

# **An Evaluation of Ground State Energy of Two-dimensional Liquid $^4\text{He}$ Interacting through Lennard-Jones the Aziz Potential at Various Densities**

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## **ABSTRACT**

Using theoretical formulation of Chung-In Um et. al., the ground state energy of two-dimensional liquid  $^4\text{He}$  interacting through Lennard-Jones and Aziz potential were calculated at various densities. Our theoretical result indicates that ground state energy of two dimensional liquid  $^4\text{He}$  interacting with Aziz potential is close to GFMC calculation.

## **INTRODUCTION**

In the previous paper,<sup>1</sup> we have presented a method of evaluation of radial distribution function  $g(r)$  of two-dimensional liquid  $^4\text{He}$  interacting through the Aziz potential at various densities using the theoretical formalism of Chung-In Um et. al.<sup>2</sup> In this paper, using the same theoretical formalism, we have evaluated the ground state energy of two dimensional liquid.  $^4\text{He}$  interacting through Lennard Jones and Aziz potential at various densities.

For many years, physicist have used hypernetted chain (HNC) and Fermi hypernetted chain (FHNC) theories to investigate the properties of highly correlated interacting boson and fermion systems such as liquid  $^4\text{He}$  and normal liquid  $^3\text{He}$ .<sup>3,4</sup> The HNC/FHNC equations

with Jastrow ground-state wave functions treat consistently both long and short correlations of the system and give agreements to some degree with experimental results. In spite of qualitative successes of the Jastrow ground-state function, there exist quantitative differences between HNC/FHNC results and experimental ones, especially the equilibrium ground-state energy, and this fact leads one to consider the contributions arising from the three-body correlation functions.<sup>5</sup> It is well known that the three-body correlations do not affect seriously the structural properties of ground states, such as the radial distribution function and liquid structure function, but contribute significantly to the ground-state energy. Since liquid  $^3\text{He}$  system is less dense than

liquid  $^4\text{He}$ , that is, the equilibrium density of the former is  $0.0166 \text{ \AA}^{-3}$  while that of the latter is  $0.02185 \text{ \AA}^{-3}$  in a three-dimensional system, effects of three-body correlations in  $^3\text{He}$  are rather small compared to those in  $^4\text{He}$ . At equilibrium density, they make up about half the difference between the Jastrow results and experimental energy in a liquid  $^3\text{He}$  system<sup>5</sup> and lower the Jastrow ground-state energy by about 10 % in liquid  $^3\text{He}$ .

A trial ground-state wave function including three-body correlation functions in addition to two-body correlation effects can be constructed in the form

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i<j}^N f_2(r_{ij}) \prod_{i<j<k}^N f_3(r_{ij}, r_{jk}, r_{ki}) |\Phi\rangle = F|\Phi\rangle$$

where  $f_2(r_{ij})$  is the two-body correlation function which describes spatial correlations and depends only upon the spatial distance  $r_{ij}$  between two particles.  $f_3(r_{ij}, r_{jk}, r_{ki})$  is a three-body correlation function, and  $|\Phi\rangle$  is the anti-symmetric product of non-interacting single-particle plane waves normalized in the system's area  $\Omega$  with  $N$  fermions, which becomes simply unity for boson systems.

In addition to the three-body correlation functions in the ground-state wave function, one should take into account the contributions coming from the elementary diagrams as well as effects of the HNC/FHNC equations to obtain better results. Unfortunately, there does not exist a general closed expression for the elementary

diagrams and therefore one must calculate each diagram individually, which is very time consuming. During the last two decades, two approximations for the estimation of the elementary diagrams have been developed. One is known as the scaling approximation,<sup>6</sup> and the other is the interpolating equation approximation.<sup>7</sup> Both techniques have shown their efficiency for central two-body correlations, providing similar results for the total ground-state energy to those of the variational Monte Carlo simulation. The scaling approximation uses the fact that successive contributions of the five, six and higher order elementary diagrams are approximately proportional to and have very similar spatial behaviour to the four-body elementary diagrams,<sup>6</sup> so that one can represent the total elementary diagram contribution by means of the readily calculable four-body elementary diagrams. The interpolating equation approximation determines a parameter such that it gives the same value for the classical isothermal compressibility obtained from both the HNC/FHNC equations and Percus-Yevick<sup>8</sup> equations using the classical pressure derivative or the compressibility integral.

