature this blob disappears into a system of smaller composites and nucleons. Qualitatively, a δ function would emerge if a finite fraction rather than an infinitesimal fraction of the blob is converted into gas with an infinitesimal increase of temperature.

In Fig. 1 we show the specific heats in the canonical model for $\rho=\rho_0/2.7$ when $A=200$ and $A=2000$. All calculations shown here will be at this ρ. The grand canonical results are also shown in the figure. For grand canonical we solve

$$\rho=\sum_{k=1}^{k_m} k\exp(k\beta\mu)\tilde{\omega}_k, \tag{1}$$

where k_m is the number of nucleons in the largest cluster allowed in the system. Here

$$\tilde{\omega}_k=\frac{(2\pi mTk)^{3/2}}{h^3}\exp[a_v k-\sigma(T)k^{2/3}+kT^2/\epsilon_0] \quad \text{for } k>1$$
$$=\frac{(2\pi mT)^{3/2}}{h^3} \quad \text{for } k=1. \tag{2}$$

To do the grand canonical calculation for $A=2000$ we set k_m in the above equation at 2000. The average value of $\langle n_k\rangle$ is then given by

$$\langle n_k\rangle=\exp(k\beta\mu)\tilde{\omega}_k V, \tag{3}$$

where V is the appropriate value of 2000 nucleons at freeze-out, i.e., $V=2000\times 2.7/\rho_0$. Denoting $\langle n_k\rangle$ as the average number of composites which has k nucleons (i.e., the average number of trimers is $\langle n_3\rangle$) we have

$$\sum_{k=1}^{2000} k\langle n_k\rangle=2000. \tag{4}$$

It should be realized that all A's (up to ∞) are included in the grand canonical ensemble but setting $k_m=2000$ in Eq. (1) signifies that the largest cluster has 2000 nucleons. In terms of canonical partition functions one has

$$Q_{gr.can}=\sum_{K=0}^{\infty} \exp(\beta\mu K)Q_{K,k_m}, \tag{5}$$

where Q_{K,k_m} is the canonical partition function of K nucleons but with the restriction that the largest cluster has only k_m $(=2000)$ nucleons. The quantity $\beta\mu$ is known from solving Eq. (1) with $k_m=2000$. Similar arguments hold when $k_m=200$ but we will not discuss this case and concentrate only on $A=k_m=2000$.

Figure 1 shows that the specific heats in the canonical and the grand canonical models are very different. In both the models, the peak value of the specific heat increases when we go from 200 to 2000 particles and the widths decrease but the results are much more dramatic in the canonical model. Since $A=2000$ is a large number in the context of nuclear physics, we try to understand the cause of this difference. In particular, it is not obvious that the specific heat in the grand

