

ON BOSE-EINSTEIN CONDENSATION

TAI TSUN WU

*Gordon McKay Laboratory, Harvard University, Cambridge, MA 02138, USA, and
Theoretical Physics Division, CERN, CH-1211 Geneva 23, Switzerland*

ABSTRACT

A most exciting recent development in physics is the first experimental observation of Bose-Einstein condensation in dilute atomic vapors. For these experiments, it is necessary to use a trap in order to keep the atomic vapor together for cooling and observation. It is the purpose of this talk to treat systematically the effect of such a trap on Bose-Einstein condensation. It also provides a simple, explicit example of non-perturbative effects in quantum field theory.

1. Introduction

About a year ago, a remarkable paper on Bose-Einstein condensation^{1,2} (BEC) was published by Anderson, Ensher, Matthews, Wieman, and Cornell.³ This is the first experimental observation of BEC in a weakly interacting system. The system used is a vapor of rubidium-87 atoms that was confined by magnetic fields. Similar experiments on different atomic vapors followed soon after.^{4,5}

BEC is a remarkable phenomenon, where a macroscopic number of bosons is in the same quantum state. In the simplest case where the particles are non-interacting and in a periodic box, the single-particle ground state is the zero-momentum state, and is the state macroscopically occupied at sufficiently low temperatures.

Before these recent experiments,³⁻⁵ BEC was already a well-known phenomenon, especially in connection with superfluids (liquid helium) and superconductivity. In these cases, the mutual interactions are fairly strong and hence difficult to treat theoretically in a quantitative way. For this reason, these experiments³⁻⁵ give a strong motivation to develop further the theory of Bose-Einstein condensation.

Aside from the fact that the atoms in the dilute atomic vapors interact with each other, a new feature is introduced in the recent experiments: the presence of the magnetic traps. From the experimental point of view, such traps are necessary in order to keep the atoms together for cooling and observation. Since the presence of a trap changes the BEC of the atomic vapor in a profound way, traps must be taken into account in any theoretical treatment. For example, the presence of a trap necessarily destroys translational invariance, and hence the macroscopically occupied quantum state cannot be the zero-momentum state. Furthermore, because of the interactions between the atoms in the vapor, this macroscopically occupied quantum state cannot be the single-particle ground state in the trap. The reason is that the single-particle ground state is very much localized near the minimum of the trap, and it is not possible to concentrate a macroscopic number of atoms in such a small region. Indeed, in the experiments,³⁻⁵ the condensate has been observed to be of macroscopic dimension.

One other point should perhaps be mentioned. Since the atoms are kept inside the trap, strictly speaking thermodynamics does not apply, because the infinite-volume limit is meaningless. However, since the total number of atoms in the vapor is quite large, ranging from the thousands to the hundred thousands,³⁻⁵ thermodynamic concepts can be applied as a reasonable approximation.

Let us now turn the attention to the theoretical treatment of Bose-Einstein condensation in a trap. The philosophy is to keep only the essential features.

1) Although it is important in the experiments to have the atoms spin-polarized so that they can be trapped by a static magnetic field, the spin of the atoms does not play a fundamental role in BEC. Therefore the atoms will be taken to have spin zero in the theoretical treatment.

2) Since the details of the magnetic trap are also not of primary concern, the trap will be replaced by an external potential. This potential is taken to be smooth and to rise rapidly at large distances.

3) With the desire to use the simplest, non-trivial interaction between the bosons,

it is chosen to be a pairwise interaction that is short-ranged and repulsive. The case of attractive interactions is believed to be much more complicated.

4) To avoid a number of complications, the system of bosons is taken to be in a single quantum state, i.e., the system is described by an N -body wave function, not incoherent superpositions of such wave functions. In the language of liquid helium-4, it is assumed that only superfluid is present, not a mixture of superfluid and normal fluid.

2. Formulation of the Problem

The main task here is to include an external potential, to be called $V_e(\mathbf{r})$, in the treatment of Bose-Einstein condensation. Since there is only one specie of bosons, the same $V_e(\mathbf{r})$ acts on each of the bosons.

