

# STATISTICAL MULTIFRAGMENTATION MODEL WITHIN THE EXTENDED MORPHOLOGICAL THERMODYNAMIC APPROACH

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## Abstract

On the basis of morphological thermodynamics we develop an exactly solvable version of statistical multifragmentation model for the nuclear liquid-gas phase transition. It is shown that the hard-core repulsion between spherical nuclei generates only the bulk (volume), surface and curvature parts of the free energy of the nucleus, while the Gaussian curvature one does not appear in the derivation. The phase diagram of nuclear liquid-gas phase transition is studied for a truncated version of the developed model.

*Keywords:* morphological thermodynamics, induced surface and surface tensions, equation of state, nuclear liquid-gas phase transition, statistical multifragmentation

## Introduction

Over the past 20 years the morphological thermodynamics approach has been extensively developed in condense matter physics to describe the behavior of dense 3- and 2-dimensional fluids [1]. It is based on the Hadwiger theorem [2, 3] and can be formulated as: the total free energy decrease  $-\Delta\Omega$  of a convex rigid body  $\mathbf{B}$  inserted into a fluid can be completely described by four thermodynamic characteristics such as the system pressure  $p$ , the mean surface tension coefficient  $\Sigma$ , the mean curvature tension coefficient  $K$  and the bending rigidity coefficient  $\Psi$ , i.e.

$$-\Delta\Omega = pv_B + \Sigma s_B + Kc_B + \Psi x_B, \quad (1)$$

where the quantities  $v_B, s_B, c_B, x_B$  are, respectively, the volume of  $\mathbf{B}$ , its surface, the mean curvature integrated over the surface of rigid body and the mean Gaussian curvature also integrated over the surface of  $\mathbf{B}$ . The last two quantities are defined via the two local principal curvature radii  $R_{c1}$  and  $R_{c2}$  as  $c_B = \int_{\partial\mathbf{B}} d^2r \frac{1}{2} \left[ \frac{1}{R_{c1}} + \frac{1}{R_{c2}} \right]$  and  $x_B = \int_{\partial\mathbf{B}} d^2r \frac{1}{R_{c1}R_{c2}}$  (the Euler characteristic). Such a treatment is usually justified, if the system exists relatively away from the critical point and, simultaneously, from wetting and drying transitions [1, 3].

Independently to the morphological thermodynamics, its analogue in the grand canonical ensemble widely known as the induced surface and curvature tensions (ISCT) equation of state (EoS) was developed recently in [4, 5, 6, 7, 8]. This cutting-edge approach was successfully applied in Ref. [4] to model the properties of the one and two-component mixtures of classical hard

spheres and hard discs. The ISCT EoS was develop not only for classical particles, but also for quantum ones [5, 6] and for relativistic particles that experience the Lorentz contraction [8]. Moreover, very recently the grand canonical ensemble formulation of morphological thermodynamics was also worked out for very small system volumes of about 100 fm<sup>3</sup>, which are typical for the nuclear reactions [7].

Here we reformulate an exactly solvable version of the statistical multifragmentation model (SMM) [9, 10] using the postulates of morphological thermodynamics. This is a highly nontrivial extension of the morphological thermodynamics to an infinite number of degrees of freedom which are the nuclear clusters of  $k$  nucleons with  $k = 1, 2, 3, \dots$ . Besides, this is an important extension of the usual morphological thermodynamics to a new domain, namely to the vicinity of (tri)critical endpoint of nuclear matter. In addition, here we discuss the possible extension of the suggested model which will improve the description of liquid phase of nuclear matter at high packing fractions.

The work is organized as follows. In Sect. 1 we heuristically derive the ISCT EoS for the SMM using the requirements of morphological thermodynamics. In Sect. 2 a truncated version of the ISCT EoS for the SMM is discussed, while our results are summarized in Conclusions.

## 1. Derivation of ISCT EoS for SMM

We start our discussion from the one-component gas of Boltzmann particles with hard-core repulsion. The potential energy  $U(r)$  between such particles depends on the distance  $r$  between their centers as

$$U(r) = \begin{cases} \infty & \text{for } r \leq 2R \\ 0 & \text{for } r > 2R \end{cases}, \quad (2)$$

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and, hence, the quantity  $R$  is the hard-core radius. Since the typical temperatures of the nuclear liquid-gas phase transition (PT) are below 20 MeV, i.e. much smaller than the nucleon mass, one can safely use the non-relativistic treatment [9, 10].