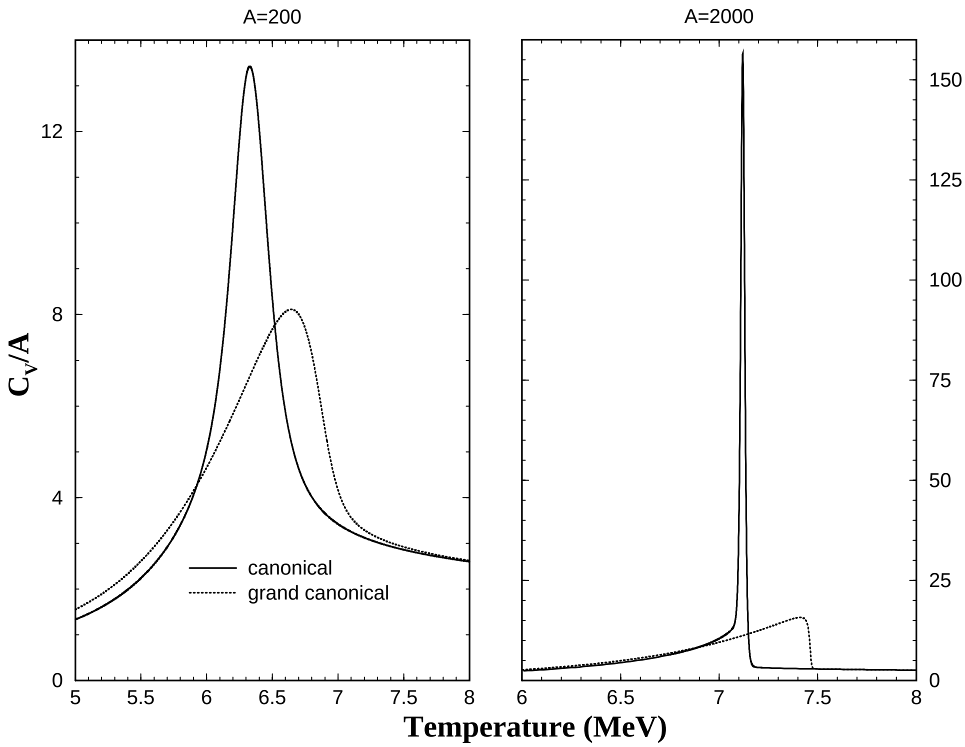

FIG. 1. Specific heat per particle at constant volume when the system has total number of particles 200 and 2000. The canonical and grand canonical values are shown.

canonical model will attain extraordinary heights and/or miniscule widths. We will show that the cause of discrepancy between the canonical and the grand canonical models is the very large fluctuation in the particle number in the grand canonical ensemble. We can investigate this in two ways, one more detailed than the other. We note that

$$Q_{gr.can}=\exp\left(\sum_{k=1}^{2000} V\tilde{\omega}_k e^{k\beta\mu}\right) \tag{6}$$

and we can calculate fluctuation exploiting the well-known relation

$$\frac{1}{\beta^2}\frac{\partial^2 \ln Q_{gr.can}}{\partial^2\mu}=\langle A^2\rangle-\langle A\rangle^2=\sum_{k=1}^{2000} k^2\langle n_k\rangle. \tag{7}$$

But we can also exploit the fact that we know Q_{K,k_m} up to rather large values of K and the value of $\beta\mu$ from the grand canonical calculation. Hence we can use Eq. (5) also to calculate fluctuation. For practical reasons, the upper limit of K will have to be cut off. The upper limit of K in the sum above was 10 000. Since we are investigating $A=2000$ one might *a priori* assume this should be adequate.

The fluctuations calculated from Eqs. (5) and (7) are shown in Fig. 2. One sees that there is a temperature above which the fluctuations are small. At these temperatures the grand canonical value of specific heat is indistinguishable from the canonical value. But as temperature is lowered, fluctuations grow rapidly and the results begin to diverge.

It is interesting to study fluctuations further. The probability of K particles being in the grand canonical ensemble is $\propto e^{K\beta\mu+\ln Q_K}$ [Eq. (5)] and we plot in Fig. 3 $\exp[\beta\mu(K-A)+\ln Q_K-\ln Q_A]$. This takes the value 1 at $K=A$ and in the normal picture of the grand canonical ensemble would drop

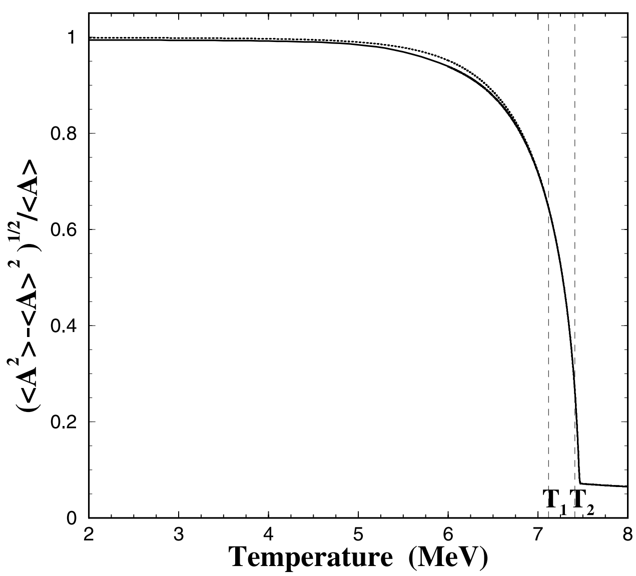

FIG. 2. Fluctuations calculated using Eqs. (5) and (7). The solid line corresponds to using Eq. (5) with K cut off at 10 000 and the dotted line corresponds to using Eq. (7). T_1 corresponds to the temperature where the specific heat maximizes in the canonical calculation and T_2 to the temperature of highest specific heat in the grand canonical calculation.