In connection with item 3) of the Introduction, it may be noted that, to the first approximation, a two-body, short-range repulsive interaction is specified by the scattering length, which is positive. Therefore, such an interaction is equivalent to a hard-sphere potential of the same scattering length.

Thirty-five years ago, various properties of a Bose system of hard spheres at extremely low temperatures were studied systematically, including non-equilibrium cases and the effect of rigid boundaries.⁶ In particular, in the treatment of rigid boundaries, no special property of this boundary condition is used, i.e., with very little modification, the procedure also works for any external potential. As emphasized in Ref. 6, the treatment is entirely quantum, and has the advantage of not making use of any concept borrowed from classical theory.

In the presence of the external potential, the Hamiltonian is ($\hbar = 2m = 1$)

$$\sum_{i=1}^N [p_i^2 + V_e(\mathbf{r}_i)] + \sum_{i<j} V_0(r_{ij}), \quad (2.1)$$

with $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. Using the method of pseudopotentials as applied to many-body problems due to Huang and Yang,⁷ this Hamiltonian (2.1) may be replaced by

$$H' = T + V', \quad (2.2)$$

with

$$T = \sum_i [p_i^2 + V_e(\mathbf{r}_i)] \quad (2.3)$$

and

$$V' = 4\pi a \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j) (\partial/\partial r_{ij}) r_{ij}, \quad (2.4)$$

where a is the scattering length. For most purposes such as the present treatment, it is sufficient to use instead the simpler

$$H = T + V, \quad (2.5)$$

where

$$V = 4\pi a \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j). \quad (2.6)$$

The only difficulty in using H instead of H' is the appearance of a familiar type of divergence, which can be easily removed.^{8,9}

In the language of quantized fields, the T and V are

$$T = \int d\mathbf{r} [|\nabla\psi(\mathbf{r})|^2 + V_e(\mathbf{r})|\psi(\mathbf{r})|^2], \quad (2.7)$$

$$V = 4\pi a \int d\mathbf{r} \psi^*(\mathbf{r})^2 \psi(\mathbf{r})^2, \quad (2.8)$$

where $\psi(\mathbf{r})$ satisfies the usual commutation rules for a boson field.

Let $\Phi(\mathbf{r}, t)$ be the condensate wave function, i.e., the wave function for the state that is macroscopically occupied. In general, this $\Phi(\mathbf{r}, t)$ depends on the time t and is complex. By item 4) of the Introduction, the occupation of this condensate state is taken to be nearly 100%. With this $\Phi(\mathbf{r}, t)$ normalized by

$$\Omega^{-1} \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^2 = 1, \quad (2.9)$$

then the creation and annihilation operators for this state are

$$a_0^*(t) = \Omega^{-1/2} \int d\mathbf{r} \psi^*(\mathbf{r}) \Phi(\mathbf{r}, t); \quad a_0(t) = \Omega^{-1/2} \int d\mathbf{r} \psi(\mathbf{r}) \Phi^*(\mathbf{r}, t). \quad (2.10)$$

The parts of $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$ corresponding to this one state may be singled out

$$\psi^*(\mathbf{r}) = \psi_0^*(\mathbf{r}, t) + \psi_1^*(\mathbf{r}, t); \quad \psi(\mathbf{r}) = \psi_0(\mathbf{r}, t) + \psi_1(\mathbf{r}, t), \quad (2.11)$$

where

$$\psi_0^*(\mathbf{r}, t) = \Omega^{-1/2} a_0^*(t) \Phi^*(\mathbf{r}, t); \quad \psi_0(\mathbf{r}, t) = \Omega^{-1/2} a_0(t) \Phi(\mathbf{r}, t). \quad (2.12)$$

In the Schrödinger picture, $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$ are time independent, but ψ_0^* , ψ_0 , ψ_1^* , and ψ_1 all may depend on the time.

