Exact Solution of the Statistical Multifragmentation Model and Liquid-Gas Phase Transition in Nuclear Matter

K.A. Bugaev\(^1,2\), M.I. Gorenstein\(^1,2\), I.N. Mishustin\(^1,3,4\) and W. Greiner\(^1\)

\(^1\) Institut für Theoretische Physik, Universität Frankfurt, Germany
\(^2\) Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine
\(^3\) The Kurchatov Institute, Russian Research Center, Moscow, Russia
\(^4\) The Niels Bohr Institute, University of Copenhagen, Denmark

(November 24, 2018)

An exact analytical solution of the statistical multifragmentation model is found in thermodynamic limit. The system of nuclear fragments exhibits a 1-st order liquid-gas phase transition. The peculiar thermodynamic properties of the model near the boundary between the mixed phase and the pure gaseous phase are studied.

**Key words:** Nuclear matter, 1-st order liquid-gas phase transition, mixed phase thermodynamics

21.65.+f, 24.10. Pa, 25.70. Pq

---

Nuclear multifragmentation is one of the most interesting and widely discussed phenomena in intermediate energy nuclear reactions. The statistical multifragmentation model (SMM) (see [13] and references therein) was recently applied to study the relationship of this phenomenon to the liquid-gas phase transition in nuclear matter [1, 14]. Numerical calculations within the canonical ensemble exhibited many intriguing peculiarities of the finite multifragment system. However, the investigation of the system’s behavior in the thermodynamic limit is still missing. Therefore, there is no rigorous proof of the phase transition existence, and the phase diagram structure of the SMM is unknown yet. In the present paper an exact analytical solution of the SMM is found within the grand canonical ensemble. The self-consistent treatment of the excluded volume effects is an important part of our study.

The system states in the SMM are specified by the multiplicity sets \(\{n_k\}\) (\(n_k = 0, 1, 2, \ldots\)) of \(k\)-nucleon fragments. The partition function of a single fragment with \(k\) nucleons is [1]:

\[
\omega_k = V (mT_k/2\pi)^{3/2} z_k ,
\]

where \(k = 1, 2, \ldots, A\) (\(A\) is the total number of nucleons in the system), \(V\) and \(T\) are, respectively, the volume and the temperature of the system, \(m\) is the nucleon mass. The first two factors in \(\omega_k\) originate from the non-relativistic thermal motion and the last factor, \(z_k\), represents the intrinsic partition function of the \(k\)-fragment. For \(k = 1\) (nucleon) we take \(z_1 = 4\) (4 internal spin-isospin states) and for fragments with \(k > 1\) we use the expression motivated by the liquid drop model (see details in Ref. [1]):

\[
\omega_k = \exp(-f_k/T) ,
\]

with fragment free energy:

\[
f_k = -[W_0 + (2/\epsilon_o) k + \sigma(T) k^{2/3}] .
\]

Here \(W_0 = 16\) MeV is the bulk binding energy per nucleon, \(T^2/\epsilon_o\) is the contribution of the excited states taken in the Fermi-gas approximation (\(\epsilon_o = 16\) MeV) and \(\sigma(T)\) is the surface tension which is parameterized in the following form:

\[
\sigma(T) = \sigma_o [(T_c^2 - T^2)/(T_c^2 + T^2)]^{5/4} ,
\]

with \(\sigma_o = 18\) MeV and \(T_c = 18\) MeV (\(\sigma = 0\) at \(T \geq T_c\)). The canonical partition function (CPF) of nuclear fragments in the SMM has the following form:

\[
Z_{A}^{\text{id}}(V, T) = \sum_{\{n_k\}} \prod_{k=1}^{A} \frac{\omega_k^{n_k}}{n_k!} \delta(A - \sum_k k n_k) .
\]  (1)

In Eq. (1) the nuclear fragments are treated as point-like objects. However, these fragments have non-zero proper volumes and they should not overlap in the coordinate space. In the excluded volume (Van der Waals) approximation this is achieved by substituting the total volume \(V\) in Eq. (1) by the free (available) volume \(V_f = V - b \sum_k k n_k\), where \(b = 1/\rho_o\) (\(\rho_o = 0.16\) fm\(^{-3}\) is the normal nuclear density). Therefore, the corrected CPF becomes:

\[
Z_A(V, T) = Z_{A}^{\text{id}}(V - b A, T) .
\]

This is a simplified version of the SMM, e.g. the symmetry and Coulomb contributions are neglected. However, its investigation appears to be of principal importance for studies of the liquid-gas phase transition.