Although large number of theoretical works regarding  $^4\text{He}$  and  $^3\text{He}$  system have been reported<sup>9-12</sup> but very few of them have been used for two-dimensional liquid.

Chung-In Um *et. al.*<sup>13</sup> have developed a theoretical model to study two-dimensional quantum fluid. By taking their model, one has evaluated the radial distribution function  $g(r)$  as a function of  $r$

for two dimensional liquid  $^4\text{He}$  interacting through Aziz potential for various densities. In section 2, we have given the mathematical formulae used in the evaluation. The discussion of the result has been given in section 3 of this paper. In the last portion, we have shown the tables of the results and the reference taken.

**MATHEMATICAL FORMULAE USED IN THE EVALUATION**

The Hamiltonian for the considered system is given by

$$H = T + V = \sum_i T_i + \sum_{i < j} V_{ij} = -\frac{\hbar}{m} \sum_i \nabla_i^2 + \sum_{i < j} V(|\vec{r}_i - \vec{r}_j|) \tag{1}$$

where  $V(r)$  is the interatomic interaction. A popular potential used in theoretical investigations is that of Lennard-Jones, which has two parameters, i.e., the hard-core radius and the well depth, and can be written as

$$V_{LJ}(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \tag{2}$$

$\varepsilon = 10.22 \text{ K}, \sigma = 2.556 \text{ \AA}$

However,  $V_{LJ}(r)$  includes only the dipole-dipole interaction and does not take into account multiple interactions. A more physically realistic potential which accounts for the self-consistent field Hartree-Fock repulsion and multiple interactions is the HFDHE2 potential of Aziz *et. al.*<sup>12</sup> presented as

$$V_{LJ}(r) = \varepsilon^* \left[ A \exp\left(-\alpha \frac{r}{r_m}\right) - \left\{ c_6 \left( \frac{r_m}{r} \right)^6 + c_8 \left( \frac{r_m}{r} \right)^8 + c_{10} \left( \frac{r_m}{r} \right)^{10} F(r) \right\} \right] \tag{3}$$

where

$$F(r) = \begin{cases} \exp\left[-(Dr_m/r - 1)^2\right] & r/r_m \leq D \\ 1 & r/r_m < D \end{cases} \tag{4}$$

The values of the constants are

$$\begin{aligned} A &= 0.54485 \times 10^6, & \varepsilon^*/k_B &= 10.8 \\ \alpha &= 13.353384, & C_6 &= 1.3732412 \\ C_8 &= 0.4253785, & C_{10} &= 0.178100 \\ D &= 1.241314, & r_m &= 2.9673 \text{ \AA} \end{aligned}$$

It is well known from the Green's function Monte Carlo simulations and other variational calculations that the Aziz potential gives closer results to experiments than  $V_{LJ}$  in three dimensions. One uses both potentials and compare the results with those in two dimensions.

The  $n$ -particle distribution function is represented as

$$p_n = (\vec{r}_1, \dots, \vec{r}_n) = v^n N(N-1) \dots (N-n+1) \times \frac{\int \psi^+(\vec{r}_1, \dots, \vec{r}_n) \psi(\vec{r}_1, \dots, \vec{r}_n) d\vec{r}_{n+1} \dots d\vec{r}_N}{\langle \psi | \psi \rangle} \tag{4}$$

where  $\vec{r}_i$  denotes the spatial coordinates of the  $i$ -th particle and  $v$  is the spin degeneracy of the system (2 for this system). In the homogeneous system, as  $N \rightarrow \infty$  and  $\Omega \rightarrow \infty$ , the single-particle distribution function reduces to the density of the system so that the radial distribution function can be expressed interms of the density and two-particle distribution function  $p_2(r)$  as

$$g(r) = \frac{1}{\rho^2} p_2(r) = \frac{N(N-1) \left( \frac{v}{\rho} \right)^2 \int \psi^+(\vec{r}_1, \dots, \vec{r}_n) \psi(\vec{r}_1, \dots, \vec{r}_n) d\vec{r}_3 \dots d\vec{r}_N}{\langle \psi | \psi \rangle} \tag{5}$$