In the grand canonical ensemble the pressure of Van der Waals (VdW) EoS of particles with hard-core repulsion can be written as

$$p = T\varphi(T) \exp\left(\frac{\mu - ap}{T}\right), \quad (3)$$

$$\varphi(T) = g \int \frac{d^3k}{(2\pi\hbar)^3} \exp\left(-\frac{\mathbf{k}^2}{2mT}\right), \quad (4)$$

where  $T$  is the system temperature and  $\mu$  is its chemical potential. In Eq. (3) the parameter  $a = \int d^3r [1 - \exp(-U(r)/T)] \equiv 4v \equiv v + sR \equiv v + \frac{1}{2}sR + \frac{1}{2}cR^2$  denotes the second virial coefficient, where  $v = \frac{4}{3}\pi R^3$  denotes the eigenvolume of particles, while  $s = 4\pi R^2$  and  $c = 4\pi R$  denote, respectively, their eigen-surface and double eigenperimeter. In Eq. (4)  $\varphi(T)$  is the thermal density of particles with mass  $m$  and the degeneracy factor  $g$ .

According to morphological thermodynamics [1, 2, 3] the free energy of rigid particle should be written as  $f = vp + s\Sigma + cK$  and, hence, the grand canonical pressure (3) should be generalized as

$$p = T\varphi(T) \exp\left(\frac{\mu - (vp + s\Sigma + cK)}{T}\right), \quad (5)$$

but this equation should be supplemented by the equations for the surface tension coefficient  $\Sigma$  and the curvature tension one  $K$  induced by hard-core repulsion. In Ref. [4] one can find how the equations for  $\Sigma$  and  $K$  can be derived rigorously. Here we generalize the heuristic derivation of Ref. [10] by including into our treatment the curvature tension coefficient  $K$ .

Since in the SMM the nuclear clusters can consist of any positive number of nucleons, we consider the system of  $N$ -sorts particles of the hard-core radii  $R_k$ , with  $k = 1, 2, \dots, N \rightarrow \infty$ . The virial expansion of the gas pressure up to the second order can be cast as [10]

$$p = T \sum_{k=1}^N \varphi_k e^{\frac{\mu_k}{T}} \left[ 1 - \sum_{n=1}^N a_{kn} \varphi_n e^{\frac{\mu_n}{T}} \right], \quad (6)$$

$$\varphi_n(T) = g_n \int \frac{d^3k}{(2\pi\hbar)^3} \exp\left[-\frac{\mathbf{k}^2}{2m_n T}\right] = g_n \left[ \frac{m_n T}{2\pi\hbar^2} \right]^{\frac{3}{2}}, \quad (7)$$

where  $\varphi_n(T)$  is the thermal density of particles of the degeneracy  $g_n$ , mass  $m_n = nm_1$  with  $m_1 = 940$  MeV. The second virial coefficient  $a_{kn}$  which has the meaning of excluded volume per particle is given by

$$\begin{aligned} a_{kn} &= \frac{2}{3}\pi(R_k + R_n)^3 = \\ &= \frac{2}{3}\pi(R_k^3 + 3R_k^2 R_n + 3R_k R_n^2 + R_n^3). \end{aligned} \quad (8)$$

Consider first the low densities at which the expansion (6) is valid. Substituting the second virial coefficients (8) into Eq. (6) and regrouping the terms with the same

powers of  $R_k$  of a  $k$ -nucleon fragment, we can write

$$\begin{aligned} p = T \sum_{k=1}^N \varphi_k e^{\frac{\mu_k}{T}} \left[ 1 - \frac{4}{3}\pi R_k^3 \sum_{n=1}^N \varphi_n e^{\frac{\mu_n}{T}} - \right. \\ \left. - \frac{4\pi R_k^2}{2} \sum_{n=1}^N R_n \varphi_n e^{\frac{\mu_n}{T}} - \frac{4\pi R_k}{2} \sum_{n=1}^N R_n^2 \varphi_n e^{\frac{\mu_n}{T}} \right]. \end{aligned} \quad (9)$$

