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# AN EVALUATION OF RADIAL DISTRIBUTION FUNCTION g (r) OF TWO-DIMENSIONAL LIQUID $^3$He INTERACTING THROUGH AZIZ POTENTIAL AT VARIOUS DENSITIES

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## ABSTRACT

Using theoretical formalism of Chung-In Um et al. the radial distribution function g (r) for two-dimensional liquid $^3$He interacting with Aziz potential has been evaluated for various densities. Our theoretical result indicates that g (r) increases with r and attains some maximum value and then becomes almost constant. Our theoretical results are good agreement with other workers.

**Key words**: Radial distribution function, Aziz potential, Two dimensional Liquid $^3$He, GFMC calculation

## INTRODUCTION

For many years, physicist have used hyper netted chain (HNC) and Fermi hyper netted chain (FHNC) theories to investigate the properties of highly correlated interacting boson and fermion systems such as liquid $^4$He and normal liquid $^3$He[1,2]. The HNC/FHNC equations with Jastrow ground-state wave functions treat consistently both long and short range 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. 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 $^3$He system is less dense than liquid $^4$He, that is, the equilibrium density of the former is 0.0166 Å$^{-3}$ while that of the latter is 0.02185 Å$^{-3}$ in a three-dimensional system, effects of three-body correlations in $^3$He are rather small compared to those in $^4$He. At equilibrium density, they make up about half the difference between the

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Jastrow results and experimental energy in a liquid $^3$He system and lower the Jastrow ground-state energy by about 10 % in liquid $^3$He[3].

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

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

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 particle $f_3$ ($r_{ij}$, $r_{jk}$, $r_{ki}$) 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 Ω 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[4] and the other is the interpolating equation approximation[5] .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 behavior to the four-body elementary diagrams, 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[5] equations using the classical pressure derivative or the compressibility integral. In this paper, one uses the scaling approximation to calculate the contribution of the elementary diagrams.

Many workers have been reported regarding the properties of three-dimensional $^4$He and $^3$He systems using the variational HNC/FHNC methods, the variational Monte Carlo method[6] and the Green's function Monte Carlo method (GFMC)[7] there are few papers on two-dimensional systems. Using the Jastrow wave functions and solving an Euler-Lagrange equation within the HNC approximation. Hatzikonstinou[8] studied the ground-state of two-dimensional liquid $^4$He interacting through a Lennard-Jones potential and explained the long-range and short-range behaviors of the correlation function to a certain extent. However, since he ignored the effects of the three-body correlation and elementary diagrams. His results give ground state energies too high compared to the GFMC[9] and diffusion Monte Carlo (DMC) results[10]. Chang calculated the ground-state energy and structure functions of two-dimensional $^4$He in liquid density ranges[11] by taking the same potential as an interatomic potential and using a self-consistent paired-phonon analysis. He included the effects of the three-body correlation in the ground-state wave function, but did not consider the elementary diagrams at all. Therefore, though he obtained very optimized liquid structure functions and radial distribution functions, his results for the ground state energy are still higher and the equilibrium density is lower than those of the GFMC and D M C calculations.

For the $^3$He system, Novaco and Campbell[12] obtained theoretically the ground-state energy of quasi-two-dimensional helium absorbed on graphite by introducing a trial wave function which has only two-body correlations, finite extent orthogonal to the substrate, and the same translational symmetry as the substrate. Furthermore, they considered the effects of Fermi Dirac statistics to only the lowest-order correction, which is the energy of the Fermi Sea. Using a variational calculation and the quantum theorem of corresponding states, Miller and Nosanow[13] analyzed properties of the two-dimensional $^3$He system. Recently Brami et al.[14] investigated two-dimensional $^3$He system absorbed on graphite through variational Monte Carlo calculations considering a one-body wave function to describe a z-delocalization of helium atoms in addition to planar correlations in the total wave function which has only two-body terms.

## 2.0 Mathematical formulae used in the evaluation

The Hamiltonian for the considered system is given by –

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

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 –

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \varepsilon = 10.22\ \text{K}, \sigma = 2.556\ \text{Å} \qquad \ldots(2)$$

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.[15] presented as –

$$V_{LJ}\,(r) = \varepsilon^{*}\left[A\exp\left(-\alpha\frac{r}{rm}\right)-\left\{C_6\left(\frac{r_m}{r}\right)^{6}+C_8\left(\frac{r_m}{r}\right)^{8}+C_{10}\left(\frac{r_m}{r}\right)^{10}F(r)\right\}\right], \qquad \ldots(3)$$

