DETERMINATION OF EQUILIBRIUM PROPERTIES OF TWO-DIMENSIONAL FLUID OF HARD DISCS

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ABSTRACT

In present paper a basic theory has been developed for calculation the leading quantum correction to the thermo dynamic properties of the two-dimensional fluid hard disc. Theoretical efforts have been made to explain the structural and thermodynamical properties of two-dimensional fluids. Although a strictly two-dimensional picture has been used in predicting the properties of absorbed film. It is required to study about hard-disc system in framing the theory of two-dimensional fluids. It is quite natural to study model fluids with only hard cores and no inter atomic attractions. The simulation results for RDF of the hard discs for same values of density solution².

Key Word:- Fluid, hard-disc, quantum correction
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INTRODUCTION

This paper is concerned with the estimation of the influence of the quantum effects on the structural and thermodynamic properties of the two-dimensional fluid whose molecules interact via a hard-disc potential. In the high density region, the behaviour of a fluid (liquid or gas) is dominated by the excluded volume effects associated with the hard-cores of its constituents. Therefore it is quite natural to study model fluids with only hard cores and no inter atomic attractions. At present the theoretical studies of liquids use almost invariably some hard-core reference fluid as basis for a perturbation expansion of the equilibrium properties of real fluids¹.². The most widely used hard-core reference fluid in two-dimensional fluid is hard discs. However the hard-disc fluid has not been studied systematically.

Several theoretical and experimental efforts have been made in recent years to understand the structural and thermodynamic properties of two-dimensional fluids. Although, ideally flat systems seldom occur, a strictly two-dimensional picture has been used in predicting the properties of absorbed film. The hard sphere fluid is treated as a reference in framing the theory of three-dimensional dense fluid. In the same way, the hard disc fluid may be treated as a reference for the two-dimensional fluid. The study of hard-disc system is essential in framing the theory of two-dimensional fluids.

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For classical hard disc fluid, considerable progress has been made. The theoretical results and simulation results are available for equation of state. The simulation results for RDF of the hard discs are also available for some values of density \( \rho d^2 \). The quantum effect increases with the decrease of temperature. At lower temperature, many terms are required to account for the quantum effects.

In this paper we study the influence of quantum effects on the equilibrium properties of the hard disc fluid. We develop a basic theory for calculating the leading quantum correction to the thermodynamic properties of the two-dimensional fluid of hard disc. The properties are expressed in terms of the RDF of the classical hard discs which is discussed in Sec. 3.

2. Basic theory:

We consider, a quantum mechanical two dimensional system of hard discs with an infinitesimal steep repulsive pair potential defined as

\[
u(r) = \begin{cases} \infty & r < d \\ 0 & r > d \end{cases}
\]

(1)

where \( d \) is the diameter of the hard discs and \( r \) denotes two-dimensional distance. The quantity of central importance in constructing the theory of quantum fluid is the Slater sum. For a two-dimensional fluid, it may be defined as

\[
W_N(1, 2, \ldots, N) = \frac{N!}{\lambda^{2N}} \exp \left( -\beta \sum_{i,j} \nu(i,j) \right)
\]

(2)

where \( \lambda \) is the thermal wavelength, \( \beta = (kT)^{-1} \) and \( \nu \) is the Hamiltonian of the system.

\[
\nu = -\frac{\beta}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i=1}^{N} \nu(i,j)
\]

(3)

Here \( \nu(i,j) \) is the pair potential between particles \( i \) and \( j \) and \( \nabla_i^2 \) is the two-dimensional Laplacian operator. In this case \( i \) denotes the position coordinate \( r_i \) of particle \( i \).

In the semiclassical limit (i.e. at high temperature limit), we can write

\[
W_N = W_N^c W_N^m
\]

(4)

where

\[
W_N^c(1, 2, \ldots, N) = \exp \left[ -\beta \sum_{i=1}^{N} \nu(i,j) \right]
\]

(5)

is the Boltzmann factor and \( W_N^m \) is a function which measures the deviation from the classical behaviour. In the case of two-dimensional fluid, \( W_N^m \) is expressed in terms of modified Ursell functions \( U_m^m \). Thus

\[
W_N^m(1,2,\ldots,N) = 1 + \sum_{i,j} U_2^m(i,j) + \sum_{i,j,k} U_3^m(i,j,k) + \sum_{i,j,k,l} U_4^m(i,j,k,l) + \ldots
\]

(6)