Apparently, for low densities each sum in Eq. (9) can be identified as

$$\sum_{n=1}^N \varphi_n e^{\frac{\mu_n}{T}} = \frac{p}{T}, \quad (10)$$

$$\frac{1}{2} \sum_{n=1}^N R_n \varphi_n e^{\frac{\mu_n}{T}} = \frac{\Sigma}{T}, \quad \frac{1}{2} \sum_{n=1}^N R_n^2 \varphi_n e^{\frac{\mu_n}{T}} = \frac{K}{T}. \quad (11)$$

The approximation (10) is valid for the low densities, since defining the second virial coefficient with the help of Eqs. (10) and (11), one modifies the third and higher virial coefficients which at these densities can be neglected. Therefore, substituting Eqs. (10) and (11) into the right hand side of Eq. (9), we obtain

$$\begin{aligned} p = T \sum_{k=1}^N \varphi_k e^{\frac{\mu_k}{T}} \times \\ \times \left[ 1 - \frac{4}{3}\pi R_k^3 \frac{p}{T} - 4\pi R_k^2 \frac{\Sigma}{T} - 4\pi R_k \frac{K}{T} \right] \simeq \end{aligned} \quad (12)$$

$$\simeq T \sum_{k=1}^N \varphi_k \exp\left[\frac{\mu_k - v_k p - s_k \Sigma - c_k K}{T}\right], \quad (13)$$

where in the last step of derivation we used the approximation  $1 - x \simeq \exp(-x)$  which is valid for low densities. In Eq. (13) we introduced the eigenvolume  $v_k = \frac{4}{3}\pi R_k^3$ , the eigen-surface  $s_k = 4\pi R_k^2$  and double eigenperimeter  $c_k = 4\pi R_k$  of the  $k$ -nucleon cluster with the hard-core radius  $R_k = R_1 k^{\frac{1}{3}}$  and  $R_1 \simeq 0.72$  fm.

Comparing Eqs. (5) and (13), we conclude that the latter one is a multicomponent version of the grand canonical pressure obtained in accord with the morphological thermodynamics. Using the same logic, we can generalize the expressions (11) for the coefficients of induced surface tension  $\Sigma$  and induced curvature tension  $K$  in accordance with the morphological thermodynamics and write

$$\Sigma = TA \sum_{k=1}^N R_k \varphi_k \exp\left[\frac{\mu_k - v_k p - s_k \Sigma - c_k K}{T}\right], \quad (14)$$

$$K = TB \sum_{k=1}^N R_k^2 \varphi_k \exp\left[\frac{\mu_k - v_k p - s_k \Sigma - c_k K}{T}\right], \quad (15)$$

where the coefficients  $A = 0.5$  and  $B = 0.5$  later on will be considered as the adjustable parameters. In Refs. [4, 5, 6] it is shown that the system (13)-(15) is the VdW EoS which can be improved at high densities by inserting the set of parameters  $\{\alpha_k > 1\}$  and  $\{\beta_k > 1\}$  for each sort of particles into Eqs. for  $\Sigma$  and  $K$  as

$$\frac{\Sigma}{T} = A \sum_{k=1}^N R_k \varphi_k \exp\left[\frac{\mu_k - v_k p - \alpha_k s_k \Sigma - c_k K}{T}\right], \quad (16)$$

$$\frac{K}{T} = B \sum_{k=1}^N R_k^2 \varphi_k \exp\left[\frac{\mu_k - v_k p - \alpha_k s_k \Sigma - \beta_k c_k K}{T}\right], \quad (17)$$

which can be now extrapolated to any particle number densities. The principal difference of the obtained system (13)-(15) from the ones analyzed previously in Refs. [4, 5, 6] is that the degeneracy factor  $g_k$  of  $k$ -nucleon cluster is a statistical partition of the ensemble of clusters with the same mean volume  $v_k$ , but different shapes [10, 11, 12]. For  $k \gg 1$  this internal partition of large clusters of  $k$ -nucleons can be expressed in terms of the mean surface  $s_k$  [10, 11, 12]. Here we generalize the internal partition  $g_k$  to high pressures by including the mean double perimeter  $c_k$  in accord with the morphological thermodynamics and write it as