One uses the FHNC approximation to sum the diagrams arising from the cluster properties of  $g(r)$ . In this scheme,  $g(r)$  can be decomposed as

$$g(\mathbf{r}_{ij}) = g_{dd}(\mathbf{r}_{ij}) + 2g_{de}(\mathbf{r}_{ij}) + g_{ee}(\mathbf{r}_{ij}) \quad (6)$$

where dd, de and ee represent terms in which both i and j are not exchanged, only j is exchanged, and both i and j are exchanged, respectively. The components of  $g(\mathbf{r}_{ij})$  are given by

$$\begin{aligned} g_{dd}(\mathbf{r}_{ij}) &= \exp\left[u_2(\mathbf{r}_{ij}) + N_{dd}(\mathbf{r}_{ij}) + E_{dd}(\mathbf{r}_{ij})\right] \\ g_{de}(\mathbf{r}_{ij}) &= g_{dd}(\mathbf{r}_{ij})\left[N_{de}(\mathbf{r}_{ij}) + E_{de}(\mathbf{r}_{ij})\right] \quad (7) \\ g_{ee}(\mathbf{r}_{ij}) &= g_{dd}(\mathbf{r}_{ij})\left[-L^2(\mathbf{r}_{ij})/v + N_{ee}(\mathbf{r}_{ij}) + E_{ee}(\mathbf{r}_{ij}) + (N_{ee}(\mathbf{r}_{ij}) + E_{ee}(\mathbf{r}_{ij}))^2\right] \\ g_{ee}(\mathbf{r}_{ij}) &= g_{dd}(\mathbf{r}_{ij})L(\mathbf{r}_{ij}) / v \end{aligned}$$

where

$$L(\mathbf{r}_{ij}) = -l(\mathbf{k}_F \mathbf{r}_{ij}) + v(N_{ee}(\mathbf{r}_{ij}) + E_{ee}(\mathbf{r}_{ij})) \quad (8)$$

$$l(\mathbf{x}) = 2j_1(\mathbf{x}) / \mathbf{x} \quad (9)$$

$k_F$  is the Fermi momentum of the system, and  $j_1(x)$  is the Bessel's function of the first kind of order 1.  $N_{mm}$  represent sums of the nodal diagrams and  $E_{mm}$  sums of the elementary diagrams. The equation  $g_{ee}(\mathbf{r}_{ij})$  denotes the terms in which both i and j are exchanged in an incomplete exchange loop, and  $N_{ee}(\mathbf{r}_{ij})$  and  $E_{ee}(\mathbf{r}_{ij})$  are sums of the nodal diagrams and the elementary diagrams in which i and j belong to the same permutation loop, respectively.

With the FHNC equation and expression for the  $g(r)$ , one now calculates the energy per particle of the system

$$\frac{E_{\text{var}}}{N} = \frac{1}{N} \frac{\langle \psi | H | \psi \rangle}{N \langle \psi | \psi \rangle} = \frac{\langle V \rangle}{N} + \frac{\langle T \rangle}{N} \quad (10)$$

The potential energy per particle is expressed by taking the thermodynamic limit, i.e., the area of system  $\Omega$  and the number of particles  $N$  are infinite, keeping the density constant as

$$\frac{\langle V \rangle}{N} = \frac{\rho}{2} \int d\bar{r}_{ij} V(\mathbf{r}_{ij}) g(\mathbf{r}_{ij}) \quad (11)$$

