Inhomogeneous 2D Lennard–Jones Fluid: Theory and Computer Simulation

R. Khordad*

Department of Physics, College of Sciences, Yasouj University, Yasouj, 75914-353, Iran

(Received July 17, 2012; revised manuscript received August 20, 2012)

Abstract *In this work, thermodynamical properties of a two-dimensional (2D) Lennard–Jones (LJ) fluid are studied. Here, to increase the accuracy of our theoretical calculations, the correlation functions in three-particle level (triplet) are applied. To obtain the triplet correlation functions, the Attard's source particle method is extended to 2D systems. In the Attard's procedure, the inhomogeneous Ornstein–Zernike (OZ) equation is solved using the Treizenberg–Zwanzwig (TZ) expression and a closure relation like the hypernetted-chain (HNC) approximation. In the present work, we also have performed the Monte Carlo (MC) simulation. The theoretical results are in fairly agreement with the MC simulation. Also, our results show that the approach proposed here is suitable to study the 2D LJ fluid.*

PACS numbers: 61.05.-a, 61.25.Em, 61.30.Cz
Key words: Lennard–Jones fluid, correlation functions, computer simulation, three-particle level

1 Introduction

The prediction of physical properties of two-dimensional (2D) fluids from information about molecular shapes and intermolecular interactions is an important goal of condensed matter physics. In the past two decades, considerable progresses have been made in the understanding of the behavior of 2D fluids at the molecular level by considering simplified potential models. In general, potential models can be classified into two groups according to the type of interaction between the molecules.[1−2]

In one group, molecules are treated as hard particles (purely repulsive) with a given shape such as hard sphere, hard ellipsoid, hard spherocylinder, hard disk, and hard ellipses.[2−7] In another group, molecules are treated as soft particles with spherical or non-spherical shapes.[2,8−11] The models include explicitly both the repulsive and attractive contributions through a convenient function of the translational and orientational degrees of freedom of the molecules. It is worth mentioning that the Lennard–Jones (for spherical particles)[2,8−9] and the Gay–Berne (for spherical particles)[11] potential models play the important roles in studying fluids.

2D fluids are interesting both from a purely theoretical and from an experimental point of view. There are examples of real systems that behave effectively as 2D fluids. The monolayers adsorbed on solid substrates[12] and surfactants adsorbed on an air/water interface[13] are examples of the 2D systems.

There are several theoretical procedures to study physical properties of 2D fluids. One of the most important procedures is the integral equations method.[2−6] Over the last two decades, integral equations method of classical equilibrium statistical mechanics has intensively been studied. This method has been used successfully to describe the thermodynamical properties and structure of simple and multi-component fluids. Examples of these fluids are the hard sphere fluid,[14−15] the hard core Yukawa fluid,[16−17] water,[18−19] hard ellipsoid fluid,[20−21] hard ellipses fluid,[6−7,22] hard disk fluid,[23−24] and 2D LJ fluid.[25−28]

The important role of triplet correlation functions has already been evidenced in several aspects of simple fluids. For example, the triplet correlation functions have been used in the characterization of fluid structure in systems like water, freezing transition of liquids, and the critical behavior of adsorbed fluids.[29−32] It is to be noted that in the systems, the pair distribution functions do not provide enough information. Therefore, we expect to obtain improved results by the triplet correlation functions instead of the pair correlation functions.

In this work, the 2D LJ fluid is studied in two phases. We have used the integral equations method and obtained triplet correlation functions for calculating the thermodynamical properties of this fluid. For this purpose, we have applied the inhomogeneous Ornstein–Zernike (OZ) equation, the Treizenberg–Zwanzwig (TZ) expression, and hypernetted-chain (HNC) approximation. To solve the OZ equation, we also used the rotational invariants in two dimensions. In addition, we have performed the Monte Carlo (MC) simulation for this system and compared with the theoretical calculations.

This article is organized as follows: In Sec. 2, the calculation method of the correlation functions in three-particle level is presented. In Sec. 3, the MC simulation technique is briefly described. For brevity, only the main steps of the simulation technique are presented here. In Sec. 4, the re-

*E-mail: khordad@mail.yu.ac.ir

sults are discussed. Finally, the conclusion is presented in Sec. 5.