Thus we obtain the expression for \( W_N \)

\[
W_N(1,2,\ldots,N) = W_N^c(1,2,\ldots,N) \left( 1 + \sum_{i,j} U_2^m(i,j) + \sum_{i,j,k} U_3^m(i,j,k) + \sum_{i,j,k,l} U_4^m(i,j,k,l) + \ldots \right)
\]

(7)

For a system of hard discs, \( U_2^m \) and \( U_3^m \) have been evaluated. \( U_2^m \) is given by

\[
U_2^m(r) = \phi_0(r) + \phi_1(r) + \ldots, \quad r > d
\]

(8)

where

\[
\phi_0(r) = -\exp(-X^2)
\]

(9a)
\[
\phi_1(r) = \left(\frac{1}{2}\sqrt{\frac{2}{\pi}}\right) \frac{\rho}{d} X^2 \text{erfc}(X)
\]  \tag{9b}

Here
\[X = \left[\frac{(2\pi)^{1/2} / (\lambda / d)}{[r / d - 1]}\right] \text{erfc}(X)
\]
and \text{erfc}(X) is the complementary error function.

In quantum statistical mechanics, the chemical potential \(\mu\) can be written as
\[
\beta \mu = -\ln \left[\frac{Q_N + 1}{Q_N}\right]
\]  \tag{10}
where \(Q_N\) is the partition function defined as
\[
Q_N = \frac{1}{N!} \left(\frac{2\pi}{\lambda}ight)^{2N} \prod_{i=1}^{N} dr_i
\]  \tag{11}

Substituting Eq. (7) in (11), we get
\[
Q_N = Q_N^c \left[1 + \frac{(1/2)\rho^2}{2} \sum_{i=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)\right]
\]  \tag{12}
where \(Q_N^c\) and \(g_N^c(1,2)\) are, respectively, the canonical partition function and RDF of the classical fluid. Using Eq. (12), Eq. (1) can be written as
\[
\beta \mu = \beta \mu^c - \left(\frac{1}{2}\right) \frac{\rho^2}{2} \sum_{i=1}^{N} \rho \frac{g_N^c(1,2)}{2} dr_1 dr_2 + O(\lambda^2)
\]  \tag{13}
where
\[
\beta \mu^c = -\ln \left[\frac{g_N^c(1,2)}{g_N^c(N,1)}\right]
\]  \tag{14}
\(\mu^c\) is the classical chemical potential.

Using the relation
\[
\rho^2 \left[\sum_{i=1}^{N} \rho g_N^c(1,2)\right] = \left(\frac{1}{N}\right) N \left[\rho^2 \sum_{i=1}^{N} \rho g_N^c(1,2)\right] = \left(\frac{1}{N}\right) N \left[\rho^2 \sum_{i=1}^{N} \rho g_N^c(1,2)\right]
\]  \tag{15}
We drop the subscript \(N\) from now on in this paper and write an expression for the chemical potential as
\[
\beta \mu = \beta \mu^c - \left(\frac{1}{2}\right) \frac{\rho^2}{2} \sum_{i=1}^{N} \rho \sum_{j=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)
\]  \tag{16}

Other thermodynamic properties can be obtained from the classical potential. Thus the Helmholtz free energy is given by
\[
\beta A/N = (\beta A^c/N) - \left(\frac{1}{2}\right) \frac{\rho^2}{2} \sum_{i=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)
\]  \tag{17}

and the pressure equation is
\[
\beta P/\rho = (\beta P^c/\rho) - \left(\frac{1}{2}\right) \frac{\rho^2}{2} \sum_{i=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)
\]  \tag{18}
where \(A^c\) and \(P^c\) are, respectively, the free energy and pressure of the classical fluid. Substituting Eq. (8) in Eq. (17), we obtain an expression for the free energy of the hard disc fluid, correct to the first order quantum correction
\[
\beta A/N = (\beta A^c/N) - \sqrt{2}\left(\frac{\rho^2}{2}\right) \eta \sum_{i=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)
\]  \tag{19}
where
\[
\eta = \frac{\pi}{4} \lambda d^2
\]
is the packing fraction and \(g_N^c(d)\) is the classical RDF at the contact. Similarly Eqs. (18) and (16) can be evaluated to give
\[
\beta P/\rho = (\beta P^c/\rho) + \sqrt{2}\left(\frac{\rho^2}{2}\right) \eta \sum_{i=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)
\]  \tag{20}
and
\[
\beta \mu = \beta \mu^c + \sqrt{2}\left(\frac{\rho^2}{2}\right) \eta \sum_{i=1}^{N} \rho g_N^c(1,2) dr_1 dr_2 + O(\lambda^2)
\]  \tag{21}
The RDF $g^c(d)$ can be obtained by solving the PY integral equation discussed in the following section. Alternately $g^c(d)$ can also be obtained using the pressure equation if the pressure is known. In the two-dimensional classical system of hard-discs, the pressure equation is given by\textsuperscript{15}

$$\beta P_c/\rho = 1 + 2\eta g^c(d)$$

(22)