$$g_{k \gg 1} = \frac{1}{k^{\tau + \frac{3}{2}}} \exp \left[ \frac{v_k p_L - s_k \sigma_0(T) - c_k K_0(T)}{T} \right], \quad (18)$$

where  $p_L$  is the pressure of nuclear liquid (internal pressure of large custers),  $\sigma_0(T)$  is the  $T$  dependent proper surface tension coefficient and  $K_0(T)$  is proper curvature tension coefficient, while  $\tau$  is the Fisher exponent [11]. Eq. (18) is a generalization of the expression found in Ref. [10] which allows us to account for the effects of proper curvature tension. It is necessary to stress that without inclusion of the proper curvature tension coefficient in Eq. (18) it is impossible to compensate the induced surface tension one and, hence, in such a model the (tri)critical point does not exist.

Existence of the curvature and even of the Gaussian curvature terms in the Bethe-Weizsäcker formula for the binding energy of large nuclei at zero temperature is discussed for about fifty years [13, 14, 15], but, so far, there was no definite conclusion reached about its existence. In this work we derived the induced curvature tension coefficient similarly to the surface one, but our analysis shows no room to introduce the Gaussian curvature terms. Therefore, we do not consider it for the SMM.

The  $T$ -dependence of both the proper and the induced surface tension coefficients of nuclear clusters are discussed for a few decades [9, 12, 14, 15, 16]. Although there exist several parameterizations for  $\sigma_0(T)$  and for  $\sigma_{tot} = \sigma_0(T) + \Sigma$ , we use the linear  $T$ -dependence of  $\sigma_0(T)$ , since it is obtained within an exactly solvable model for the surface partition [12]. Besides, a thorough analysis of experimental data performed in Ref. [16] shows that there is a wide range of temperatures at which the total surface tension coefficient  $\sigma_{tot}$  is a linear function of  $T$ . Below it is shown that even a truncated version of the ISCT EoS provides an existence of two regions of such a  $T$ -dependence of  $\sigma_{tot}$ .

## 2. Truncated ISCT EoS for low densities

The system (13)-(15) can be used to describe the properties of nuclear matter at high particle number densities and to clarify a principal question what is the value of total surface tension coefficient  $\sigma_{tot}$  at supercritical temperatures. In the famous Fisher droplet model [11] and in the solvable version of SMM [9] it is assumed that  $\sigma_{tot} = 0$  for  $T \geq T_{cep}$ , while in the SMM with compressible nuclear liquid it is argued that  $\sigma_{tot} < 0$  for  $T > T_{cep}$ , while  $\sigma_{tot} = 0$  at  $T = T_{cep}$ . Apparently, this problem can be solved only experimen-

tally. On the other hand, it is expected that the critical point of nuclear matter is located at particle number densities about  $\rho_c \simeq \frac{\rho_0}{3}$  [10, 14], where  $\rho_0 \simeq 0.16 \text{ fm}^{-3}$  is the normal nuclear density. Therefore, to study the properties of nuclear matter at the vicinity of critical endpoint it is sufficient to work out a simpler EoS.

Using the fact that at low particle number densities the contributions of surface and curvature tensions to the second virial coefficient are the same, i.e.  $\sum_{k=1}^N \varphi_k e^{\frac{\mu_k}{T}} R_k^2 \Sigma = \sum_{k=1}^N \varphi_k e^{\frac{\mu_k}{T}} R_k K$ , one can account for the curvature tension effects by doubling down the contribution of  $\Sigma$  on the right hand side of Eqs. (13) and (16) [10]. Hence, instead of the system (13)-(15) one can write

$$p = T \sum_{k=1}^N \varphi_k \exp \left[ \frac{\mu_k - v_k p - s_k \Sigma}{T} \right], \quad (19)$$

$$\Sigma = T \sum_{k=1}^N R_k \varphi_k \exp \left[ \frac{\mu_k - v_k p - \alpha s_k \Sigma}{T} \right], \quad (20)$$

