On Pair–Particle Distribution in Imperfect Bose Gas

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Abstract

A simple model of estimating the radial distribution function of an imperfect Bose gas in the ground state is presented. The model is based on integro–differential equations derived by considering the space boson distribution in an external field. With the approach proposed, the particular case of dilute Bose gas is investigated within the hard sphere approximation and beyond.

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1 Introduction

This letter is devoted to investigation of spatial particle correlations in many–body systems in the spirit of the approach of Ref.1 which consists in the following. Let us consider a uniform many–body system with the interaction potential \( \Phi(r) \) at the particle density \( n = N/V \). As it has been shown for the classical case \([1]\), the radial distribution function of this system \( g(r) \) can be calculated with

\[
g(r) = \frac{n_{\text{str}}(r)}{n},
\]

where \( n_{\text{str}}(r) \) denotes the density of the mentioned particles at the point \( \vec{r} \) \( (r \equiv | \vec{r} |) \) of the nonuniform structure appearing under the action of the external field \( \Phi(r) \) on the system considered. Here it is implied that

\( \Phi(r) \to 0, n_{\text{str}}(r) \to n \ (r \to \infty). \)

Relation (1) seems quite natural because the quantity \( g(| \vec{r}_1 - \vec{r}_2 |)/V \) is the probability of finding the second particle of the system at the point \( \vec{r}_2 \) provided that the first one is at the point \( \vec{r}_1 \). Therefore, we are able to calculate \( g(r) \) by considering the space distribution of the particles with the numbers 2, ..., \( N \) in the external field generated by the first particle fixed at the origin of the coordinates.

The aim of the present article is to clarify to what extent relation (1) is suitable for the case of an imperfect Bose gas at zero temperature. The paper is organized as follows. To simplify understanding of the subject, the results of investigating relation (1) in the classical case are briefly discussed in the second section. The third paragraph contains the main items of
deriving integro–differential equations for $g(r)$ of a Bose gas in the ground state on the basis of (1). To check validity of the equations, in the fourth section the Bose gas of the hard spheres is considered in the weak coupling approximation. At last, the fifth paragraph is the consideration of a dilute Bose gas beyond the hard sphere simplification.

2 Classical Case

To demonstrate reasonable character of relation (1) and simplify understanding of further arguments, let us consider a many–body system of classical particles interacting with each other by means of the potential $\Phi(r)$ and being in the external field $\Phi(r)$. In this case we are able to calculate the structure function $n_{str}(r)$ with the well–known Thomas–Fermi approximation [2]. According to this method, $n_{str}(r)$ can be found with the following condition:

$$\mu(n_{str}(r)) + \Phi(r) + U(r) = const \quad (\forall \vec{r}),$$

where $\mu(n_{str}(r))$ is the chemical potential of the ideal gas of the given particles at the density $n_{str}(r)$; $U(r)$ denotes the energy of the interaction of the particle at the point $\vec{r}$ with the surrounding particles. To complete the calculational procedure, we use the reasonable integral relation

$$U(r) = \int_V \Phi(|\vec{r} - \vec{y}|) n_{str}(y) d\vec{y}.$$  

Now, we have got everything to obtain an integral equation for $g(r)$ in the classical case. At some point $\vec{r}_{far}$ being far enough from the origin of the external field, expression (2) is written as

$$\mu(n) + n \int_V \Phi(|\vec{r}_{far} - \vec{y}|) d\vec{y} = const$$

provided that we limit ourselves to the situation

$$\lim_{r \to \infty} \Phi(r) = 0.$$  

Using formulae (1)–(4), the classical approximation

$$\mu(n) - \mu(n_{str}(r)) = -\theta \ln (n_{str}(r)/n)$$

and the relation

$$\lim_{V \to \infty} \frac{\int_V \Phi(|\vec{r}_{far} - \vec{y}|) - \Phi(|\vec{r} - \vec{y}|)d\vec{y}}{\int_V \Phi(|\vec{r} - \vec{y}|)d\vec{y}} = 0,$$

we arrive at

$$-\theta \ln g(r) = \Phi(r) + n \int_V (g(y) - 1)\Phi(|\vec{r} - \vec{y}|)d\vec{y}$$

Note that relation (5) is valid for lots of the known potentials, in particular, for the integrable and Coulomb—like potentials.