Where

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

The values of the constants are -

$A = 0.54485 \times 106$, $\frac{\varepsilon^{*}}{k_B} = 10.8$

$\alpha = 13.353384$, $C_6 = 1.3732412$

$C_8 = 0.4253785$, $C_{10} = 0.178100$

$D = 1.241314$, $r_m = 2.9673$ Å

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 –

$$P_n = \left(\vec{r}_1,\ldots\vec{r}_n\right) = V^{n}N\,(N-1)\ldots(N-1)\times\frac{\int \psi+(\vec{r}_1,\ldots\vec{r}_n)\,\psi+(\vec{r}_1,\ldots\vec{r}_n)\,d\vec{r}_{n+1}\ldots d\vec{r}_N}{\langle\psi|\psi\rangle} \qquad \ldots(5)$$

Where $\vec{\mathbf{r}}_1$ 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 → ∞ and **Ω** → ∞, the single-particle distribution function reduces to the density of the system so that the radial distribution function can be expressed in terms of the density and two-particle distribution function $P_2(r)$ as –

$$g(r) = \frac{1}{\rho^2} P_2(r) = N\ (N–1) \left(\frac{\nu}{\rho}\right)^2 \frac{\int \psi + (\vec{r}_1,...\vec{r}_n)\ \psi(\vec{r}_1,...\vec{r}_n)\ d\vec{r}_3\ ...d\vec{r}_N}{\langle\psi|\psi\rangle} \quad ...(6)$$

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 –

$$g(r) = g_{dd}\ (r_{ij}) + 2g_{de}\ (r_{ji}) + g_{ee}\ (r_{ij}) \quad ...(7)$$

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 $g(r_{ij})$ are given by –

$$g_{dd}\ (r_{ij}) = \exp\ [u_2\ (r_{ij}) + N_{dd}\ (r_{ij}) + E_{dd}\ (r_{ij})]$$

$$g_{de}\ (r_{ij}) = g_{dd}\ (r_{ij})\ [N_{dd}\ (r_{ij}) + E_{dd}\ (r_{ij})]$$

$$g_{de}\ (r_{ij}) = g_{dd}\ (r_{ij}) \left[ -\frac{L^2(r_{ij})}{v} + N_{ee}(r_{ij}) + E_{ee}(r_{ij}) + N_{ee}(r_{ij}) + E_{ed}(r_{ij}))^2 \right]$$

$$g_{de}\ (r_{ij}) = \frac{g_{dd}\ (r_{ij})\ L\ (r_{ij})}{v} \quad ...(8)$$

Where

$$L\ (r_{ij}) = –1\ (k_F r_{ij}) + v\ (N_{ee}\ (r_{ij}) + E_{ed}\ (r_{ij})) \quad ...(9)$$

$$1\ (x) = \frac{2_{j1}(x)}{x} \quad ...(10)$$

$k_F$ 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 $E_{nm}$ sums of the elementary diagrams. The equation $g_{ee}$ denotes the terms in which both i and j are exchanged in an incomplete exchange loop, and $N_{ee}$ $(r_{ij})$ and $E_{ee}$ $(r_{ij})$ are sums of the nodal diagrams and the elementary diagrams in which i and j belong to the same permutation loop, respectively.

The sums of nodal diagrams are given by the following integral equation:

$$N_{dd}\,(r_{ij}) = r_2\,[(g_{dd} + g_{de} - N_{dd} - N_{de} - 1)_{ik}, (g_{dd} - 1)_{ik}] + r_2[(g_{dd} - N_{dd} - 1)_{1k}, (g_{de})_{1k},]$$

$$N_{de}(r_{ij}) = r_2[(g_{dd} + g_{de} - N_{dd} - N_{de} - 1)_{ik}, (g_{de} - 1)_{kj}] + r_2[(g_{dd} - N_{dd} - 1)_{1k}, (g_{ee})_{1k},] \qquad \ldots(11)$$

$$N_{dd}(r_{ij}) = r_2[(g_{de} + g_{ee} - N_{de} - N_{ee} - 1)_{ik}, (g_{de})_{kj}] + r_2[(g_{de} - N_{de} - 1)_{1k}, (g_{ee})_{1k},]$$

$$N_{ee}\,(r_{ij}) = r_2 \left[ \left( g_{ee} - N_{ee} + \frac{1}{\mathrm{v}} \right)_{1k}, (g_{ee})1k \right] \qquad \ldots(12)$$

Where Γ $[x_{ik}, y_{kj}]$ is the convolution in integral of $x_{ik}$ and $y_{kj}$ and defined as –

$$\Gamma_2\,(x_{ik}, y_{kj}) = \rho \int d^3\, r_k x\,(r_{ik})_y\,(r_{ik}) \qquad \ldots(13)$$