The basic idea is to treat ψ_1^* and ψ_1 as small compared with ψ_0^* and ψ_0 . In the first-order approximation to be discussed in Sec. 3, only terms linear in ψ_1^* and ψ_1 are kept. Similarly, in the second-order approximation of Sec. 4, terms quadratic in ψ_1^* and ψ_1 are also kept. As an example, the total number N of particles, which is of course independent of t , can be written as

$$N = \int d\mathbf{r} \psi^*(\mathbf{r})\psi(\mathbf{r}) = a_0^*(t)a_0(t) + \int d\mathbf{r} \psi_1^*(\mathbf{r}, t)\psi_1(\mathbf{r}, t). \quad (2.13)$$

In the second-order approximation, both terms on the right-hand side are kept. However, in the first-order approximation, only the first term $a_0^*(t)a_0(t)$ can be kept.

3. First-Order Approximation

In this first-order approximation, we keep in T and V of Eqs. (2.7) and (2.8) three types of terms: i) terms independent of ψ_1^* and ψ_1 ; ii) terms linear in ψ_1^* and independent of ψ_1 ; and iii) terms linear in ψ_1 and independent of ψ_1^* . Therefore,

$$\begin{aligned} T_1 = & N[\bar{\zeta}(t) + \zeta_e(t)] + \Omega^{-1/2}a_0(t) \int d\mathbf{r} [-\nabla^2\Phi(\mathbf{r}, t) + V_e(\mathbf{r})\Phi(\mathbf{r}, t)]\psi_1^*(\mathbf{r}, t) \\ & + \Omega^{-1/2}a_0^*(t) \int d\mathbf{r} [-\nabla^2\Phi^*(\mathbf{r}, t) + V_e(\mathbf{r})\Phi^*(\mathbf{r}, t)]\psi_1(\mathbf{r}, t) \end{aligned} \quad (3.1)$$

and

$$\begin{aligned} V_1 = & \frac{4\pi aN}{\Omega} \left[N\zeta(t) + 2\Omega^{-1/2}a_0(t) \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^2\Phi(\mathbf{r}, t)\psi_1^*(\mathbf{r}, t) \right. \\ & \left. + 2\Omega^{-1/2}a_0^*(t) \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^2\Phi^*(\mathbf{r}, t)\psi_1(\mathbf{r}, t) \right], \end{aligned} \quad (3.2)$$

where

$$\bar{\zeta}(t) = \Omega^{-1} \int d\mathbf{r} |\nabla\Phi(\mathbf{r}, t)|^2, \quad \zeta(t) = \Omega^{-1} \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^4,$$

and

$$\zeta_e(t) = \Omega^{-1} \int d\mathbf{r} V_e(\mathbf{r})|\Phi(\mathbf{r}, t)|^2. \quad (3.3)$$

Accordingly, in this approximation the N -body wave function is of the form

$$\Psi(t) = (N!)^{-1/2}a_0^*(t)^N|\text{vac}\rangle, \quad (3.4)$$

leading to a non-linear Schrödinger equation for the condensate wave function

$$i\left(\frac{\partial}{\partial t}\right)\Phi(\mathbf{r}, t) = \left[-\nabla^2 + V_e(\mathbf{r}) + \frac{8\pi aN}{\Omega}|\Phi(\mathbf{r}, t)|^2 - \frac{4\pi aN}{\Omega}\zeta(t)\right]\Phi(\mathbf{r}, t). \quad (3.5)$$

This is essentially Eq. (2.21) of Ref. 6.

In Eq. (3.5), there are two basic lengths:

- i) the length over which the external potential $V_e(\mathbf{r})$ varies; and
- ii) the length scale determined by $(4\pi aN/\Omega)|\Phi(\mathbf{r}, t)|^2$.

In the absence of the external potential $V_e(\mathbf{r})$, the first length is just the size $\Omega^{1/3}$ of the box. For the Dirichlet boundary condition, ordinary perturbation expansion in the scattering length a applies only when the second length is larger than the first length. Otherwise, non-perturbative effects become dominant. A more detailed discussion of this point may be found in Sec. 3 of Ref. 6.