We have derived integral equation (6) neglecting spatial particle correlations when calculating $U(r)$ [1]. Therefore, it can only be used for the integrable and Coulomb–like potentials but not for the strongly singular potentials with the short range behaviour of the Lennard–Jones
type. To include the correlations, we should be based on a more accurate approximation of $U(r)$. The simplest one is the following [1]:

$$U(r) = \int_V g(|\vec{r} - \vec{y}|) \Phi(|\vec{r} - \vec{y}|) n_{str}(y) d\vec{y}. \quad (7)$$

With (1), (2) and (7) we find

$$-\theta \ln g(r) = \Phi(r) + n \int_V (g(y) - 1) g(|\vec{r} - \vec{y}|) \Phi(|\vec{r} - \vec{y}|) d\vec{y}. \quad (8)$$

In spite of the simplest version of approximating $U(r)$ with the space particle correlations taken into account, integral equation (8) is very similar to the well–known Bogoliubov equation for $g(r)$ (see discussion in Ref.1). As it is seen, relations (1) and (8) can be used for the integrable, Coulomb–like as well as Lennard–Jones potentials because $g(r)\Phi(r) \rightarrow 0$ ($r \rightarrow 0$) for the strongly singular $\Phi(r)$. Thus, in this paragraph we have been convinced of the correctness of relation (1) for the classical many–body systems. To elucidate the problem of using (1) in the quantum case, we further investigate many–boson system in the ground state.

### 3 Bose Gas in the Ground State

One could expect that in the quantum case being essentially more complicated than the classical one, such a simple approach based on expression (1) is not able to provide us with satisfactory results. However, in the situation with no exchange effects, for the Bose gas in the ground state, relation (1) yields a quite reasonable estimate of $g(r)$ with only one obvious correction. To obtain more accurate data on $g(r)$ for a uniform many–body system of bosons with the mass $m$, we need to investigate a nonuniform Bose gas made of particles with the mass $m/2$. It should be noted, that as the quantity $m$ does not appear in the integral equations of the previous paragraph, the mentioned correction does not contradict the classical case either.

Now, let us consider the system of $N - 1$ zero-spin bosons with the mass $m/2$ at zero temperature and in the external field $\Phi(r)$. As before, we assume the interparticle potential to be $\Phi(r)$. The simplest way to find $n_{str}(r)$ in this case is to adopt the Hartree approximation for the wave function of the system

$$\psi_s = \prod_{i=1}^{N-1} \psi(\vec{r}_i), \quad (9)$$

where $\psi(\vec{r}_i)$ denotes the normalized wave function of the $i$–th boson in the ground state. As $\psi(\vec{r})$ can be chosen to be a real function [3], we have

$$n_{str}(r) = (N - 1) \psi^2(\vec{r}), \quad (10)$$

and, therefore, $\psi(\vec{r}) = \psi(r)$. Thus, to calculate $n_{str}(r)$, we need evaluating $\psi(r)$ which obeys the following Schrödinger equation:

$$-\frac{\hbar^2}{m} \Delta \psi(r) + \Phi(r)\psi(r) + (N - 2)\psi(r) \int_V \Phi(|\vec{r} - \vec{y}|)\psi^2(y) d\vec{y} = E_0 \psi(r). \quad (11)$$
Here $E_0$ denotes the energy of a boson in the ground state. Not to solve the eigenvalue problem, let us take into account that at the point $\vec{r}_{\text{far}}$ being far enough from the origin of the coordinates

$$\psi(r_{\text{far}}) = \frac{1}{\sqrt{V}} \quad (\Phi(r_{\text{far}}) = 0).$$  

(12)