Then it can be shown that

$$\frac{d}{d} \left( \frac{\beta A^c}{N} \right) = \pi \rho d^2 g^c(d)$$

(23)

$$\frac{d}{d} \left( \frac{\beta P^c}{\rho} \right) = \pi \rho d^2 g^c(d) + \eta( g^c(d)/\eta)$$

(24)

and

$$\frac{d}{d} \left( \beta \mu^c \right) = \pi \rho d^2 \left[ 2g^c(d) + \eta( g^c(d)/\eta) \right]$$

(25)

and one can write Eqs.(17) and (19) in the form

$$A = A^c + A^\lambda$$

(26)

$$P = P^c + AP^\lambda$$

(27)

$$\mu = \mu^c + \mu^\lambda$$

(28)

where

$$A^\lambda = d( A^c/ d)$$

(29)

$$P^\lambda = d( \partial P^c/ d)$$

(30)

$$\mu^\lambda = d( \partial \mu^c/ d)$$

(31)

and

$$\Lambda = (1/2\sqrt{2}) (\lambda/d)$$

(32)

Thus the leading quantum corrections to the thermodynamic properties of the hard disc fluid can be obtained by replacing the actual diameter $d$ by and effective diameter $(d + 2^{3/2} \Lambda)$. This is identical to those found for hard sphere\textsuperscript{9,16}. Recently it is generalised for hard sphere fluid\textsuperscript{17}.

### 3. Percus-Yevick integral equation for Radial distribution function of hard-disc fluid:

In this section, we consider the RDF of the two-dimensional fluid of hard-discs.

We employ the Percus-Yevick (PY) integral equation, which can be solved analytically for the hard-disk fluid.

In the PY approximation we have a relation

$$Y(1,2) + C(1,2) - g(1,2) = 0$$

(33)

Using the relation

$$g(1,2) = [1 + f(1,2)] Y(1,2)$$

(34)

where

$$f(1,2) = \exp [-\beta u(1,2)] - 1$$

we have

$$c(1,2) = f(1,2) Y(1,2)$$

(35)

This equation, when substituted in the Ornstein-Zernicke equation\textsuperscript{18}

$$g(1,2) - 1 = c(1,2) + \rho c(1,3) [g(3,2) - 1] dr_3$$

(36)

gives the PY-integral equation for $g(1,2)$

$$g(1,2) = \exp [-\beta u(1,2)] [1 + \rho [1 - \exp [-\beta u(1,3)] g(1,3) (g(2,3) - 1) dr_3$$

(37)

This gives an expression for $Y(1,2)$

$$Y(1,2) = 1 + \rho \{ 1 - \exp (-\beta u(1,3)) g(1,3) (g(2,3) - 1)dr_3$$

(38)

The PY-approximation is found to be superior, when the repulsive forces are dominant.

For hard discs of diameter $d$, we have the condition that

$$g(r) = 0 \quad r < d$$

(39)

On the other hand the function $Y(r)$ is given by

$$Y(r) = \exp [ -\beta u(r)] g(r)$$

(40)

Which remains continuous at $r = d$.

In case of the hard-disc fluid, Eq.(35) reduces to
Table 1. The RDF for hard disc fluid for $0.1 \leq \rho d^2 \leq 0.55$