4. Second-Order Approximation

We discuss briefly the second-order approximation, where terms of the six types 1, ψ^* , ψ , $\psi^*\psi^*$, $\psi^*\psi$, and $\psi\psi$ are kept in the T and V of Eqs. (2.7) and (2.8). This means that all terms in T have to be kept, and V is approximated by

$$\begin{aligned}
V_2 = & \frac{4\pi aN}{\Omega} \left[N\zeta(t) + 2\Omega^{-1/2}a_0(t) \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^2 \Phi(\mathbf{r}, t) \psi_1^*(\mathbf{r}, t) \right. \\
& + 2\Omega^{-1/2}a_0^*(t) \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^2 \Phi^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \\
& + \int d\mathbf{r} \{ [-2\zeta(t) + 4|\Phi(\mathbf{r}, t)|^2] \psi_1^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \\
& \left. + N^{-1}a_0(t)^2 \Phi(\mathbf{r}, t)^2 \psi_1^*(\mathbf{r}, t)^2 + N^{-1}a_0^*(t)^2 \Phi^*(\mathbf{r}, t)^2 \psi_1(\mathbf{r}, t)^2 \} \right]. \quad (4.1)
\end{aligned}$$

In this case, the N -body wave function takes the form

$$\Psi(t) = \mathcal{N}(t) e^{\mathcal{P}(t)} (N!)^{-1/2} a_0^*(t)^N |\text{vac}\rangle, \quad (4.2)$$

where $\mathcal{P}(t)$ describes the creation of pairs from the condensate

$$\mathcal{P}(t) = [2N_0(t)]^{-1} \int d\mathbf{r} d\mathbf{r}' \psi_1^*(\mathbf{r}, t) \psi_1^*(\mathbf{r}', t) K_0(\mathbf{r}, \mathbf{r}'; t) a_0(t)^2. \quad (4.3)$$

The equations of motion are easily obtained from Sec. 7 of Ref. 6 with the following replacements:

$$-\nabla^2 \rightarrow -\nabla^2 + V_e(\mathbf{r}); \quad -\nabla'^2 \rightarrow -\nabla'^2 + V_e(\mathbf{r}'); \quad \bar{\zeta} \rightarrow \bar{\zeta} + \zeta_e. \quad (4.4)$$

5. Discussion

It remains to discuss the nature of the present expansion, where ψ_1^* and ψ_1 are considered to be small compared with ψ_0^* and ψ_0 .

So far as the Hamiltonian is concerned, such an expansion is well defined. For example, in the first-order approximation of Sec. 3, the Hamiltonian is linear in ψ_1^* and ψ_1 . Similarly, in the second-order approximation of Sec. 4, it is quadratic in ψ_1^* and ψ_1 .

In these two approximations, the N -body wave function can be written down explicitly, as given by Eqs. (3.4) and (4.2), respectively.

To higher orders, the expansion for the Hamiltonian remains unambiguous. However, the N -body wave function corresponding to such a Hamiltonian cannot be found exactly, and further approximations must be introduced. There are already a number of interesting unsolved problems in the third-order approximation.

As a reminder of the type of complications to be encountered, let us return briefly to the simplest case of the periodic boundary condition without external potential. In this case, the expansion parameter is $(\rho a^3)^{1/2}$, where $\rho = N/\Omega$. However, in higher orders, the logarithm of this expansion parameter occurs; in particular, the ground-state energy per particle is given by⁹⁻¹²

$$4\pi a\rho \left\{ 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + \rho a^3 \left[8 \left(\frac{4\pi}{3} - \sqrt{3} \right) \ln(\rho a^3) + C \right] \right\}, \quad (5.1)$$

where the constant C is determined by the solution to the three-body problem. The order of magnitude of the next term is expected to be $(\rho a^3)^{3/2}[\ln(\rho a^3)]^n$, but it is not clear whether n is 1 or 2 or some other value. This and other complications are surely going to occur also in the study of Bose-Einstein condensation in an external potential.

Acknowledgments

I am greatly indebted to Professor Harry Lehmann and Professor Chen Ning Yang for their most helpful discussions. I am grateful as well to the organizers of this Workshop, especially to Herbert Fried, for such an interesting and pleasant meeting. I also wish to thank the Theoretical Physics Division of CERN for their kind hospitality. This work was supported in part by the the U.S. Department of Energy under Grant No. DE-FG02-84ER40158 with Harvard University.

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