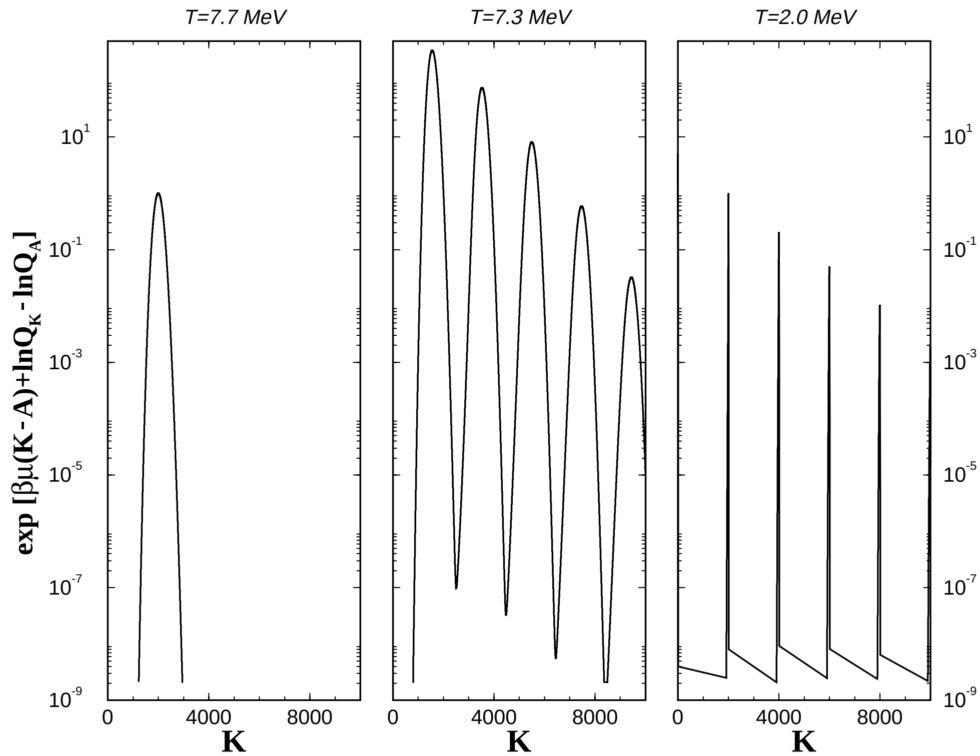

FIG. 3. These graphs show the spread of particle numbers in the grand canonical ensemble when the average particle number is 2000. The spread is very narrow at temperature 7.7 MeV but becomes quite wide at lower temperatures.

off rapidly on either side of A. This does happen at a temperature higher than the boiling temperature. The case at temperature $T=7.7$ MeV corresponds to a standard scenario. But the situation at temperature 7.3 MeV is drastically different. The probability does not maximize at $K=A$ but at a lower value. It is also very spread out with a periodic structure. At temperature 2.0 MeV, the probability of having no particle is higher than the probability of having $K=A$. We notice that here also there is a periodicity in the probability distribution. The periodicity is 2000 and is linked with the fact that in the case studied the largest composite has 2000 nucleons and at low temperatures, this composite will play a significant role.

We can now understand why the specific heat curve is so flat in the grand canonical ensemble in Fig. 1. Even though the average number of A is 2000, the ensemble contains large components of $K<A$ (thus have lower density and peaks of specific heat below 7.1 MeV) and $K>A$ (which have peaks at higher than 7.1 MeV). It is this smearing which makes the specific heat peak much lower and much wider.

In Fig. 4 we have shown canonical and grand canonical results for the total energy of 2000 particles. The canonical result suggests that starting from a low temperature, energy increases at a finite rate (implies a finite value of C_V), followed by a sudden rise (will lead to infinite specific heat), followed again by a regular behavior. Thus the transition region is marked by two different values of C_V with a δ function switched in between. In the grand canonical model for 2000 particles one sees only the discontinuity in the value of C_V. If one was calculating C_V directly in either the canonical or the grand canonical model and for a very large system there is indeed a δ function in C_V, one will miss the δ function since it has zero width. To see that there is indeed one, we should instead calculate the total energy and see that at a given temperature T there is a huge difference in the total energy for an infinitesimal increase in T.