Substituting (12) into (11) one can obtain

$$\frac{N - 2}{V} \int_V \Phi(| \vec{r}_{\text{far}} - \vec{y} |) d\vec{y} = E_0.$$  

(13)

Further, with the use of relations (5), (11) and (13) we arrive at

$$\frac{\hbar^2}{m} \triangle \psi(r) = \Phi(r) \psi(r) +$$

$$+ \frac{(N - 2)}{V} \psi(r) \int_V \Phi(| \vec{r} - \vec{y} |) \left(V \psi^2(y) - 1\right) d\vec{y}.$$  

(14)

Taking into account that in the thermodynamic limit

$$\frac{N - 2}{V} \approx \frac{N}{V} = n$$

and using (5), (10) and (14), we derive the following integro–differential equation for $g(r)$ of a cold Bose gas:

$$\frac{\hbar^2}{mg^{1/2}(r)} \triangle g^{1/2}(r) = \Phi(r) +$$

$$+ n \int_V \Phi(| \vec{r} - \vec{y} |) (g(y) - 1) d\vec{y}.$$  

(15)

By analogy with the classical case this equation can be generalized to the situation of strongly singular potentials

$$\frac{\hbar^2}{mg^{1/2}(r)} \triangle g^{1/2}(r) = \Phi(r) +$$

$$+ n \int_V g(| \vec{r} - \vec{y} |) \Phi(| \vec{r} - \vec{y} |) (g(y) - 1) d\vec{y}.$$  

(16)

Remark that equations (15) and (16) have been derived for the spinless bosons but they are also valid for bosons with nonzero spin.
4 Bose Gas with the Hard Sphere Interaction

To verify the reasonable character of equations (15) and (16), let us consider the well–known example of the hard–sphere Bose gas in the weak coupling approximation characterized by the relation

\[ g(r) = 1 - \varepsilon(r), \quad \varepsilon(r) \ll 1. \]

Taking account of this relation and limiting oneself to the first order in \( \varepsilon(r) \), one can rewrite equation (15) (or (16)) as

\[ -\frac{\hbar^2}{2m} \Delta \varepsilon(r) = \Phi(r) - n \int V \Phi(|\vec{r} - \vec{y}|) \varepsilon(y) d\vec{y}. \]  

(17)

The new equation is solved with the Fourier transformation and gives the following result:

\[ g(r) = 1 - \frac{1}{(2\pi)^3} \int \frac{\tilde{\Phi}(q) \exp(i\vec{q}\cdot\vec{r})}{\hbar^2 q^2 / 2m + n\Phi(q)} d\vec{q}, \]

(18)

where \( \tilde{\Phi}(q) \) denotes the Fourier transform of \( \Phi(r) \). Inserting \( \tilde{\Phi}(q) = \frac{4\pi \hbar^2 a}{m} \), where \( a \) denotes the sphere radius, we find

\[ g(r) = 1 - \frac{4a}{r} f_{est}(x), \quad x \equiv 4r\sqrt{\pi an}, \]

(19)

here \( f_{est}(x) = 0.5 \exp(-x/\sqrt{2}) \). How well this estimate is coordinated with the explicit expression (see Ref.4)

\[ g(r) = 1 - \frac{4a}{r} f_{expl}(x), \]

