Bimodality Phenomenon in Finite and Infinite Systems Within an Exactly Solvable Statistical Model

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We present a few explicit counterexamples to the widely spread belief about an exclusive role of the bimodal nuclear fragment size distributions as the first order phase transition signal. In thermodynamic limit the bimodality may appear at the supercritical temperatures due to the negative values of the surface tension coefficient. Such a result is found within a novel exactly solvable formulation of the simplified statistical multifragmentation model based on the virial expansion for a system of the nuclear fragments of all sizes. The developed statistical model corresponds to the compressible nuclear liquid with the tricritical endpoint located at one third of the normal nuclear density. Its exact solution for finite volumes demonstrates the bimodal fragment size distribution right inside the finite volume analog of a gaseous phase. These counterexamples clearly demonstrate the pitfalls of Hill approach to phase transitions in finite systems.

1 Introduction

Despite many efforts the phase transition (PT) thermodynamics of finite systems is far from being completed. Its consistent formulation remains a real theoretical challenge for the researchers working in statistical mechanics. On the other hand, nowadays it is of great practical importance since at intermediate and high energies the modern nuclear physics is dealing with the phase transformations of liquid-gas type occurring in finite or even small systems. The central issue of this field is related to a rigorous definition of finite volume analogs of phases.

The first attempt [1] to rigorously define the gaseous and liquid phases in finite systems was based on the properties of phases existing in infinite systems in which two phases coexist at phase equilibrium and generate two local maxima, i.e. a bimodality, of some order parameter. Each maximum is associated with a pure phase [1]. Since a few years ago such a concept of nuclear liquid-gas PT [2, 3] completely dominates in nuclear physics of intermediate energies. It considers the bimodal distributions as a robust signal of a PT in finite systems. However, this concept does not seem to be correct since in a finite system an analog of mixed phase is not just a simple mixture of two pure phases as it is explicitly shown within an exactly solvable statistical model [4, 5, 6]. The aim of this work is to demonstrate that in finite and infinite systems the bimodal distributions can appear without a PT and, hence, they cannot serve as robust signal of a PT in finite systems.

1.1 Constrained SMM with the compressible nuclear matter

The simplified statistical multifragmentation model (SMM) which has no Coulomb and no asymmetry energy was exactly solved in thermodynamic limit in [7], while its generalization constrained for finite systems, the CSMM, was solved in [4]. For a volume V the grand canonical partition of the CSMM can be identically written as [4, 5, 6]

$$\mathcal{Z}(V,T,\mu) \;=\; \sum_{\{\lambda_n\}} e^{\lambda_n V}\left[1 - \frac{\partial \mathcal{F}(V,\lambda_n)}{\partial \lambda_n}\right]^{-1}, \tag{1}$$

where the set of λ_n $(n = 0, 1, 2, 3, ..)$ are all the roots of the equation $\lambda_n \;=\; \mathcal{F}(V, \lambda_n)$.

The volume spectrum of our model $\mathcal{F}(V, \lambda)$ depends on the eigen volume $b = 1/\rho_0$ of a nucleon at the normal nuclear density $\rho_0 \simeq 0.17$ fm^3 taken at $T = 0$ and zero pressure, mass $m \simeq 940$ MeV, degeneracy factor $z_1 = 4$ of nucleons and it is defined as

$$\mathcal{F}(V,\lambda) = \left(\frac{mT}{2\pi}\right)^{\frac{3}{2}} z_1 \exp\left\{\frac{\mu - \lambda T b}{T}\right\} + \sum_{k=2}^{K(V)} \phi_k(T) \exp\left\{\frac{(p_L(T,\mu) - \lambda T)bk}{T}\right\} . \tag{2}$$