where the parameter  $\alpha = 1.5$  is chosen according to Ref. [10]. To parameterize the degeneracy of large clusters according to Eq. (18) and to account for the fact that nucleons have no proper surface tension, we assume the thermal density of  $k$ -nucleon fragments to be as

$$\varphi_1 = z_1 \left[ \frac{mT}{2\pi\hbar^2} \right]^{\frac{3}{2}} \exp \left[ -\frac{\sigma_0(T)}{T} \right] \quad (21)$$

$$\varphi_{k \geq 2} = \frac{1}{k^\tau} \left[ \frac{mT}{2\pi\hbar^2} \right]^{\frac{3}{2}} \exp \left[ \frac{(k p_L V_1 - \mu_k) - \sigma_0(T) k^{\frac{2}{3}}}{T} \right], \quad (22)$$

where the chemical potential of a  $k$ -nucleon fragment is  $\mu_k = k\mu$  [9, 10], and value of  $\tau = 1.9$  provides the existence of 1-st order PT for  $T < T_{cep}$  [10]. In Eq. (21)  $z_1 = 4$  is the degeneracy factor of nucleons. For  $k \geq 1$  one finds  $v_k = V_1 k = \frac{4}{3} \pi R_k^3$  with  $V_1 = \frac{1}{\rho_0}$ . For  $\varphi_{k \geq 2}$  the binding energy of nucleons is included into the pressure of liquid phase

$$p_L = \frac{\mu + W_F(T) + W_0 + a_\nu [\mu + W_0]^\nu}{V_1}, \quad (23)$$

with  $\nu = 2, 3, 4$ . The binding energy per nucleon is given by  $W(T) = W_0 + W_F(T)$ , where  $W_0 = 16 \text{ MeV}$  is the bulk binding energy per nucleon at  $T = 0$  and  $W_F(T) = \frac{T^2}{\varepsilon_0}$  (with  $\varepsilon_0 = 16 \text{ MeV}$ ) accounts for the Fermi motion of nucleons inside a nucleus at  $T > 0$  [9]. The constant  $a_\nu$  in Eq. (23) should be found by requiring that at  $T = 0$  and normal nuclear density  $\rho_L = \frac{\partial p_L}{\partial \mu} = \rho_0$  the liquid pressure is zero [10]. For definiteness, in this work we assume that  $a_2 = 1.261 \cdot 10^{-2} \text{ MeV}^{-1}$  and  $\nu = 2$ . Hence now the system (19), (20) becomes

$$\frac{p}{T} = \left[ \frac{mT}{2\pi\hbar^2} \right]^{\frac{3}{2}} \sum_{k=1}^N \frac{b_k}{k^\tau} \exp \left[ \frac{(p_L - p) V_1 k - (\Sigma + \sigma_0) k^{\frac{2}{3}}}{T} \right], \quad (24)$$

$$\frac{\Sigma}{3V_1 T} = \left[ \frac{mT}{2\pi\hbar^2} \right]^{\frac{3}{2}} \sum_{k=1}^N \frac{b_k}{k^{\tau - \frac{1}{3}}} \exp \left[ \frac{(p_L - p) V_1 k - (\alpha \Sigma + \sigma_0) k^{\frac{2}{3}}}{T} \right], \quad (25)$$

where the degeneracies  $b_k$  are defined as  $b_1 = 4 \exp \left[ \frac{-W(T)}{T} \right]$  and  $b_{k > 1} = 1$ . The proper surface ten-

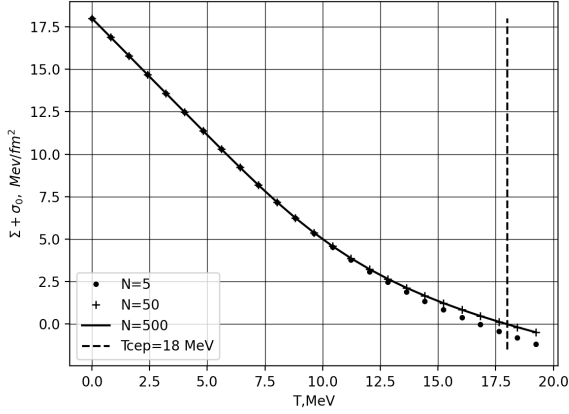


Fig. 1. Total surface tension coefficient  $\sigma_{tot}(\mu_c(T), T)$  at the PT curve  $\mu_c(T)$  as a function of  $T$  is shown for several sizes of largest nucleus  $N$ . A vertical line defines the critical temperature  $T_{cep} = 18$  MeV.