The calculation of \(Z_A(V, T)\) is difficult because of the constraint \(\sum_k k n_k = A\). This difficulty can be partly avoided by calculating the grand canonical partition function:

\[
Z(V, T, \mu) = \sum_{A=0}^{\infty} \exp \left( \frac{A \mu}{k_B T} \right) Z_A(V, T) \Theta(V - b A) ,
\]  (2)

where chemical potential \(\mu\) is introduced. The calculation of \(Z\) is still rather difficult. The summation over \(\{n_k\}\) sets in \(Z_A\) cannot be performed analytically because of additional \(A\)-dependence in the free volume \(V_f\) and the restriction \(V_f > 0\). The problem can be solved by in-
Introducing the so-called isobaric partition function (IPF) which is calculated in a straightforward way:

\[
\hat{Z}(s, T, \mu) = \int_0^\infty dV \exp(-sV) \frac{Z(V, T, \mu)}{s - F(s, T, \mu)},
\]

(3)

where

\[
F(s, T, \mu) = \left(\frac{mT}{2\pi}\right)^{3/2} \frac{z_1 \exp\left(\frac{\mu - sbT}{T}\right)}{s} + \sum_{k=2}^{\infty} k^{3/2} \exp\left(\frac{(\nu - sbT)k - \sigma k^{2/3}}{T}\right),
\]

(4)

with \(\nu \equiv \mu + W_\omega + T^2/\epsilon_\omega\). In the thermodynamic limit \(V \to \infty\) the pressure of the system is defined by the farthest-right singularity, \(s^*(T, \mu)\), of the IPF \(\hat{Z}(s, T, \mu)\) (see Ref. [7] for details):

\[
p(T, \mu) = T \lim_{V \to \infty} \frac{\ln Z(V, T, \mu)}{V} = T s^*(T, \mu).
\]

(5)

The study of the system’s behavior in the thermodynamic limit is therefore reduced to the investigation of the singularities of \(\hat{Z}\).

FIG. 1. Phase diagram in the \((T, \rho)\)-plane. The mixed phase and pure gaseous phase boundary is shown by the solid line. The pure liquid phase (shown by crosses) corresponds to the fixed density \(\rho = \rho_0\). Point C is the critical point, at \(T > T_c\) only the pure gaseous phase exists.

The IPF (3) has two types of singularities: 1) the simple pole singularity defined by the equation \(s_g(T, \mu) = F(s_g, T, \mu)\); 2) the singularity of the function \(F\) itself at the point \(s_l(T, \mu) = \nu/7b\) where the coefficient in linear over \(k\) terms of the exponent in Eq. (3) is equal to zero.

The simple pole singularity corresponds to the gaseous phase where pressure \(p_g = Ts_g\) is determined by the transcendental equation: \(p_g(T, \mu) = T F(p_g/T, T, \mu)\). The singularity \(s_l(T, \mu)\) of the function \(F\) defines the liquid pressure: \(p_l(T, \mu) = Ts_l(T, \mu) = \nu/b\). Here the liquid is represented by an infinite fragment with \(k = \infty\).

In the region of the \((T, \mu)\)-plane where \(\nu < bp_g(T, \mu)\) the gaseous phase is realized \((p_g > p_l)\), while the liquid phase dominates at \(\nu > bp_g(T, \mu)\). The liquid-gas phase transition occurs when the two singularities coincide, i.e. \(s_g(T, \mu) = s_l(T, \mu)\). As \(F\) in Eq. (3) is a monotonously decreasing function of \(s\) the necessary condition for the phase transition is that the function \(F\) is finite in its singular point \(s_l\). This condition requires \(\sigma(T) > 0\) and, therefore, \(T < T_c\). Otherwise, \(F(s_l, T, \mu) = \infty\) and the system is always in the gaseous phase as \(s_g > s_l\).

At \(T < T_c\) the system undergoes a 1-st order phase transition across the line \(\mu^* = \mu^*(T)\) defined by the condition of coinciding singularities: \(s_l = s_g\). The baryonic density \(\rho\) in the liquid and gas phases is given by the following formulae, respectively: \(\rho_l \equiv (\partial p_l/\partial \mu)_T = 1/b\), \(\rho_g \equiv (\partial p_g/\partial \mu)_T = \rho_{id}/(1 + bp_{id})\), where the function \(\rho_{id}\) is the density of point-like nuclear fragments with shifted, \(\mu \to \mu - bp_g\), chemical potential:

\[
\rho_{id}(T, \mu) = \left(\frac{mT}{2\pi}\right)^{3/2} \frac{z_1 \exp\left(\frac{\mu - bp_g}{T}\right)}{s} + \sum_{k=2}^{\infty} k^{3/2} \exp\left(\frac{(\nu - bp_g)k - \sigma k^{2/3}}{T}\right).
\]

(6)

A similar expression for \(\rho_g\) within the excluded volume model for the pure nucleon gas was obtained in Ref. [8]. The phase transition line \(\mu^*(T)\) in the \((T, \mu)\)-plane corresponds to the mixed liquid and gas states. This line is transformed into the finite mixed-phase region in the \((T, \rho)\)-plane shown in Fig. 1. The baryonic density in the mixed phase is a superposition of the liquid and gas baryonic densities: \(\rho = \lambda \rho_l + (1 - \lambda)\rho_g\), where \(\lambda\) is a fraction of the system’s volume occupied by the liquid inside the mixed phase. Similar linear combinations are also valid for the entropy density \(s\) and the energy density \(\varepsilon\) with \(i = l, g\) \(s_i = (\partial p_i/\partial T)_\mu\), \(\varepsilon_i = T (\partial p_i/\partial T)_\mu + \mu (\partial p_i/\partial \mu)_T - p_i\).