2 Theory

In the late eighties, Attard described a source particle method to determine the triplet distribution functions in three dimensions.[33−34] Attard extended the inhomogeneous OZ equation to the study of triplet correlation functions using the Percus's source particle method.[35] Until then, the study of inhomogeneous integral equations had mostly focused in confined fluids.

Here, we extend the Attard's method for the 2D systems and obtain the triplet distribution function of 2D LJ fluid. The 2D LJ potential can be written as

$$u_{\rm LJ}(r) = 4\epsilon\Big[\Big(\frac{\sigma}{r}\Big)^{12} - \Big(\frac{\sigma}{r}\Big)^{6}\Big], \tag{1}$$

where ϵ sets the energy scale (the LJ energy parameter) and σ the length scale (the LJ size parameter). Also r is the center-center distance between two molecules.

To obtain the triplet correlation functions we consider a 2D inhomogeneous fluid with the inhomogeneity caused by an atom fixed at the origin. Therefore, the triplet distribution function of a uniform fluid is simply related to the inhomogeneous pair distribution function in the presence of the source particle. In the following, we briefly express the required equations that define our method. Also, we explain our computational algorithm and numerical results.

2.1 *The HNC3 Approximation*

It is to be noted that in 2D LJ fluid, the atoms interact with circularly symmetric pair potential, $u(1,2) = u(r_{12})$. Therefore, one can use the source particle method for determining the triplet distribution function. The external potential representing the atom fixed at the origin is given by

$$V(1) = V(r_1) = u(r_1)\,. \tag{2}$$

Note that the singlet density of a circularly inhomogeneous fluid is a function of the distance from the origin, $\rho(1) = \rho(r_1)$, and the inhomogeneous pair correlation functions depend only on the distances of the two particles from the origin and their mutual angle.

$$h(1,2) = h(r_1, r_2, \theta_1, \theta_2) = h(r_1, r_2, \theta_{12})\,, \tag{3}$$

$$c(1,2) = c(r_1, r_2, \theta_1, \theta_2) = c(r_1, r_2, \theta_{12})\,. \tag{4}$$

The 2D OZ equation can be written as[2,7]

$$h(r_1, r_2, \theta_{12}) = c(r_1, r_2, \theta_{12}) + \int \mathrm{d}\boldsymbol{r}_3 c(r_1, r_3, \theta_{13}) \times \rho(r_3) h(r_3, r_2, \theta_{32})\,, \tag{5}$$

where $h \equiv g - 1$ is the total correlation function, g is the radial distribution function, c is the direct correlation function, and ρ is the singlet density profile. The surface element in the polar coordinates is $\mathrm{d}\boldsymbol{r} = r\,\mathrm{d}r\,\mathrm{d}\theta$.

The rotational invariant basis in two-dimensional is given by[36]

$$f(r_1, r_2, \theta_{12}) = f(1,2) = \sum_{m,n=-\infty}^{\infty} f^{mn}(r_1, r_2)\Psi^{mn}(\theta_1, \theta_2)\,, \tag{6}$$

where f is an arbitrary function and the invariants $\Psi^{mn}(\theta_1, \theta_2)$ are given by

$$\Psi^{mn}(\theta_1, \theta_2) = \mathrm{e}^{\mathrm{i}(m\theta_1 + n\theta_2)}\,. \tag{7}$$

These invariants are orthogonal and the projections (or the expansion coefficients) f^{mn} can be expressed as

$$f^{mn}(r_1, r_2) = \frac{1}{4\pi^2}\int_0^{2\pi} \mathrm{d}\theta_1 \int_0^{2\pi} \mathrm{d}\theta_2 f(r_1, r_2, \theta_{12})\Psi^{mn}(\theta_1, \theta_2)\,. \tag{8}$$

We expand the correlation functions in Eqs. (3), (4) and use the orthogonality of invariants to achieve the desired factorization

$$y^{mn}(r_1, r_2) = h^{mn}(r_1, r_2) - c^{mn}(r_1, r_2) = 2\pi \sum_{m'=-\infty}^{\infty} \int_0^{\infty} r_3\,\mathrm{d}r_3 \rho(r_3) c^{m,-m'}(r_1, r_3) h^{m',n}(r_3, r_2)\,. \tag{9}$$