sion coefficient  $\sigma_0 = \sigma_{01} - \sigma_{02} \frac{T}{T_{cep}}$  is chosen according to the exact result found for the surface partition [12], where  $\sigma_{01} = 18$  MeV,  $\sigma_{02} = 24.76$  MeV,  $T_{cep} = 18$  MeV.

Assuming in Eqs. (24, 25) that  $p = p_L$ , one obtains the equations for the PT curve

$$\frac{p_L}{T} = \left[ \frac{mT}{2\pi\hbar^2} \right]^{\frac{3}{2}} \sum_{k=1}^N \frac{b_k}{k^{\tau}} \exp\left[ -\frac{(\Sigma + \sigma_0)}{T} k^{\frac{2}{3}} \right], \quad (26)$$

$$\frac{\Sigma}{3V_1 T} = \left[ \frac{mT}{2\pi\hbar^2} \right]^{\frac{3}{2}} \sum_{k=1}^N \frac{b_k}{k^{\tau - \frac{1}{3}}} \exp\left[ -\frac{(\alpha\Sigma + \sigma_0)}{T} k^{\frac{2}{3}} \right]. \quad (27)$$

Solving Eq. (27) for  $\Sigma$  and substituting it into Eq. (26), one gets the pressure  $p_c = p_L$  at the PT curve. Then Eq. (23) for  $\mu$  with  $\nu = 2$  can be written as

$$\mu^2 + \mu(1 + 2a_2 W_0) + W(T) + a_2 W_0^2 - p_c V_1 = 0. \quad (28)$$

Solving Eq. (28) for  $\mu$ , one obtains  $\mu_c(T)$  at the PT curve. The  $T$ -dependence of total surface tension coefficient  $\sigma_{tot}(\mu_c(T), T) = \Sigma + \sigma_0$  is shown in Fig. 1, while the function  $\mu_c(T)$  is presented in Fig. 2. From Fig. 1 one can see that  $\sigma_{tot}(\mu, T)$  vanishes at  $T = T_{cep} = 18$  MeV even for a small size of largest nucleus  $N = 50$ , although the true PT exists only for  $N \rightarrow \infty$ .

In Fig. 2 the solutions  $\mu_c(T)$  of Eq. (28) are shown. It is evident that the upper curve describes the gas-liquid PT curve for nuclear matter, while the lower one corresponds to anti-matter.

## Conclusions

In this work we develop an exactly solvable version of statistical multifragmentation model for nuclear liquid-gas PT using the requirements of morphological thermodynamics. By evaluating the second virial coefficients we explicitly demonstrate that the hard-core repulsion between spherical nuclei generates only the bulk (volume), surface and curvature parts of the free energy of nuclei and does not produce the Gaussian curvature one. For a truncated version of the developed ISCT EoS we studied the  $T - \mu$  phase diagram of nuclear liquid-gas PT for several sizes of largest nucleus.

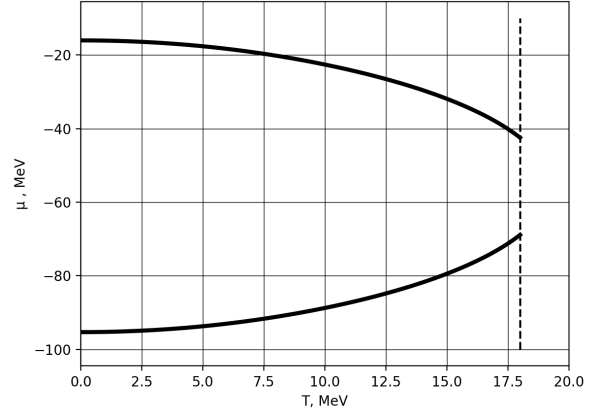


Fig. 2. The PT curves  $\mu_c(T)$  in the plane of temperature  $T$  and nuclear chemical potential  $\mu$ .

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