On pressure versus density dependence in statistical multifragmentation models

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Abstract

We show that the statistical multifragmentation model with the standard parameterization of the free volume predicts a constant pressure as density approaches the normal nuclear density. This is contrary to the Raduta&Raduta result obtained by disregarding the center of mass constraint. It is demonstrated that in finite nuclear systems the partitions with small number of fragments play an important role.

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In recent years much efforts have been directed to investigating thermodynamical properties of finite nuclear systems (see e.g. refs. \cite{1}). In the paper \cite{2} the authors study the phase diagram of finite systems with a statistical model designed for describing nuclear multifragmentation. The authors’ model follows the theoretical prescriptions developed earlier in refs. \cite{3–5} and based on the assumption that fragments are formed at a low density freeze-out stage. Consequently, the thermodynamical characteristics calculated within such kind of models have adequate physical meaning at low densities only, e.g. \( \rho < \left( \frac{1}{2} - \frac{1}{3} \right) \rho_0 \) (\( \rho_0 \approx 0.15 \text{fm}^{-3} \) is the normal nuclear density), when individual fragments are singled out from the surrounding nuclear matter \cite{3, 4}. However, the authors of ref. \cite{2} have tried to apply their model for the higher densities \( \rho \to \rho_0 \) by removing the physical assumption that fragments do not overlap. They have found that the model predicts a Van der Waals kind of phase diagram. In particular, the pressure \( P \to \infty \) at \( \rho \to \rho_0 \), as seen from Fig. 3 of ref. \cite{2}. In this comment we want to demonstrate that this result can be misleading, even under assumption of overlapping fragments. Within the standard statistical treatment of finite systems, when the conservation laws are properly implemented, the pressure always remains finite, even in the limit \( \rho \to \rho_0 \).

In the statistical models \cite{2–5} the volume (density) affects the partition probabilities via so called free volume \( V_f \) determining the phase space available for the translational motion of fragments. It differs from the actual physical volume of the system \( V \) because of the finite size of the fragments and fragment-fragment interaction. In the standard canonical description

\footnote{1A comment on “Investigating the phase diagram of finite extensive and nonextensive systems” by Al.H. Raduta and Ad.R. Raduta, Phys. Rev. Lett. 87, 202701 (2001)}
of multifragmentation the free volume enters in the partition probabilities through the factor \((V_f/\lambda_T^3)^{N-1}\), where \(N\) is the number of fragments in the partition and \(\lambda_T = 2\pi\hbar/\sqrt{m_N T}\) is the thermal wavelength of nucleons at temperature \(T\). The exponent \((N - 1)\) comes from the integration over momenta and coordinates of fragments under constraints that total momentum and center of mass position are fixed for all partitions. These constraints are crucial for finite systems in contrast to the thermodynamic limit \((N \to \infty , V \to \infty , N/V = \text{const})\), where this factor is usually taken as \((V_f/\lambda_T^3)^N\). In the canonical ensemble, for a finite system with the number of nucleons \(A_0\), the free energy can be represented as

\[
F = -T \cdot \ln \left( \sum_{N=1}^{A_0} V_f^{N-1} C_N \right),
\]

where \(C_N\) is the volume-independent weight of \(N\)-fragment partitions which is influenced by combinatorial factors as well as by internal excitation of fragments and their interaction. For simplicity, below we disregard the Coulomb interaction in the system. In the microcanonical ensemble the structure of the statistical weights with respect to the volume will be practically the same, and thus our conclusions concerning the volume dependence of the pressure in the limit \(V_f \to 0\) will not change. Though the weights \(C_N\) can significantly vary from partition to partition, they are finite for any finite system. Therefore, the behavior of the free energy in the limit \(V_f \to 0\) is similar for different assumptions on the fragments’ relative motion in the freeze-out volume. To illustrate our point we use the excluded volume approximation \(V_f = V - V_0\), where \(V_0 = A_0/\rho_0\) is the normal nuclear volume of all fragments. In this approximation one gets straightforwardly:

\[
P = -\frac{\partial F}{\partial V} = T \frac{\sum_{N=2}^{A_0} (N - 1)V_f^{N-2} C_N}{\sum_{N=1}^{A_0} V_f^{N-1} C_N}.
\]

Now it is obvious that in the limit \(V \to V_0\) the pressure goes to a constant, \(P \to T \cdot (C_2/C_1) = \text{const}\). It is interesting to note that a similar behavior for this kind of model was also found in the thermodynamic limit [3]. In this case constant parts of pressure isotherms appear in the coexistence region of liquid and gaseous phases. And the liquid phase is represented by an infinite cluster which in a finite system would correspond to the compound-like nucleus.

