Dilute Hard “Sphere” Bose Gas in Dimensions 2, 4 and 5

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(Dated: July 20, 2008)

The ground state energy for a dilute hard “sphere” Bose gas in various dimensions is studied theoretically.

PACS numbers: 03.75.Hh, 05.30.Jp, 67.85.Bc, 03.65.-w

Consider a collection of $N$ Bose hard spheres in a periodic $L \times L \times L$ box. The ground state energy $E_0$ of the system was given \cite{1} in an asymptotic expansion in 1957:

$$
\frac{E_0}{N} = 4 \pi a \rho [1 + \frac{128}{15 \sqrt{\pi}} \sqrt{\rho a^3} + ...]
$$

(1)

in the limit that $N \to \infty$ at fixed density $\rho = N/\Omega$, for small value of $\rho a^3$. We follow the notation of reference 1, now usually called LHY. At that time equation (1) was a purely theoretical result. Today with the amazing developments of laser technology and computer power it has become possible \cite{2} to test the validity of the expansion (1). In the present paper we attempt to find similar expansions for the same problem in dimensions 2, 4 and 5.

For dimension 1, the problem had been solved in reference 3.

**REVIEW OF DIMENSION 3**

The one dimensional problem is special since there is no diffraction, only reflection, in one dimension. In higher dimensions diffraction is present.

For the ground state only S-wave scattering need be \cite{3} considered in the limit of fixed $\rho$, $N \to \infty$ and $a \to 0$. In this section, we review the derivation of equation (1) in dimension 3.

The boundary condition that the wave function vanishes when $|r_i - r_j| = 0$ is mathematically simple to define, but difficult to analyze. We shall therefore replace it by a potential energy called the “pseudopotential” originally \cite{3} due to Fermi:

$$
H = - \sum_i \nabla_i^2 + V
\]

$$

$$
V = 4 \pi a \int d^3 r_1 d^3 r_2 \psi^*(r_1) \psi^*(r_2) \delta^3(r_1 - r_2) \frac{\partial}{\partial r_{12}} \quad [2]
$$

$$
\times [r_{12} \psi(r_1) \psi(r_2)].
$$

All equations with a square bracket refer to equations in LHY.

To generalize to other dimensions we need to understand why the pseudopotential can replace the boundary condition when two spheres touch, at least in low orders of $a$. Now it is known from electrostatics that

$$
\nabla^2 \frac{1}{r} = -4 \pi \delta^3(r).
$$

(2)

Thus for 2 bodies

$$
[-\nabla^2 + 4 \pi a \delta^3(r) \frac{\partial}{\partial r}] \psi = 4 \pi a \delta^3(r) \frac{\partial}{\partial r} \psi - 1],
$$

(3)

if

$$
\psi = 1 - \frac{a}{r}.
$$

(4)

Now (a) the RHS of (3) when operating on any function that is not singular at $r = 0$ gives zero. (b) $\psi$ satisfies the boundary condition that $\psi = 0$ at $r = a$, so that $\psi$ is the correct $S$ wave scattered wave function for the collision of particles 1 and 2. This means that the $N = 2$ problem can be replaced by a pseudopotential

$$
V = 8 \pi a \delta^3(r_{12}) \frac{\partial}{\partial r_{12}} r_{12},
$$

(PP3)

where we have taken into account the reduced mass for the 2 body system. For the $N$ body problem we thus obtain the potential $V$ of equation [2] in LHY.

The next step is to use the simpler potential $V'$ [3] in LHY which operating on any nonsingular wave function gives the same result as $V$.

With $V'$ LHY obtained for the ground state the first order perturbation energy and wave function. With $V'$ the second order perturbation energy, however, diverges. LHY showed that is due to the fact $V'$ is not $V$ in the second order calculation. Using $V$ and not $V'$ in the second order calculation, LHY showed that

$$
E_0 = 4 \pi a \rho N - \sum \left[ k^2 + k_0^2 - k \sqrt{k^2 + 2 k_0^2} - \frac{k_0^4}{2 k^2} \right],
$$

(23)

which is convergent and gave equation (1) above.

**DIMENSION 4**

To generalize to dimension 4 we need generalizations of equations (2)–(4):

$$
\nabla^2 \frac{1}{r^2} = -4 \pi^2 \delta^4(r).
$$

(5)


\[-\nabla^2 + 4\pi^2 a^2 \delta^4 (r) \frac{\partial^2}{2\partial \tau^2} r^2] \varphi = 4\pi^2 a^2 \delta^4 (r) \times [\frac{\partial^2}{2\partial \tau^2} r^2 - 1], \quad (6)\]

and

\[\varphi = 1 - \frac{a^2}{r^2}. \quad (7)\]

The pseudopotential now becomes

\[V = 8\pi^2 a^2 \delta^4 (r) \frac{\partial^2}{2(\partial \tau)^2} r^2 \quad \text{(PP4)}\]

and

\[V' = 4\pi^2 a^2 \int d^3 r \psi^*(r) \psi^*(r) \psi(r) \psi(r) \quad (8)\]

We can now follow the steps in LHY to arrive at the energy $E_0$:

\[E_0 = 4\pi^2 a^2 \rho N - \sum' [k^2 + k_0^2 - k \sqrt{k^2 + 2k_0^2} - \frac{k_0^2}{2k^2}], \quad (9)\]

where now

\[k_0 = \sqrt{8\pi^2 \rho a^2}. \quad (10)\]