The OZ equation contains three unknown functions: i) the density, ii) the inhomogeneous direct, and iii) total correlation functions. Thus, two more equations are required. There are several approximate closures which relate the correlation functions and can hence be applied directly to the inhomogeneous problem. Two common examples are Percus–Yevick (PY)[2]

$$c(r_1, r_2, \theta_{12}) = g(r_1, r_2, \theta_{12})\{1 - \exp[\beta u(r_1, r_2, \theta_{12})]\}\,, \tag{10}$$

and the hypernetted-chain (HNC)[2]

$$h(r_1, r_2, \theta_{12}) = \exp[h(r_1, r_2, \theta_{12}) - c(r_1, r_2, \theta_{12}) - \beta u(r_1, r_2, \theta_{12})] - 1\,. \tag{11}$$

Here $\beta = 1/k_B T$ is the inverse temperature, and u is the pair potential.

There are several exact equations that relate the density profile to the external potential field V and the inhomogeneous pair correlation functions.[37−42] One of these popular equations is the Treizenberg and Zwanzwig (TZ) equation which involves the total correlation function.[37−38] The TZ equation is expressed by

$$\nabla\rho(\boldsymbol{r}_1) = -\beta\rho(\boldsymbol{r}_1)\nabla V(\boldsymbol{r}_1) - \beta\rho(\boldsymbol{r}_1)\int \mathrm{d}\boldsymbol{r}_2 \rho(\boldsymbol{r}_2) h(\boldsymbol{r}_1, \boldsymbol{r}_2)\nabla V(\boldsymbol{r}_2)\,. \tag{12}$$

For circularly inhomogeneous systems, one can write

$$\rho'(r_1) = -\beta\rho(r_1)V'(r_1) - \beta\rho(r_1)\int_0^\infty\int_0^{2\pi} r_2\,\mathrm{d}r_2\,\mathrm{d}\theta_2\rho(r_2)h(r_1,r_2,\theta_{12})\cos\theta_{12}V'(r_2)$$
$$= -\beta\rho(r_1)V'(r_1) - \pi\beta\rho(r_1)\int_0^\infty r_2\,\mathrm{d}r_2\rho(r_2)[h^{1-1}(r_1,r_2)+h^{-11}(r_1,r_2)]V'(r_2)\,, \quad (13)$$

where the prime denotes differentiation with respect to argument.

2.2 *Solution of the OZ Equation*

The calculation method can be summarized into several steps. i) We apply the below relation

$$y^{mn}(r_1,r_2) = h^{mn}(r_1,r_2) - c^{mn}(r_1,r_2)\,. \quad (14)$$

This function obtains from a first approximation which sets it equal to the bulk pair correlation function calculated from the HNC closure for a uniform fluid. ii) The HNC closure [Eq. (10)] can be applied to form a new $h(r_1,r_2,\theta_{12})$. iii) A new direct correlation function determines from

$$c(r_1,r_2,\theta_{12}) = h(r_1,r_2,\theta_{12}) - b(r_1,r_2,\theta_{12})\,. \quad (15)$$

iv) A new density profile obtains by calculating the right-hand side of Eq. (13), and this is mixed with the old density. As we know, a first approximation for the density profile is simply the bulk HNC. v) A new $y^{mn}(r_1,r_2)$ can be obtained from the OZ Eq. (9), and this is also mixed with the previous estimate. This procedure repeats until satisfactory convergence and self consistency is achieved in the various thermodynamic properties.