(20)

is shown in the following table:

| \( x \) | \( f_{est}(x) \) | \( f_{expl}(x) \) | \( x \) | \( f_{est}(x) \) | \( f_{expl}(x) \) | \( x \) | \( f_{est}(x) \) | \( f_{expl}(x) \) | \( x \) | \( f_{est}(x) \) | \( f_{expl}(x) \) |
|-------|-----------------|-----------------|-------|-----------------|-----------------|-------|-----------------|-----------------|
| 0.0   | 0.500           | 0.500           | 2.0   | 0.122           | 0.098           | 5.0   | 0.015           | 0.012           | 10.0  | 0.004          | 0.001           |
| 0.5   | 0.351           | 0.328           | 2.5   | 0.085           | 0.067           | 10.0  | 0.0004         | 0.001           |
| 1.0   | 0.246           | 0.217           | 3.0   | 0.060           | 0.046           | 20.0  | 3.6 \times 10^{-6} | 0.0002         |
| 1.5   | 0.173           | 0.145           | 4.0   | 0.030           | 0.023           |       |                 |                 |

As it is seen, estimate (19) is in reasonable agreement with the explicit result (20) except the region of large distances

\[ r > \frac{10}{\sqrt{2}} r_c, \]

where the correlation length

\[ r_c = \sqrt{\frac{1}{8\pi an}} \]

is the same for both the (19) and (20) expressions. Note that in the case of (19) the correlation length can be found from \( \exp(-x/\sqrt{2}) = \exp(-1) \). Estimation (19) does not give the known
$1/r^4$—decay of $g(r)$ for $r \gg r_c$ [4, 5]. Therefore, we need to be careful investigating the spectrum of the low-lying excitations in a Bose gas with $g(r)$ estimated from equations (13) and (16). However, the model proposed can yield satisfactory evaluations for the main thermodynamic characteristics which are essentially determined by the values of $g(r)$ at $r < r_c$ and $r \sim r_c$. For example, the ground state energy calculated with (19) is given by

$$E = \frac{2\pi \hbar^2}{m} \frac{a^2}{V} \left( 1 + 4.01 \sqrt{\frac{a^3 N}{V}} \right).$$

(21)

The explicit result (20) leads [6] to the expression

$$E = \frac{2\pi \hbar^2}{m} \frac{a^2}{V} \left( 1 + 4.81 \sqrt{\frac{a^3 N}{V}} \right)$$

(22)

first found by Lee and Yang [7]. Besides, we can improve our estimates treating the boson mass in equations (15) and (16) as a free parameter of the model. In particular, to derive (22) we should replace $m$ by $1.13m$ in (15) or (16).

5 Natural Dilute Bose Gas

A helpful feature of equations (15) and (16) consists in the possibility of operating with them beyond the weak coupling and hard spheres. In particular, in investigating a natural dilute Bose gas the expansion in powers of $n$ for $g(r)$ may be of interest. To find it let us assume that

$$g^{1/2}(r) = u_0(r) + n u_1(r) + \ldots$$

(23)

and substitute (23) into, say, equation (16). We arrive at the following differential equations:

$$\frac{\hbar^2}{m} \Delta u_0(r) - \Phi(r) u_0(r) = 0,$$

(24)

and

$$\frac{\hbar^2}{m} \Delta u_1(r) - \Phi(r) u_1(r) = u_0(r) \int_V u_0^2(|\vec{r} - \vec{y}|) \Phi(|\vec{r} - \vec{y}|) (u_0^2(y) - 1) d\vec{y}. $$

(25)

Relation (24) is exactly the equation which is often used to find the zero density limit for the function of the boson two–body distribution [8]. Equations (24) and (25) testify to that $g(r)$ of a natural Bose gas in the ground state is an analytical function of $n$ contrary to the case of the weakly interacting Bose gas of the hard spheres.
6 Summary

The integro–differential equations for the radial distribution function of a cold Bose gas with the interaction potential \( \Phi(r) \), have been found via investigating the spatial boson distribution in the external field \( \Phi(r) \). Checking the validity of these equations, we have considered the weakly interacting Bose gas of the hard spheres and derived the reasonable picture of the two–body correlations and the satisfactory estimate of the mean energy. In the case of a natural Bose gas ( beyond the hard spheres and weak coupling ), the equations have provided us with the expansion in powers of \( n \) for \( g(r) \) that can be useful at investigating a dilute many–boson system.

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