| $\rho d^2 \rightarrow$ | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.55 |
|------------------------|-----|-----|-----|-----|-----|------|
| 1.000                  | 1.136 | 1.306 | 1.522 | 1.802 | 2.177 | 2.414 |
| 1.048                  | 1.126 | 1.280 | 1.470 | 1.711 | 2.021 | 2.210 |
| 1.096                  | 1.116 | 1.254 | 1.421 | 1.625 | 1.876 | 2.202 |
| 1.143                  | 1.106 | 1.230 | 1.375 | 1.544 | 1.741 | 1.849 |
| 1.191                  | 1.097 | 1.206 | 1.330 | 1.468 | 1.616 | 1.691 |
| 1.239                  | 1.088 | 1.184 | 1.288 | 1.397 | 1.502 | 1.549 |
| 1.287                  | 1.079 | 1.162 | 1.248 | 1.330 | 1.398 | 1.420 |
| 1.334                  | 1.070 | 1.141 | 1.210 | 1.269 | 1.304 | 1.306 |
| 1.382                  | 1.061 | 1.121 | 1.175 | 1.212 | 1.220 | 1.205 |
| 1.430                  | 1.053 | 1.102 | 1.141 | 1.160 | 1.144 | 1.116 |
| 1.478                  | 1.046 | 1.085 | 1.110 | 1.113 | 1.077 | 1.040 |
| 1.525                  | 1.3038 | 1.068 | 1.082 | 1.070 | 1.019 | 0.974 |
| 1.573                  | 1.032 | 1.053 | 1.056 | 1.032 | 0.969 | 0.919 |
| 1.621                  | 1.025 | 1.038 | 1.032 | 0.998 | 0.927 | 0.875 |
| 1.669                  | 1.019 | 1.025 | 1.011 | 0.969 | 0.893 | 0.839 |
| 1.717                  | 1.013 | 1.013 | 0.992 | 0.944 | 0.865 | 0.814 |
| 1.764                  | 1.009 | 1.003 | 0.976 | 0.925 | 0.846 | 0.797 |
| 1.813                  | 1.004 | 0.993 | 0.963 | 0.910 | 0.834 | 0.790 |
| 1.860                  | 1.000 | 0.986 | 0.953 | 0.900 | 0.830 | 0.792 |
| 1.908                  | 1.997 | 0.980 | 0.946 | 0.896 | 0.835 | 0.805 |
| 1.956                  | 0.995 | 0.977 | 0.944 | 0.900 | 0.852 | 0.833 |
| 2.003                  | 0.994 | 0.978 | 0.950 | 0.916 | 0.890 | 0.887 |
| 2.051                  | 0.995 | 0.982 | 0.962 | 0.944 | 0.944 | 0.960 |
| 2.099                  | 0.996 | 0.986 | 0.972 | 0.966 | 0.986 | 1.015 |
| 2.147                  | 0.997 | 0.989 | 0.981 | 0.984 | 1.017 | 1.053 |
| 2.195                  | 0.997 | 0.991 | 0.989 | 0.999 | 1.040 | 1.079 |
| 2.243                  | 0.998 | 0.994 | 0.994 | 1.010 | 1.054 | 1.093 |
| 2.290                  | 0.998 | 0.996 | 0.9999 | 1.017 | 1.062 | 1.098 |
| 2.338                  | 0.999 | 0.998 | 1.002 | 1.022 | 1.065 | 1.096 |
| 2.386                  | 0.999 | 0.999 | 1.006 | 1.025 | 1.063 | 1.088 |
| 2.434                  | 0.999 | 1.000 | 1.007 | 1.026 | 1.059 | 1.077 |
| 2.482                  | 1.000 | 1.001 | 1.008 | 1.026 | 1.051 | 1.063 |
| 2.530                  | 1.000 | 1.001 | 1.009 | 1.024 | 1.042 | 1.048 |
| 2.578                  | 1.000 | 1.001 | 1.009 | 1.021 | 1.033 | 1.031 |
| 2.625                  | 1.000 | 1.002 | 1.008 | 1.018 | 1.022 | 1.016 |
\[ C(r) = -Y(r), \quad r < d \]
\[ = 0, \quad r > d \]  

(41)

Substituting Eqs. (39) and (41) in Eq. (38) leads to an integral equation for \( Y(r) \)

\[ Y(r) = 1 + \rho \int_{r'} Y(r) Y(|r-r'|) \, dr' \quad \text{for} \quad r < d \]
\[ + \int_{r'} Y(r) \, dr' \quad \text{for} \quad r > d \]  

(42)