The expression for the or the kinetic energy part is more complicated. There are three well-known expression for the helium system i.e., Jackson–Freeberg,<sup>10</sup> Clark–Westhous<sup>11</sup> and Bethe–Pandharipande.<sup>12</sup> Among expressions for the kinetic energy per particle. The Jackson–Feenberg form is popular and easily tractable since its three–particle distribution part is not more significant than others. One uses here the Jackson–Feenberg and the Bethe–Pandharipande forms so that we make use of the scaling approximation for the elementary diagrams. From the identity

$$\int \psi^\dagger \nabla^2 \psi d\bar{r} = \frac{1}{4} \int \left[ \psi^\dagger (\nabla^2 \psi) (\nabla^2 \psi^\dagger) + 2(\nabla \psi^\dagger) \cdot (\nabla \psi) \right] d\bar{r} \quad (12)$$

the Jackson–Feenberg energy form is obtained as

$$\begin{aligned} \frac{E_{\text{JF}}}{N} &= \frac{-\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \langle \Phi | F^2 \nabla^2 \nabla_i^2 + \frac{1}{2} F \nabla_i^2 F - \frac{1}{2} (\nabla_i F)^2 | \Phi \rangle \\ &+ \frac{\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \langle F^2 \nabla_i^2 | \Phi |^2 \rangle d\bar{r}_1 \dots d\bar{r}_N + \frac{\langle V \rangle}{N} \\ &= T_F = W_B + W_\phi + U_\phi \quad (13) \end{aligned}$$

The first term of Eq. (13),  $T_F = \hbar^2 k_F^2 / 4m$ , is the noninteracting fermion energy with the Fermi momentum  $k_F = \sqrt{4\pi\rho/v}$ , and the second,  $W_B$  is the energy of the boson system.

$$W_n = \frac{\rho}{2} \int d^2r g(r) \left[ v(r) - \frac{\hbar^2}{2m} \frac{\nabla^2 f_2(r) - (\nabla f_2(r))^2}{f_2(r)} \right] \quad (14)$$

The forms of  $W_\phi$  and  $U_\phi$  are

$$W_\phi = \frac{\hbar^2 \rho}{4m v} \int d^2r \left\{ g_{dd}(r) - 1 \left[ I(k_F r) - v(N_{cc}(r) + E_{cc}(r)) \right] \nabla^2 I(k_F r) + \nabla I(k_F r)^2 - v d_{dd}(r) E_{cc}(r) \nabla^2 I(k_F r) \right\} \quad (15)$$

$$U_\phi = \frac{\hbar^2 \rho^2}{8m} \int d^2r_1 d^2r_2 g_{dd}(r_{12}) - 1 \nabla I(k_F r_{12}) \cdot (g_{dd}(r_{13}) - 1) \times \nabla I(k_F r_{13}) g_{cc}(r_{23}) \quad (16)$$

$$U_\tau = \frac{\hbar^2 \rho}{16m} \int d^2r_1 d^2r_2 g_3(r_{12}, r_{23}, r_{13}) \nabla^2 u_3(r_{12}, r_{23}, r_{13}) \quad (17)$$

The Pandharipande–Bethe energy form is obtained by expanding the kinetic energy per particle as

$$-\frac{\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \langle \Phi | F \nabla_i^2 [F | \Phi] \rangle = \frac{\langle T \rangle_{PB}}{N} \quad (18)$$

which yields

$$\frac{\langle T \rangle_{PB}}{N} - \frac{\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \langle \Phi | F [\nabla_i^2 + \nabla_i^2 + 2(\nabla_i F)] | \Phi \rangle \quad (19)$$

After some calculations, we obtained  $E_{PB}/N$

$$\text{as} \quad \frac{E_{PB}}{N} = T_F + W + W_r + U + U_F \quad (20)$$

where  $W$  and  $U$  are the bosonic energies per particle, and  $W_F$  and  $U_F$  are from the last term of Eq. (19)

$$W = \frac{\rho}{2} \int d^2r g(r) \left[ v(r) - \left( \frac{\hbar^2}{m} \right) \frac{\nabla^2 f_2(r)}{f_2(r)} \right] \quad (21)$$

$$U = -\frac{\hbar^2 \rho^2}{2m} \int d^2r_1 d^2r_2 g_3(r_{12}, r_{23}, r_{13}) \left[ \frac{\nabla_1 f_2(r_{12}) \cdot \nabla_1 f_2(r_{13})}{f_2(r_{12}) f_2(r_{13})} \right] \quad (22)$$

$$W_F = -\frac{\hbar^2 \rho}{2m} \int d^2r g_{cc}(r) \left[ \frac{\nabla f_2(r) \cdot \nabla I(k_F r)}{f_2(r)} \right] \quad (23)$$

$$U_F = -\frac{\hbar^2 \rho^2}{2m} \int d^2r_{12} \nabla f_2(r_{12}) \cdot \nabla I(k_F r_{13}) \times \{ g_{cc}(r_{13}) g_{dy}(r_{12}) (g_{dy}(r_{32}) - 1) + g_{dd}(r_{13}) g_{cc}(r_{23}) g_{cc}(r_{31}) \} \quad (24)$$