Note that all functions used in the calculations are defined on some finite grid with cutoff D. Also, a correction ought be made for the truncation of the infinite integrals, Eqs. (9) and (13). Now, the OZ equation reads as

$$y^{mn}(r_1,r_2) = 2\pi\sum_{m'=-\infty}^{\infty}\int_0^D r_3\,\mathrm{d}r_3\rho(r_3)c^{m,-m'}(r_1,r_3)h^{m',n}(r_3,r_2) + y_\infty^{mn}(r_1,r_2)\,, \quad (16)$$

where the contribution from beyond the grid can be approximated by

$$y_\infty^{mn}(r_1,r_2) \approx 2\pi\rho\sum_{m'=-\infty}^{\infty}\int_D^{2D} r_3\,\mathrm{d}r_3 c_\infty^{m,-m'}(r_1,r_3)h_\infty^{m',n}(r_3,r_2)\,. \quad (17)$$

As we see, the inhomogeneous pair correlation functions are only required on the grid, $r_1 < D$, $r_2 < D$. Here, we correct the Eq. (13) as below

$$\rho'(r_1) = -\beta\rho(r_1)V'(r_1) - \pi\beta\rho(r_1)\int_0^D r_2\,\mathrm{d}r_2\rho(r_2)[h^{1-1}(r_1,r_2)+h^{-11}(r_1,r_2)]V'(r_2) - \rho(r_1)\rho'_\infty(r_1)\,, \quad (18)$$

where

$$\rho'_\infty(r_1) \approx -\pi\beta\rho\int_D^{2D} r_2\,\mathrm{d}r_2[h^{1-1}(r_1,r_2)+h^{-11}(r_1,r_2)]V'(r_2)\,. \quad (19)$$

The density itself can be obtained by below relation

$$\rho(r_1) = \int_D^{r_1}\rho'(r_2)\,\mathrm{d}r_2 + \rho(D)\,. \quad (20)$$

3 Simulation Techniques

Phase transitions of real and model complex fluids are of significant scientific and technological interest. From a modeling point of view, it is often of considerable interest to predict the phase behavior of a simplified system containing the essential interactions of interest. Computer simulations are a natural choice for this purpose. The focus of the present section in on a relatively simple and computationally inexpensive set of techniques known collectively under the name of Gibbs ensemble method. Although the Gibbs ensemble does not necessarily provide data of the highest possible accuracy and is not applicable to many important classes of systems, it is now commonly used for obtaining the phase behavior of fluids and mixtures. The main reason for this widespread use is probably the simplicity of the method. Also, this method is easy to describe and program, and has an intuitive physical basis.

3.1 *Gibbs Ensemble Simulation*

The Gibbs ensemble Monte Carlo simulation (GEMCS) technique is the most direct way of computing phase equilibria, and therefore of comparing the vapour-liquid equilibrium properties of the LJ fluid. In this part, a description is given of the simulation techniques that are used in the present work. A more extensive description of the Gibbs ensemble technique can be found in the literatures.[41−44]

Let us consider a macroscopic system with two phases coexisting at equilibrium. Simulations in the Gibbs ensemble are performed using two boxes, each box is simulated within standard periodic boundary conditions. The

boxes are kept at a constant temperature T, the total volume of the two boxes is fixed at V, and a fixed number of N particles are distributed over the two boxes. The algorithm consists of three basic moves: displacement of particles within each box (displacement step), fluctuations in the volume of the two boxes (volume exchange step), and transfer of particles between the boxes (particle exchange step). The details of the theoretical basis of the Gibbs ensemble Monte Carlo algorithm are described by Panagiotopoulos.[43−44] Here, we mention some details to clarify our implementation of GEMCS.

We perform the MC simulation technique in the Gibbs ensemble to calculate the thermodynamical properties of the 2D LJ fluid. In addition to the Gibbs ensemble, the canonical ensemble also can be done to calculate the thermodynamical properties. A formal proof of the equivalence of two ensembles can be found in Ref. [45]. A convenient method in the Gibbs ensemble is to perform a simulation in cycles. A cycle consisted of N_1 attempt to change the position of a particle in one of the boxes, N_2 attempt to change the volume of the subsystems, and N_3 attempt to exchange particles between the boxes. It is to be noted that at each step of the simulation, the equilibration condition must be fulfilled. In this work, we perform a random choice at each MC step instead of performing the sequential method. In Ref. [43], a more serious disadvantage of the sequential method was mentioned by Panagiotopoulos.