We believe that the main reason of the \(P \to \infty\) behavior obtained in ref. [2] is in disregarding the center of mass constraint [3]. The unconstrained integration over coordinates of all fragments in the freeze-out volume results in a factor proportional to \(V_f^N\). If in eqs. (1) and (2) we take \(V_f^N\) instead of \(V_f^{N-1}\), we get formally \(P \sim 1/V_f\) at \(V \to V_0\), i.e. \(P \to \infty\). One can easily see that \(V_{\text{free}}\) adopted in ref. [3] (their eq. (4)) gives the same limiting behavior as \(V_f^N\).

For illustration, in Fig. 1 we show the phase diagram obtained with the canonical calculations for partitioning a one-component system containing \(A_0=100\) nucleons into all possible fragments characterized by the mass number \(A\) only. Contributions of all 190569292 partitions were calculated directly, in order to achieve the best accuracy [4]. We adopt the liquid-drop description for individual fragments disregarding the Coulomb interaction and

\[\text{Because of this and other approximations used in the model [3], depicting it as "exact" in comparison with other models does not seem justified.}\]
Figure 1: Pressure versus free volume (in units of normal nuclear volume) in multifragmentation of one component system with \(A_0=100\) nucleons calculated within the canonical ensemble. Solid lines are calculations taking into account the center-of-mass constraint in the fragmentation statistical weights, dashed lines correspond to a similar calculation but without this constraint. The temperatures (in MeV) are given by numbers at the curves.

Internal excitation of fragments. The statistical weight of a partition with \(N\) fragments with individual multiplicities \(N_A\) is taken as

\[
W(\{N_A\}) \sim \left(\frac{V_f}{\lambda_f^3}\right)^{N-1} \prod_A \frac{1}{N_A!} \left[ A^{3/2} \exp\left(\frac{B(A)}{T}\right) \right]^{N_A},
\]

where \(B(A) = a_V \cdot A - a_S \cdot A^{2/3}\) is the liquid-drop binding energy of fragment \(A\) with parameters \(a_V \approx a_S \approx 16\) MeV. In this case the pressure is \(P = T \cdot (\langle N \rangle - 1)/V_f\), where \(\langle N \rangle\) is the mean fragment multiplicity. It is seen that at large \(V_f\) the phase diagram is consistent with expectations for a gas system. Here the system disintegrates into many fragments and the fragment mass distribution falls off nearly exponentially with \(A\). By decreasing \(V_f\) we move into region where the partitions with low fragment multiplicity dominate. The mass distribution turns into "U-shape"-like one, which is associated with the phase transition.
Namely in this region the pressure has a slight "backbending" (at low temperatures) and then approaches a constant. Formally this behavior at small volumes sets in because probabilities of the channels with $N > 1$ are suppressed by factors $\propto V_f^{N-1}$. The compound nucleus (a partition with $N=1$) dominates in this case, however, it does not contribute to the pressure. This is a trivial consequence of the conservation laws: the compound nucleus is at rest in its center of mass frame. For $N > 1$ only relative momenta and positions of fragments have physical meaning.

We have also simulated the effect of non-conservation of the center-of-mass by introducing an additional factor $\propto V_f$ in the weights of all partitions in the formula (3). This effect is shown by dashed lines in Fig. 1, corresponding to the pressure $P = T \cdot \langle N \rangle / V_f$. This means that compound nucleus can "move" and "exert a pressure" in the freeze-out volume, and as a result $P \to \infty$ at $V_f \to 0$. Moreover, in this case the phase diagram looks like a Van der Waals one, that in fact does not correspond to the physical content of the model. Even in the region of large volumes relevant for the model this effect can considerably change many thermodynamical characteristics, such as the critical temperature or the caloric curve at constant pressure.

This example shows that phase diagrams of finite systems depend sensitively on physical assumptions adopted in the model. In particular, in the study of a liquid-gas type phase transition a careful treatment of the partitions with small multiplicities becomes extremely important. However, in order to investigate realistically the phase diagram at $\rho > \frac{1}{2} \rho_0$ it is necessary to introduce a really new physics in the statistical models, e.g. instead of the picture of individual fragments surrounded by the nucleon gas to consider the bubbles of the nuclear gas inside the nuclear matter.

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