For numerical calculations, one adopts the McMillan type function as a trial two–body correlation functions, which is widely used in variational and Monte Carlo calculations for liquid and solid helium systems.

$$u_2(r) = -\left( \frac{b}{r} \right)^5 \quad (25)$$

where  $b$  is a variational parameter chosen to give an optimized radial distribution function at a given density. To obtain more precise results, we include three–body correlation effects in the following forms:

$$u_3(r_{ij}, r_{jk}, r_{ki}) = \sum_{cyc} \eta(r_{ij}) \eta(r_{jk}) (\hat{r}_{ij} \cdot \hat{r}_{jk}) \quad (26)$$

$$\eta(r) = \sqrt{\lambda_1} r \exp \left[ -\left( \frac{r - r_1}{\omega_1} \right)^2 \right] \quad (27)$$

where  $cyc$  denotes the cyclic permutation among the three particle coordinates  $i, j$  and  $k$ , and  $\hat{r}_{ij}$  is a unit vector along the line

connecting particle  $i$  and  $j$ . Since it was first used in a variational Monte Carlo calculation,<sup>13</sup> this form for the three-body correlations is generally used in variational HNC/FHN methods.<sup>14</sup>

## DISCUSSION OF RESULTS

In this paper, we have evaluated the ground state energy of two dimensional liquid  $^4\text{He}$  interacting through Lennard-Jones and Aziz potential at various densities. We have used the theoretical formalism of Chung-In Um *et. al.*<sup>2</sup> in our evaluation. Chung-In Um<sup>2</sup> calculated ground state energy of two dimensional liquid  $^4\text{He}$  with a

Jastrow two body correlation function in the trial wavefunction and within the HNC approximation. His other calculation for energy per particle is by taking two body correlation and contribution of four order elementary diagrams. We have taken three body as well as two-body correlations within the scaling approximation.<sup>15</sup> Our theoretical calculation indicates that the two dimensional liquid  $^4\text{He}$  system interesting through Aziz potential is more close to the GFMC calculation.<sup>14</sup> Comparing with two potential, one conclude that Aziz potential is more suitable to describe, the ground state of the two dimensional helium system, similar to bulk case.<sup>16</sup>

Table T<sub>1</sub>

Evaluated results of ground state energy of two-dimensional liquid  $^4\text{He}$  interacting through the Lennard-Jones potential at various density

$\rho(\text{\AA}^{-2})$	Ground state energy $E(k)/N$		
	Our's	Chang's <sup>13</sup> results	GFMC Calculations <sup>14</sup>
0.020	-0.520	-0.628	-0.504
0.025	-0.546	-0.637	-0.546
0.030	-0.624	-0.658	-0.589
0.035	-0.658	-0.586	-0.627
0.040	-0.748	-0.552	-0.553
0.045	-0.786	-0.505	-0.524
0.050	-0.842	-0.486	-0.508
0.055	-0.725	-0.453	-0.493
0.060	-0.556	-0.446	-0.486

Table T<sub>2</sub>

Evaluated results of ground state energy [E(k)/N] of two-dimensional liquid <sup>4</sup>He interacting through Aziz potential at various densities

$\rho(\text{\AA}^{-2})$	Ground state energy E(k)/N		
	Our's	Chang's <sup>13</sup> results	GFMC Calculations <sup>14</sup>
0.020	-0.487	-0.586	-0.523
0.025	-0.509	-0.603	-0.588
0.030	-0.586	-0.658	-0.602
0.035	-0.627	-0.709	-0.657
0.040	-0.723	-0.682	-0.697
0.045	-0.706	-0.596	-0.602
0.050	-0.658	-0.542	-0.524
0.055	-0.532	-0.506	-0.486
0.060	-0.456	-0.487	-0.442

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