In the present work, we used 216 particles for he Lennard–Jones calculations. Exchanges attempts were made after every displacement attempts of a randomly selected particle in both boxes. Volume change attempts were performed after every 100 displacement and exchange attempts. Each calculation used a spherical cutoff on the interactions based on the distances of the center of masses. In this work, we used a spherical cutoff, 2.5σ, for the calculations of the LJ fluid. Also, the number of attempts per cycle to insert a particle were 100 for 216 particles. The number of cycles are given in Tables 1, 2, and 3.

4 Results and Discussion

As we know there are few numerical results, theoretically, for the thermodynamical properties of the 2D LJ fluid especially at three-particle level. For this reason, we tried to obtain the thermodynamical properties (such as pressure, energy, and chemical potential) of this fluid at three-particle level. For this goal, we first used the rotational invariants in two dimensions. Then, we solved numerically the inhomogeneous OZ equation in two dimensions by using the TZ equation and the HNC approximation. Therefore, we determined the energy, pressure, and chemical potential for this particular fluid. We also compared the results with our computer simulation.

In the numerical calculations and MC simulation, we have used the reduced parameters. These parameters are defined as [46]

$$T^* = k_B T/\epsilon, \quad P^* = P\sigma^2/\epsilon, \quad \rho^* = \rho\sigma^2. \tag{21}$$

Table 1 shows the pressure values of the 2D LJ fluid in the gas and liquid phases. These data obtained by the HNC3 method and compared with our simulation results.

In Table 2, we have reported the energy of the 2D LJ fluid in gas and liquid phases which obtained from the HNC3 procedure. We also compared these results with our simulation results.

Table 1 Pressure values (P^*) in gas and liquid phases: simulation $P^*_{\rm sim}$, and theoretical results $P^*_{\rm th}$ for the 2D LJ fluid.

	T^*	ρ^*	$P^*_{\rm sim}$	$P^*_{\rm th}$	$P^{*\rm a}_{\rm sim}$
Gas phase	0.450	0.030	0.0120	0.0118	0.011
	0.460	0.036	0.0130	0.0127	0.012
	0.470	0.050	0.0180	0.0176	0.017
	0.480	0.053	0.0180	0.0176	0.017
	0.490	0.064	0.0210	0.0206	0.020
	0.495	0.070	0.0220	0.0216	0.021
	0.500	0.090	0.0250	0.0245	0.024
	0.505	0.090	0.0280	0.0274	0.027
	0.515	0.28	0.0270	0.0265	0.026
Liquid phase	0.450	0.722	0.020	0.019	0.01
	0.460	0.72	0.020	0.019	0.01
	0.470	0.70	0.020	0.019	0.01
	0.480	0.68	0.020	0.019	0.01
	0.490	0.65	0.030	0.029	0.02
	0.495	0.65	0.030	0.029	0.02
	0.500	0.65	0.040	0.039	0.03
	0.505	0.64	0.040	0.039	0.03
	0.515	0.43	0.040	0.039	0.03

[a] The simulation results of Ref. [41].

Table 2 Energy values (E) in gas and liquid phases: simulation $E_{\rm sim}$, and theoretical results $E_{\rm th}$ for the 2D LJ fluid.

	T^*	ρ^*	$-E_{\rm sim}$	$-E_{\rm th}$	$-E^{\rm a}_{\rm sim}$
Gas phase	0.450	0.030	0.4	0.39	0.3
	0.460	0.036	0.4	0.39	0.3
	0.470	0.050	0.5	0.49	0.45
	0.480	0.053	0.45	0.44	0.4
	0.490	0.064	0.55	0.53	0.5
	0.495	0.070	0.65	0.63	0.6
	0.500	0.090	0.65	0.63	0.6
	0.505	0.090	0.95	0.93	0.9
Liquid phase	0.450	0.722	2.28	2.23	2.26
	0.460	0.72	2.25	2.20	2.23
	0.470	0.70	2.21	2.17	2.19
	0.480	0.68	2.13	2.08	2.11
	0.490	0.65	2.07	2.03	2.05
	0.495	0.65	2.02	1.98	2.0
	0.500	0.65	2.05	2.01	2.03
	0.505	0.64	2.02	1.98	2.0

[a] The simulation results of Ref. [41].