We follow the method of Lado\(^{18}\) to evaluate Eq. (42) and obtain the values of \( g(r) \) for the hard disc fluid over the range of density \( \rho d^2 \). The values of \( g(r) \) of the hard disc fluid are reported in Tables 1 and 2 for \( 0.10 \leq \rho d^2 \leq 0.55 \) and \( 0.60 \leq \rho d^2 \leq 0.75 \), respectively. For these states the simulation results are not available. So no comparison can be made. However, in order to check the accuracy of two results, we employ them to calculate the equation of state, using the relation....
| \( \rho d^2 \rightarrow \) | 0.60 | 0.65 | 0.70 | 0.75 |
|----------------|------|------|------|------|
| \( r/d \)      |      |      |      |      |
| 1.000           | 2.697| 3.039| 3.457| 3.978|
| 1.053           | 2.398| 2.644| 2.931| 3.269|
| 1.107           | 2.127| 2.292| 2.470| 2.661|
| 1.161           | 1.885| 1.983| 2.076| 2.055|
| 1.215           | 1.672| 1.716| 1.742| 1.740|
| 1.269           | 1.485| 1.488| 1.465| 1.405|
| 1.323           | 1.324| 1.295| 1.238| 1.143|
| 1.377           | 1.187| 1.135| 1.056| 0.942|
| 1.430           | 1.071| 1.005| 0.913| 0.792|
| 1.484           | 0.975| 0.900| 0.804| 0.687|
| 1.538           | 0.897| 0.820| 0.726| 0.617|
| 1.591           | 0.837| 0.761| 0.673| 0.579|
| 1.646           | 0.792| 0.720| 0.643| 0.566|
| 1.699           | 0.763| 0.698| 0.633| 0.575|
| 1.753           | 0.747| 0.692| 0.612| 0.604|
| 1.807           | 0.745| 0.702| 0.668| 0.651|
| 1.861           | 0.757| 0.728| 0.713| 0.718|
| 1.915           | 0.786| 0.774| 0.780| 0.808|
| 1.969           | 0.838| 0.847| 0.878| 0.937|
| 2.022           | 0.938| 0.980| 1.053| 1.65 |
| 2.076           | 1.032| 1.100| 1.202| 1.342|
| 2.130           | 1.094| 1.171| 1.276| 1.409|
| 2.184           | 1.129| 1.202| 1.295| 1.400|
| 2.238           | 1.143| 1.206| 2.278| 1.344|
| 2.291           | 1.141| 1.190| 1.234| 1.262|
| 2.345           | 1.128| 1.160| 1.179| 1.170|
| 2.399           | 1.108| 1.122| 1.117| 1.078|
| 2.453           | 1.083| 1.081| 1.056| 0.995|
| 2.507           | 1.055| 1.040| 1.000| 0.925|
| 2.560           | 1.028| 1.003| 0.952| 0.871|
| 2.614           | 1.033| 0.970| 0.914| 0.835|
| 2.668           | 0.981| 0.943| 0.887| 0.815|
| 2.722           | 0.963| 0.923| 0.870| 0.811|
| 2.776           | 0.909| 0.911| 0.866| 0.811|
| 2.829           | 0.940| 0.907| 0.871| 0.845|
Table 3. Equation of state $\beta P / \rho$ for hard disc fluid

| $\eta$ | From Eq.(43) | From Eq.(44) |
|--------|--------------|--------------|
| 0.10   | 1.1785       | 1.1787       |
| 0.20   | 1.4104       | 1.4119       |
| 0.30   | 1.7170       | 1.7237       |
| 0.40   | 2.1320       | 2.1528       |
| 0.50   | 2.7094       | 2.7649       |
| 0.55   | 3.0858       | 3.1733       |
| 0.60   | 3.5421       | 3.6783       |
| 0.65   | 4.1027       | 4.3128       |
| 0.70   | 4.8012       | 5.1243       |
| 0.75   | 5.6864       | 6.1843       |
\[ \beta P_c/\rho = 1 + 2\eta g^2(d) \]  

(43)

The results are demonstrated in Table 3. We have also calculated the equation of state using the expression

\[ \beta P_c/\rho = (1 + 0.126\eta^2) / (1 - \eta)^2 \]  

(44)

The argument is good for \( \rho d^2 \leq 0.50 \). Descripancy increases with densities. One is expected to improve the results by using the PY2 approximation. However it is time consuming, so it is not attempted here.

4. RESULT AND DISCUSSION

A method has been developed for calculating the leading quantum correction to the thermodynamical properties and classical RDF of the two-dimensional fluid of hard discs. This gives good results at high temperature where quantum effects are small. The estimation of the influence of the quantum effects on the structural and thermodynamical properties of the two-dimensional fluid whose molecules interact via a hard-disc potential. At present the theoretical studies of liquids are almost invariably some hard core reference fluid as basis for a perturbation expansion of the equilibrium properties of real fluids\textsuperscript{1,2}.

The quantum effects increases with the decreases of temperature. At lower temperatures, many terms are required to account for quantum for quantum effects. In the semiclassical limit (i.e. at high temperature) where quantum limit (i.e. at high temperature) whence quantum effects are small and treated as a correction to the classical behaviour, the usual way is to expand the properties about this classical values.

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