The summation in (9) converts into an integral:

\[N64\pi^4 a^6 \rho^2 \int_0^\infty \xi^2 d\xi [1 + \xi^2 - \xi \sqrt{\xi^2 + 2} - \frac{1}{2\xi}], \quad (11)\]

where $k = k_0 \xi$. This last integral has a ultra violet divergence:

\[\int \cong - \int_0^{\infty} \frac{d\xi}{2\xi} = -\frac{1}{2} \ln \xi \cong -\frac{1}{2} \ln k \cong \infty. \quad (12)\]

The cutoff for large $k$ is $\sim \frac{1}{\xi}$. Thus the integral is equal to $-\sim \frac{1}{2} \ln k_0$. We have thus

\[\frac{E_0}{N} = 4\pi^2 a^2 \rho + 32\pi^4 a^6 \rho^2 [\ln k_0 + \cdot \cdot \cdot]. \quad (13)\]

The depletion of the $k = 0$ state for dimension 3 was given in LHY:

\[\langle n_{k=0} \rangle = N[1 - \frac{8}{3\sqrt{\pi}} \sqrt{\rho a^3} + \cdot \cdot \cdot]. \quad \text{(40b)}\]

One arrives at a similar expression for dimension 4:

\[\langle n_{k=0} \rangle = N[1 - \beta \rho a^4 [\ln \rho a^4] + \cdot \cdot \cdot]. \quad (14)\]

where the logarithmic factor has the same origin as in (13) above. Here $\beta$ is a numerical coefficient. Comparing equations (1) and [40b] for dimension 3 with equations (13) and (14) for dimension 4, we see that the expansion parameter changes from dimensions 3 to 4 as follows:

\[\sqrt{\rho a^3} \rightarrow \rho a^4 [\ln \rho a^4]. \quad (15)\]

**DIMENSION 5**

Generalization of these perturbation calculations to dimension 5 proceeds seemingly without problem, but what replaces (14) becomes

\[\langle n_{k=0} \rangle = N[1 - \infty] \quad (16)\]

where $\infty$ represents a linear divergence at large $k$. This means that the single particle state $k = 0$ will be totally depleted by converting into many pairs ($k$, - $k$) of single particle states. In other words for interacting systems the BEC in dimensions 5 has [40] basic group of 2 instead of 1, unlike the BEC of dimensions 3 and 4. The details of this BEC need further study.

**DIMENSION 2**

In dimension 2 what replace (2) and (4) for dimension 3 are

\[\nabla^2 (-lnr) = -2\pi \delta^2 (r). \quad (17)\]

and

\[\varphi = \ln \frac{r}{a}. \quad (18)\]

$\varphi$ is the correct scattering amplitude, but it is impossible to generalize (3) to dimension 2 because unlike in dimensions 3 and 4, (18) does not approach a limit as $r \rightarrow \infty$. However it changes very slowly at large $r$. To approximately solve this problem we search for a $V$ which satisfies approximately $-\nabla^2 \varphi \cong -V \varphi$. Using (17) and (18) this equation become

\[-2\pi \delta^2 (r) \cong -V[\ln (r/a)]. \quad (19)\]

Now for a dilute system, the particles are at a large distance of order

\[R = \sqrt{\rho}^{-1}. \quad (20)\]

from each other. Thus we may put $r \cong R$ in the RHS of (19) and get

\[-2\pi \delta^2 (r) \cong -V[\ln (R/a)]. \quad (21)\]

or

\[V \cong \frac{1}{\ln (R/a)} \frac{2\pi \delta^2 (r)}{\ln (\rho a^4)}. \quad \text{(PP2)}\]

Here we take advantage of the fact that the logarithm varies very slowly with its argument if the latter is large. (The above derivation is not rigorous but I believe it to be correct.)

With (PP2) we proceed as in LHY and obtain

\[E_0 = \frac{4\pi \rho N}{\ln (\rho a^4)} - \sum' [k^2 + k_0^2 - k \sqrt{k^2 + 2k_0^2}] \quad (21)\]
where

\[ k_0^2 = \frac{8\pi \rho}{|\ln \rho a^2|}. \]  

(22)

There is no subtraction term in (21), unlike [23], because now \( V' = V \). The summation gives a contribution to \( E_0/N \):

\[ -\frac{16\pi \rho \ln A}{A^2} \]

where \( A = |\ln \rho a^2| \). But it is not clear that this term is reliable.

We summarize the results for dimension \( n \) in Table I for dilute interacting Boson systems.

With incredible new technology it has been possible to study experimentally 2D and 1D systems [7]. Perhaps the qualitative and quantitative features exhibited in Table I above for different dimensions could be studied with these new technologies and with powerful computers.

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Table I: Comparison of BEC in dilute interacting Boson gases for different dimensions. (BG = basic group [6])

| Dimension | Pseudopotential for fixed scatterer | \( E_0/N \) | Comments |
|-----------|-------------------------------------|-------------|----------|
| 1         | \( \sim 4\pi \delta^2 \) \[ \ln(\rho a^2) \] | \( \pi^2 \rho^2 / 3(1 - \rho a) \) \[ 3 \] | No BEC |
| 2         | \( \sim 4\pi \rho \) \[ \ln(\rho a^2) \] \[ \pm \cdots \] | | Almost BEC |
| 3         | \( 8\pi a^3 \delta^4 \frac{\partial r}{\partial r} \) | \( 4\pi \rho a(1 + \frac{128}{15\sqrt{\pi}} \rho a^3 + \cdots) \) \[ BEC, BG = 1 Boson \] |
| 4         | \( 8\pi a^2 \delta^4 \frac{\partial^2 r}{\partial r^2} \) | \( 4\pi^2 \rho a^2(1 + 4\pi \rho a^4 \ln(\rho a^4) + \cdots) \) \[ BEC, BG = 1 Boson \] |
| 5         | \( ? \) | \[ BEC, BG = \text{pair of Bosons} \] |

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