Here $\phi_{k>1}(T) \equiv \left(\frac{mT}{2\pi}\right)^{\frac{3}{2}} k^{-\tau} \exp\left[-\frac{\sigma(T)\ k^{\varsigma}}{T}\right]$ is a reduced distribution function of the k-nucleon fragment, τ is the Fisher topological exponent and $\sigma(T)$ is the T-dependent surface tension coefficient. Usually, the constant, parameterizing the dimension of surface in terms of the volume is $\varsigma = \frac{2}{3}$. In the expression for $\mathcal{F}(V, \lambda)$ the maximal size of fragment is denoted as $K(V)$. In the usual SMM [8] and in its simplified version SMM the nuclear liquid pressure $p_L^{SMM} = \frac{\mu + W(T)}{b}$ corresponds to an incompressible matter. Since this is in contradiction with the experimental heavy ions collisions data [9], here we analyze the following equation of state with non-zero compressibility

$$p_L = \frac{W(T) + \mu + a_\nu(\mu - \mu_0)^\nu}{b} \tag{3}$$

which contains an additional term to the usual SMM liquid pressure. Here an integer power is $\nu = 2$ or $\nu = 4$, $W(T) = W_0 + \frac{T^2}{W_0}$ denotes the usual temperature dependent binding energy per nucleon with $W_0 = 16$ MeV [7], while the constants $\mu_0 = -W_0$, $a_2 \simeq 1.233 \cdot 10^{-2}$ MeV^{-1} and $a_4 \simeq 4.099 \cdot 10^{-7}$ MeV^{-3} are fixed in order to reproduce the properties of normal nuclear matter, i.e. at vanishing temperature $T = 0$ and normal nuclear density $\rho = \rho_0$ the liquid pressure must be zero. Under a new ansatz for p_L the nuclear liquid of CSMM becomes compressible [6, 10]. A careful analysis of the proposed parameterization [10] shows that it is fully consistent with the L. van Hove axioms of statistical mechanics [11].

In addition to a more general parameterization of the bulk free energy of nuclear fragments we also consider a more general parameterization of the surface tension coefficient

$$\sigma(T) = \sigma_0 \left|\frac{T_{cep} - T}{T_{cep}}\right|^{\zeta} \mathrm{sign}(T_{cep} - T) , \tag{4}$$

with $\zeta = const \geq 1$, $T_{cep} = 18$ MeV and $\sigma_0 = 18$ MeV the SMM. In contrast to the Fisher droplet model [12] and the usual SMM [8], the CSMM surface tension (4) is negative above the critical temperature T_{cep}. An extended discussion on the validity of such a parameterization can be found in Refs. [5, 6].

1.2 Infinite system

In the thermodynamic limit, i.e. for $V \to \infty$ and $K(V) \to \infty$, in the CSMM there is always a single solution λ_0 of the equation $\lambda_n = \mathcal{F}(V \to \infty, \lambda_n)$, but it can be of two kinds [4]: either the gaseous pole $\lambda_0(T,\mu) = p_g(T,\mu)/T$ for $\mathcal{F}(V \to \infty, \lambda_0 - 0) < \infty$ or the liquid essential singularity $\lambda_0(T,\mu) = p_L(T,\mu)/T$ for $\mathcal{F}(V \to \infty, \lambda_0 - 0) \to \infty$.

This model has a PT which occurs when the gaseous pole is changed by the liquid essential singularity or vice versa. The PT curve $\mu = \mu_c(T)$ is a solution of the equation $p_g(T,\mu) = p_L(T,\mu)$, which is just the Gibbs criterion of phase equilibrium. The properties of a PT are defined only by the liquid phase pressure $p_L(T,\mu)$ and by the temperature dependence of surface tension $\sigma(T)$. The phase diagram of the present model in thermodynamic limit in the plane of baryonic chemical potential μ and temperature T is shown in the left panel of Fig. 1.