Table 3 displays the chemical potential of the 2D LJ fluid in gas and liquid phases which calculated by the HNC3 method. The results also have been compared with our simulation data. In Tables 1–3, our results have also been compared with simulation data of Ref. [47]. It is seen from Tables 2 and 3 that there is a turning point for the energy and chemical potential values of the liquid phase. It is worth mentioning that such turning points have been observed in previous works like Refs. [47–48]. From the obtained data, one can deduce that there is a critical phenomenon. To clarify this problem, we have plotted ρ-T curve for a 2D LJ fluid in Fig. 2. Other authors in the previous works[47−48] have predicted this phenomenon. They could obtain the critical temperature and density. To obtain more information, the reader can refer to [47–50].

Table 3 Chemical potential values (μ) in gas and liquid phases : simulation $\mu_{\rm sim}$, and theoretical results $\mu_{\rm th}$ for the 2D LJ fluid.

	T^*	ρ^*	$-\mu_{\rm sim}$	$-\mu_{\rm th}$	$-\mu_{\rm sim}^{\rm a}$
Gas phase	0.450	0.030	1.79	1.75	1.77
	0.460	0.036	1.78	1.74	1.76
	0.470	0.050	1.74	1.70	1.72
	0.480	0.053	1.76	1.73	1.74
	0.490	0.064	1.74	1.70	1.72
	0.495	0.070	1.72	1.69	1.70
	0.500	0.090	1.72	1.69	1.70
	0.505	0.090	1.71	1.68	1.69
	0.515	0.28	1.70	1.67	1.68
Liquid phase	0.450	0.722	1.84	1.80	1.82
	0.460	0.72	1.84	1.80	1.82
	0.470	0.70	1.75	1.71	1.73
	0.480	0.68	1.73	1.70	1.71
	0.490	0.65	1.71	1.68	1.69
	0.495	0.65	1.73	1.70	1.71
	0.500	0.65	1.73	1.70	1.71
	0.505	0.64	1.68	1.65	1.66
	0.515	0.43	1.73	1.70	1.71

[a] The simulation results of Ref. [41].

One of the approximate theories for the 2D LJ fluid is the perturbation theory. In this theory, the hard disks system considers as a reference system. There are several perturbation theories such as the Zwanzig (Z), the Gibbs–Bogoliubov (GB), and the Weeks–Chandler–Andersen (WCA).[8]

In Fig. 1, we have plotted the P-T curve obtained from the present work, the WCA perturbation theory,[48] the GB perturbation theory, and simulation data.[47] One can see an important and interesting problem in this figure. At higher temperatures, it is obvious from the figure that our theoretical results (HNC3) deviate from the simulation data from Ref. [41]. Related to this deviation, four points should be noted: (i) Including all terms in Eq. (16) is not possible. (ii) There are different functions in our calculations which have various ranges. Hence, at higher temperatures, these functions have different values. (iii) All functions used in the calculations are defined on some finite grid with cutoff D. This cutoff can be temperature-dependent. (iv) In the Attard's source particle method, the external potential has been considered as hard particles [Eq. (13)]. At higher temperatures, these particles may not be as hard particles and they can penetrate to each other.

Figure 2 shows the reduced density as a function of reduced temperature. This figure presents liquid-gas coexistence curve of a 2D Lennard–Jones fluid.

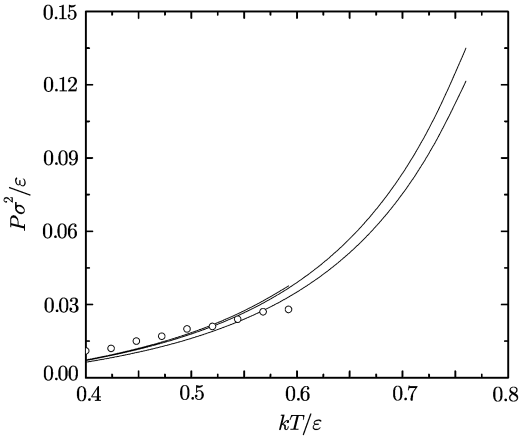

Fig. 1 P-T liquid-gas curve for a 2D LJ system. The results of this work (solid line) are compared with the simulation results[41] (open circles), the Gibbs–Bogoliubov variational method[42] (dashed curve), and Weeks–Chandler–Andersen theory[42] (dotted curve).