Where the sum over each is over all allowed combination of x, y, z, z', y' and z' which form proper exchange, and the sums of the Abe contributions in the FHNC approximation are neglected. The Abe contributions will be taken into consideration when we include the elementary diagrams through the scaling approximation. To include three body correlation effects, one replace $N_{nm}\,(r_{ij}) + E_{nm}\,(r_{ij})$ in Eqs. (7) and (8) by $N_{nm}\,(r_{ij}) + E_{nm}\,(r_{ij})\;C_{mn}\,(r_{ij})$. Here $C_{mn}\,(r_{ij})$ are diagrams dressed with chains due to the three body correlation functions, represented as –

$$C_{dd} = \Gamma_3\,[(g_{dd} - 2g_{de})_{ik}, (g_{dd})_{kj}]$$

$$C_{de} = \Gamma_3\,[(g_{ee} - g_{de})_{ik}, (g_{dd})_{ik} + r_3\,(g_{de})_{kj}, (g_{de})_{ik}]$$

$$C_{de} = \Gamma_3\,[(2\,g_{de} - g_{de})_{ik}, (g_{dd})_{ik}]$$

$$C_{ee} = \Gamma_3\,[(g_{ee})_{ik}, (g_{ee})_{ik}]$$

Where

$$\Gamma_3\,(x_{ik}, y_{kj}) = \rho \int d^3\, r_k\,[f_3^2\,(r_{ik}, r_{jk}, r_{ki}) - 1]\,x\,(r_{ik})_y\,(r_{ki})$$

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

$$u_3\,(r_{ij}, r_{jk}, r_{ki}) = \sum_{cyc} \eta(r_{ij})\eta\,(r_{ik})\,(\hat{r}_{ij}\hat{r}_{ik}) \qquad \ldots(20)$$

Where

$$H(r) = \sqrt{\lambda_1}\, r \exp\left[-\left(\frac{r - r_1}{\omega_1}\right)^2\right] \quad \ldots(21)$$

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 particles i and j. Since it was first used in a variational Monte Carlo calculations[12], this form for the three body correlations is generally used in variational HNC/FHNC methods[16]. The above parameters $\lambda_1$, $r_1$ and $\omega_1$ can be determined through a variational procedure also. In the three dimensional calculations, the value of the parameters from the Monte Carlo simulations are used, but one should determine these parameters for a two dimensional system through a variational procedure and HNC scheme because they are different in the two systems and the Monte Carlo results do not exist in two dimensions. They depend very weakly on the density, so that one use values at the equilibrium density for all density ranges.

## RESULTS AND DISCUSSION

In this paper, we have evaluated the radial distribution function g (r) as a function of r for two dimensional liquid $^3$He interacting through Aziz potential at various densities. The evaluation has been performed with the help of Chung-In-Um et al.[17] formalism. Our theoretical calculation indicates that g(r) increases with r and attains some maximum value at some value of r and thereafter it becomes almost a constant value. This behavior is something different from g(r) of liquid $^4$He in which g(r) increases and attains some maxim value and then decreases. We repeated our calculation for four densities $\rho = 0.01A^{0-2}$, $\rho = 0.015A^{0-2}$, $\rho = 0.02A^{0-2}$ and $\rho = 0.025A^{0-2}$. The trend is same for all four densities. However the values of g(r) is large for $\rho = 0.01A^{0-2}$. The results are shown in Table 1. Some recent results[18-20] also confirm the above facts.

**Table 1: An evaluated results of radial distribution function g(r) as a function of r interacting through Aziz potential at various densities.**

| $r(A^0)$ | g(r) | | | |
|---|---|---|---|---|
| | $\rho = 0.01A^{0-2}$ | $\rho = 0.015A^{0-2}$ | $\rho = 0.020A^{0-2}$ | $\rho = 0.025A^{0-2}$ |
| 2.0 | 0.825 | 0.804 | 0.786 | 0.774 |
| 2.5 | 0.917 | 0.827 | 0.800 | 0.785 |
| 3.0 | 0.958 | 0.846 | 0.829 | 0.794 |

Cont…

| **r($A^0$)** | **g(r)** | | | |
|---|---|---|---|---|
| | **ρ = 0.01$A^{0-2}$** | **ρ = 0.015$A^{0-2}$** | **ρ = 0.020$A^{0-2}$** | **ρ = 0.025$A^{0-2}$** |
| 3.5 | 0.974 | 0.855 | 0.843 | 0.816 |
| 4.0 | 0.902 | 0.864 | 0.855 | 0.833 |
| 4.5 | 0.874 | 0.843 | 0.867 | 0.854 |
| 5.0 | 0.843 | 0.825 | 0.822 | 0.867 |
| 5.5 | 0.827 | 0.806 | 0.805 | 0.845 |
| 6.0 | 0.806 | 0.795 | 0.783 | 0.812 |
| 6.5 | 0.835 | 0.822 | 0.812 | 0.807 |
| 7.0 | 0.867 | 0.854 | 0.843 | 0.842 |
| 7.5 | 0.892 | 0.866 | 0.866 | 0.862 |
| 8.0 | 0.905 | 0.873 | 0.870 | 0.885 |
| 9.0 | 0.923 | 0.885 | 0.882 | 0.892 |
| 10.0 | 0.946 | 0.897 | 0.894 | 0.899 |

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