1.3 Finite system

The treatment of the model for finite volumes is more complicated, since the roots λ_n of (1) have not only the real part R_n, but an imaginary part I_n as well ($\lambda_n = R_n + iI_n$). Therefore, equation for λ_n can be cast as a system of coupled transcendental equations for R_n and I_n

$$R_n = \sum_{k=1}^{K(V)} \phi_k(T) \; \exp\left[\frac{Re(\nu_n)\, k}{T}\right] \cos(I_n b k)\,, \tag{5}$$

$$I_n = - \sum_{k=1}^{K(V)} \phi_k(T) \; \exp\left[\frac{Re(\nu_n)\, k}{T}\right] \sin(I_n b k)\,, \tag{6}$$

where for convenience we introduced the following set of the effective chemical potentials ν_n

$$\nu_n \equiv \nu(\lambda_n) = p_l(T,\mu) b - (R_n + iI_n) b T\,, \tag{7}$$

and the reduced distribution for nucleons $\phi_1(T) = \left(\frac{mT}{2\pi}\right)^{\frac{3}{2}} z_1 \exp((\mu - p_l(T,\mu)b)/T)$.

Consider the real root ($R_0 > 0, I_0 = 0$), first. The real root $\lambda_0 = R_0$ of the CSMM exists for any T and μ. From (1) and (5) for $R_n = R_0$ and $I_0 = 0$ one can see that TR_0 is a constrained grand canonical pressure of the mixture of ideal gases with the chemical potential ν_0. Hence, a single real solution $\lambda_0 = R_0$ with $I_0 = 0$ of the system (5, 6) corresponds to a gaseous phase (for more details see [7]). If for some thermodynamic parameters we have a real solution λ_0 and any finite number $n = 1, 2, 3, ...$ of the complex conjugate pairs of roots $\lambda_{n\geq 1}$, then such a system corresponds to a finite volume analog of mixed phase [7]. Note that, each pair of complex conjugate roots $\lambda_{n\geq 1}$ represents a metastable state with a complex value of chemical potential ν_n. Since $\nu_{n1} \neq \nu_{n2\neq n1}$ these metastable states are not in a true chemical equilibrium with the gas and with each other. A finite system analog of a liquid phase corresponds to an infinite number of the complex roots of the system (5, 6), but in finite system it exists at infinite pressure only. Using these definitions, one can build up the finite system analog of the $T - \mu$ phase diagram (see the right panel of Fig.1).

Therefore, in contrast to assumptions of Refs. [2, 3], in finite systems the pure liquid phase cannot exist at finite pressures. Instead, in finite system and finite pressures we are dealing with the finite volume analogs of gaseous or mixed phases [4].

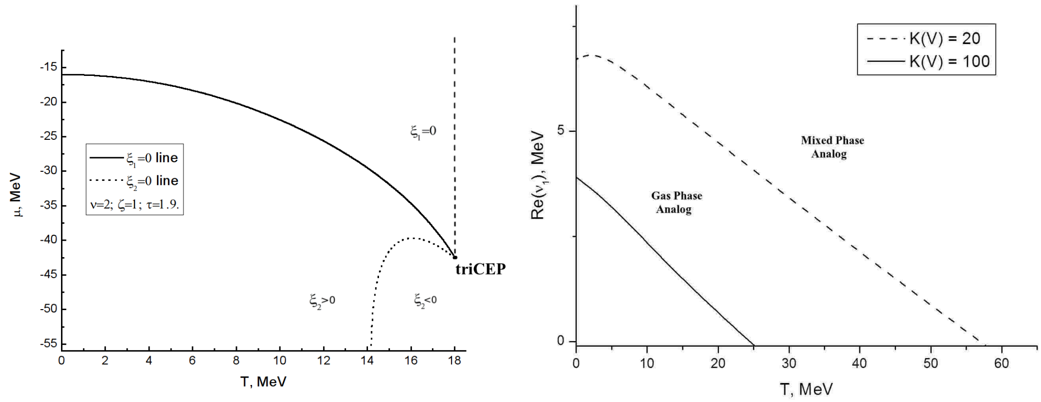

Figure 1: **Left panel:** Phase diagram in $T-\mu$ plane for the case $\nu = 2$, $\tau = 1.9$ with tricritical point at temperature $T_{cep} = 18$ MeV in thermodynamic limit. The solid line corresponds to the 1-st order PT, the dashed line shows the 2-nd order PT, while at the dotted line the surface tension coefficient vanishes. **Right panel:** the finite volume analog of the phase diagram in $T - Re(\nu_1)$ plane for given values of $K(V) = 20$ (dashed curve) and $K(V) = 100$ (solid curve). Below each of these phase boundaries there exists a gaseous phase only, but at and above each curve there are three or more solutions of the system (5, 6).