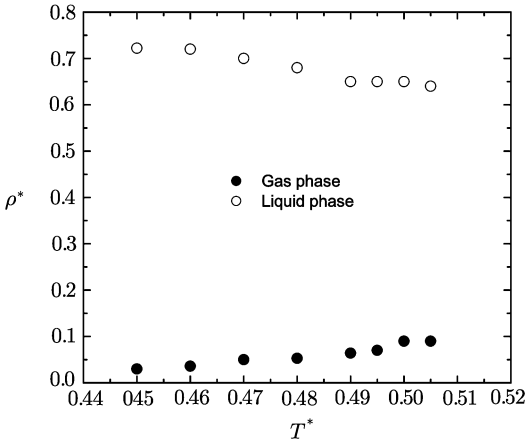

Fig. 2 ρ-T liquid-gas coexistence curve of a 2D Lennard–Jones fluid. Open and solid circles correspond to liquid and gas phases, respectively. We have obtained these results from simulation method.

5 Conlusion

In the present work, we have theoretically studied thermodynamical properties of a 2D fluid. We have obtained pressure, energy, and chemical potential of a 2D Lennard–Jones fluid. In the previous works, researchers have calculated these properties by using the pair correlation functions. But, in this paper, we have obtained these ther-

modynamical properties by using triplet correlation functions. To calculate the triplet correlation functions, we have solved the OZ and TZ equations by using HNC closure relation. We also have applied the Attard's source particle method and extended to 2D fluids. In addition to numerical calculations, we also have performed the MC simulations.

According to the results obtained from the present work for the thermodynamical properties of the 2D LJ fluid reveals that these properties can be obtained relatively from integral equations method using the HNC approximation. For the 2D LJ fluid, we have reported the pressure, energy, chemical potential, and P-T curves. Our theoretical results are in fairly agreement with numerical calculations obtained from our computer simulation results and other results from Refs. [47–48]. The simulation results demonstrate that the our theoretical approach proposed here is suitable to determine thermodynamical properties 2D LJ fluid. We also have obtained the coexistence curve [ρ-T curve] of a 2D Lennard–Jones fluid.

In summary, the Attard's source particle method is extensible to 2D systems. Using this method and triplet correlation functions, one can obtain thermodynamical properties of 2D fluids.

References

[1] M.P. Allen, in *Observation, Prediction and Simulation of Phase Transitions in Complex Fluids*, ed. M. Baus, L.F. Rull, and J.P. Ryckaert, NATO ASI Series, Kluwer, Durdre cht (1995).

[2] J.P. Hansen and I.R. McDonald, *Theory of Simple Liquids*, Academic, London (1986).

[3] C.N. Patra and S.K. Ghosh, J. Chem. Phys. **118** (2003) 3668.

[4] M. Moradi and R. Khordad, J. Chem. Phys. **125** (2006) 214504.

[5] M. Moradi and R. Khordad, Int. J. Mod. Phys. B **25** (2011) 301.

[6] D.A. Ward and F. Lado, Mol. Phys. **63** (1988) 623.

[7] M. Moradi and R. Khordad, Physica A **384** (2007) 187.

[8] R. Khordad, Physica A **387** (2008) 4519.

[9] M.M. Papari, R. Khordad, and Z. Akbari, Physica A **388** (2009) 585.

[10] R. Khordad, F. Hosseini, and M.M. Papari, Chem. Phys. **360** (2009) 123.

[11] R. Khordad, M. Mohebbi, A. Keshavarzi, A. Poostforush, and F.G. Haghighi, Int. J. Mod. Phys. B **23** (2009) 753.

[12] W.A. Steele, *The Interaction of Gases with Solid Surfaces*, Pergamon, Oxford (1974).

[13] D.J. Shaw, *Introduction to Colloid Surface Chemistry*, Butterworths, London (1980).

[14] J.K. Percus and G.J. Yevick, Phys. Rev. **110** (1958) 1.

[15] J.L. Lebowitz, Phys. Rev. **133** (1964) A895.