Inside the mixed phase at constant density \(\rho\) the parameter \(\lambda\) has a specific temperature dependence shown in Fig. 2: from an approximately constant value \(\rho/\rho_0\) at small \(T\) the function \(\lambda(T)\) drops to zero in a narrow vicinity of the boundary separating the mixed phase and the pure gaseous phase. Such an abrupt decrease of \(\lambda(T)\) near this boundary causes a strong increase of the energy density as a function of temperature. This is evident from Fig. 3 which shows the caloric curves at different baryonic densities. One can clearly see a plateau-like behavior. As a consequence this leads to a sharp peak in the specific heat per nucleon at constant density,
\[ c_\rho(T) \equiv \left( \frac{\partial \varepsilon}{\partial T} \right)_\rho / \rho, \] shown in Fig. 4.

![Fig. 2](image1.png)

**FIG. 2.** Volume fraction \( \lambda(T) \) of the liquid inside the mixed phase is shown as a function of temperature for fixed nucleon densities \( \rho/\rho_0 = 1/6, 1/3, 1/2, 2/3, 5/6 \) (from bottom to top).

The peculiar thermodynamic property of the considered model is a finite discontinuity of \( c_\rho(T) \) at the boundary of the mixed and gaseous phases seen in Fig. 4. This finite discontinuity is due to the fact that \( \lambda(T) = 0 \), but \( (\partial \lambda / \partial T)_\rho \neq 0 \) at this boundary inside the mixed phase (see Fig. 2). It should be emphasized that the energy density is continuous at the boundary of the mixed phase and the gaseous phase, hence the sharpness of the peak in \( c_\rho \) is entirely due to the strong temperature dependence of \( \lambda(T) \) near this boundary. Therefore, in contrast to the expectation in Refs. [4,5], the maximum value of \( c_\rho \) remains finite and the peak width in \( c_\rho(T) \) is not zero in the thermodynamic limit considered in our study.

![Fig. 3](image2.png)

**FIG. 3.** Temperature as a function of energy density per nucleon (caloric curve) is shown for fixed nucleon densities \( \rho/\rho_0 = 1/6, 1/3, 1/2, 2/3 \).

![Fig. 4](image3.png)

**FIG. 4.** Specific heat per nucleon as a function of temperature at fixed nucleon density \( \rho/\rho_0 = 1/3 \). The dashed line shows the finite discontinuity of \( c_\rho(T) \) at the boundary of the mixed and gaseous phases.

In conclusion, the simplified version of the SMM is solved analytically in the grand canonical ensemble. The progress is achieved by reducing the description of phase transitions to the investigation of the isobaric partition function singularities. The model clearly demonstrates a 1-st order phase transition of the liquid-gas type. The considered system has peculiar properties near the boundary of the mixed and gaseous phases seen in the behavior of the specific heat.

**Acknowledgments.** The authors are thankful to A.S. Botvina, Ph. Chomaz, D.H.E. Gross, A.D. Jackson and J. Randrup for useful discussions. We are thankful to the Alexander von Humboldt Foundation and DFG, Germany for the financial support. The research described in this publication was made possible in part by Award No. UP1-2119 of the U.S. Civilian Research & Development Foundation for the Independent States of the Former Soviet Union (CRDF).

[1] J.P. Bondorf, A.S. Botvina, A.S. Iljinov, I.N. Mishustin, K.S. Sneppen, Phys. Rep. 257 (1995) 131.
[2] D.H.E. Gross, Phys. Rep. 279 (1997) 119.
[3] K.C. Chase and A.Z. Mekjian, Phys. Rev. C 52 (1995) R2339.
[4] S. Das Gupta and A.Z. Mekjian, Phys. Rev. C 57 (1998) 1361.
[5] S. Das Gupta, A. Majumder, S. Pratt and A. Mekjian, nucl-th/9903007 (1999).
[6] M.I. Gorenstein, V.K. Petrov and G.M. Zinovjev, Phys. Lett. 327B 106 (1981) 327.
[7] M.I. Gorenstein, W. Greiner and S.N. Yang, J. Phys. G 24 (1998) 725.
[8] D. H. Rischke, M. I. Gorenstein, H. Stöcker and W. Greiner, Z. Phys. C 51, 485 (1991).