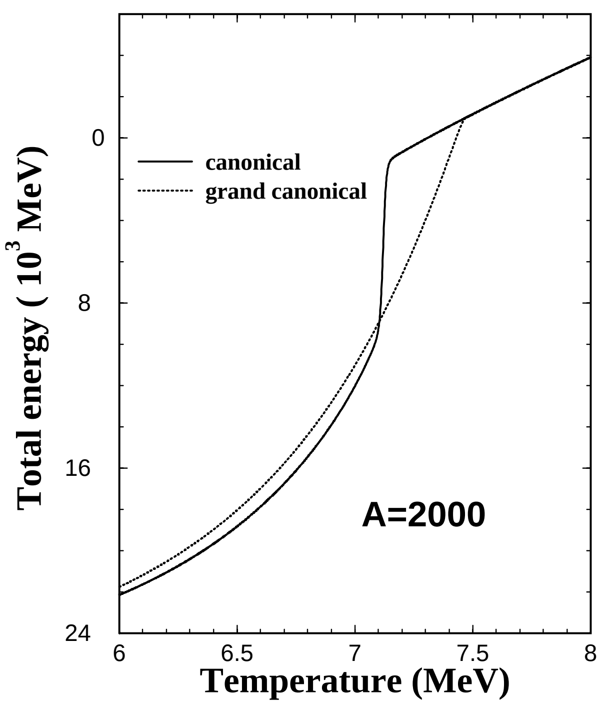

FIG. 4. Caloric curves in the canonical and the grand canonical models for a system of 2000 particles.

One might get the impression that for finite systems the use of a grand canonical ensemble is very dangerous. For many observables it is quite acceptable. However, a recent work shows [7] that interpreting data according to grand canonical ensemble can lead to a serious error in estimating temperature. It thus depends on the particular observable being calculated.

Returning briefly to the interesting periodicity seen in Fig. 3, it arises because at low temperatures it is advantageous for the system to form large clusters. In the example studied in Fig. 3 where the largest cluster size was 2000, at temperature 2 MeV when the system has 8000 nucleons, we have essentially four clusters, each of size 2000 (we are confining ourselves to canonical calculation of course). This becomes less precise at higher temperature. For example, at 6 MeV temperature if the system has 4100 nucleons, nearly 4000 of them are distributed in large clusters (more precisely, on an average, 3950.22 nucleons are bound in clusters of sizes between 1800 and 2000) and nearly 100 of them are in lighter clusters (149.78 on an average). If we now go to a system of 6100 nucleons, on an average 5940.22 are bound in very heavy clusters and 159.78 in lighter clusters. Approximately, at low temperatures, $\ln Q_{K+2000} \approx \ln Q_K + \ln(V\tilde{\omega}_{2000})$.

The low temperature periodic structure at $T=2$ MeV can be qualitatively understood using the following results. As $T \to 0$, the system will go to the largest cluster allowed, and in this case, $k_m = 2000$. For example, at $K = 10\,000$ (the total number of nucleons in the system) a result of five clusters of size 2000 follows. The mean number of cluster of size k_m $(=2000)$ is

$$\langle n_{k_m} \rangle = \omega_{k_m} \frac{Q_{K-k_m}}{Q_K}.$$

Also the factorial moment $\langle n_{k_m}(n_{k_m}-1)\rangle$ is given by

$$\langle n_{k_m}(n_{k_m}-1)\rangle = (\omega_{k_m})^2 \left(\frac{Q_{K-2k_m}}{Q_K} \right).$$

And in general,

$$\langle n_{k_m}(n_{k_m}-1)\cdots(n_{k_m}-n+1)\rangle = (\omega_{k_m})^n \left(\frac{Q_{K-nk_m}}{Q_K} \right). \quad (8)$$

Thus the points at 8000, 6000, 4000, 2000, and 0 can be related to the factorial moments of the n_{k_m} distributions as $T \to 0$. At $T=0$ these are $5\times4\times3\times2\times1, 5\times4\times3\times2, 5\times4\times3, 5\times4$, and 5 at $K=0, 2000, 4000, 6000$, and 8000, respectively. The heights of the peaks in Fig. 3 will be determined by

$$\frac{1}{\omega_m^{\;n}} \langle n_{k_m}(n_{k_m}-1)\cdots(n_{k_m}-n+1)\rangle \frac{Q_K}{Q_{k_m}} e^{\beta\mu[K-(n+1)k_m]}$$

as $T \to 0$. Even at $T=2$ MeV, this expression is very accurate.

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