[16] M. Yasutomi and M. Ginoza, J. Phys. Condens. Matter. **12** (2000) L605.

[17] D. Henderson, L. Blum, and J.P. Noworyta, J. Chem. Phys. **102** (1995) 4973.

[18] T. Urbic, V. Vlachy, Y.V. Kalyuzhnyi, N.T. Southall, and K.A. Dill, J. Chem. Phys. **112** (2000) 2843.

[19] T. Urbic, V. Vlachy, Y.V. Kalyuzhnyi, and K.A. Dill, J. Chem. Phys. **118** (2003) 5516.

[20] M. Letz and A. Latz, Phys. Rev. E **60** (1999) 5865.

[21] A. Perera, P.G. Kusalik, and G.N. Patey, J. Chem. Phys. **87** (1987) 1295.

[22] P.G. Ferreira, A. Perera, M. Moreau, and M.M.T. da Gama, J. Chem. Phys. **95** (1991) 7591.

[23] E. Leutheusser, J. Chem. Phys. **84** (1986) 1050.

[24] F. Lado, J. Chem. Phys. **49** (1968) 3092.

[25] P.L. Fehder, J. Chem. Phys. **50** (1969) 2617.

[26] F. Tsien and J.P. Valeau, Mol. Phys. **27** (1974) 177.

[27] J.H. Sikkenk, H.J. Hilhorst, and A.F. Barker, Physica A **131** (1985) 587.

[28] J.H. Sikkenk, J.M.J. van Leeuwen, E.O. Vossnack, and A.F. Barker, Physica A **146** (1987) 622.

[29] M. Lombardero, C. Martin, S. Jorge, F. Lado, and E. Lomba, J. Chem. Phys. **110** (1999) 1148.

[30] J.L. Barrat, J.P. Hansen, and G. Pastore, Mol. Phys. **63** (1988) 747.

[31] D.A. Huckaby and L. Blum, J. Chem. Phys. **97** (1992) 5773.

[32] S. Jorge, E. Lomba, and J.L.F. Abascal, J. Chem. Phys. **114** (2001) 3562.

[33] P. Attard, J. Chem. Phys. **91** (1989) 3072.

[34] P. Attard, J. Chem. Phys. **95** (1991) 4471.

[35] J.K. Percus, in *The Equilibrium Theory of Classical Fluids*, ed. H.L. Frisch, J.L. Lebowitz, and W.A. Benjamin, John Wiley, New York (1964).

[36] J.M. Caillol, D. Levesque, and J.J. Weis, Mol. Phys. **44** (1981) 733.

[37] D.G. Triezenberg and R. Zwanzig, Phys. Rev. Lett. **28** (1972) 1183.

[38] R.A. Lovett, C.Y. Mou, and F.P. Buff, J. Chem. Phys. **58** (1976) 1880.

[39] M.S. Wertheim, J. Chem. Phys. **65** (1976) 2377.

[40] M. Born and H.S. Green, Proc. R. Soc. London Ser. A **188** (1946) 10.

[41] J. Yvon, Act. Sci. Ind. Hermann **203** (1935) 938.

[42] N.N. Bogoliubov, J. Phys. (Moscow) **10** (1946) 256.

[43] A.Z. Panagiotopoulos, Mol. Phys. **61** (1987) 813.

[44] A.Z. Panagiotopoulos, N. Quirke, M. Stapleton, and D.J. Tildesley, Mol. Phys. **63** (1988) 527.

[45] B. Smit, Ph. de Smedt, and D. Frenkel, Mol. Phys. **68** (1989) 931.

[46] B. Cao, M. Chen, and Z. Guo, Chin. Sci. Bullet. **49** (2004) 1101.

[47] B. Smit and D. Frenkel, J. Chem. Phys. **94** (1991) 5663.

[48] O.H. Scalise, G.J. Zarragoicoechea, L.E. Gonzalez, and M. Silbert, Mol. Phys. **93** (1998) 751.

[49] R.R. Singh, K.S. Pitzer, J.J. De Pablo, and J.M. Prausnitz, J. Chem. Phys. **92** (1990) 5463.

[50] M.R. Reddy and S.F. O'Shea, Can. J. Phys. **64** (1986) 677.