1.4 Bimodality phenomenon in finite and infinite systems

In this section we discuss another typical mistake of the approaches [2, 3] based on the bimodal properties of the first order PT in finite systems. The authors of [2, 3] implicitly assume that, like in the infinite systems, in finite systems there exist exactly two 'pure' phases and they exactly correspond to two peaks in the bimodal distribution of the order parameter. As two counterexamples to these assumptions we present the bimodal fragment distributions obtained for an infinite system at the supercritical temperature where the surface tension coefficient is negative (the left panel of Fig.2) and the one obtained inside the finite volume analog of a gaseous phase corresponding to positive values of the effective chemical potential ν_0 (the right panel of Fig.2). As one can see from Fig.2, in contrast to expectations of [2, 3], the bimodal fragment distributions occur without a PT.

2 Conclusions

A novel version of the CSMM is presented here. Its detailed analysis is performed in order to clarify an origin of the bimodality appearing both in finite and in infinite systems. An exact analytical solution of the present model allows us to perform a robust analysis of the fragment size distributions in the regions where there is and there is no PT. It is shown that the fragment size distribution can be bimodal-like inside of the finite volume analog of gaseous phase. Also we demonstrate that a bimodal fragment size distribution can be caused by negative values of the surface tension and, hence, it is not a robust signal of PT existence in finite systems.

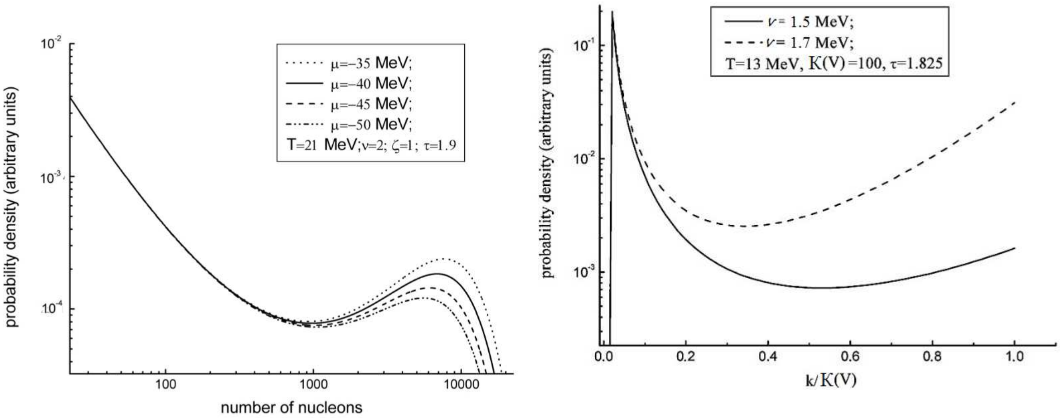

Figure 2: **Left panel:** Fragment size distributions of the model are shown for a fixed temperature $T = 21$ MeV and four values of the baryonic chemical potential μ for an infinite system. This region of phase diagram is characterised by the negative surface tension coefficient which prevents an existing of a PT. **Right panel:** Bimodal distributions existing inside the finite system analog of gaseous phase for a fixed temperature $T = 13$ MeV and different values of the effective chemical potential ν_0. Even in the region of fragments gas we observe a bimodal like shape of the fragment distribution. The maximal size of nuclear fragment is $K(V)=k=100$ nucleons.

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