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Time Evolution of a Bose-Einstein Condensate in a Trap

—A Field Theoretical Approach—

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The recent observations of Bose-Einstein condensation (BEC) in magnetically trapped atomic gases[1,2]have stimulated the theoretical study of these phenomena. In this work, we investigate the particle distribution in a condensate of neutral boson field under the trapping potential and its time evolution immediately after the trapping potential is switched off, taking the interaction between the particles into account.

We consider a collection of interacting Bose particles trapped in a harmonic oscillator potential $1/2\ \Sigma_{i=1}^{3} w_i^2 x_i^2$, whose Hamiltonian is given by

$$H_B=\int dx\phi^\dagger(x)\left\{-\frac{1}{2}\Delta+\frac{1}{2}\sum_{i=1}^{3} w_i^2 x_i^2\right\}\phi(x)$$

$$+\frac{1}{2}g\int dx\,dx'\phi^\dagger(x)\phi^\dagger(x')V(x-x')\phi(x)\phi(x'), \tag{1}$$

where we set particle mass $=\hbar=1$.

In a classical paper on BEC[3], Bogoliubov treated a similar Hamiltonian but without the trapping potential. The key idea in his theory is that the creation and annihilation operators for the zero momentum particle should be replaced by a c-number $\sqrt{N_0}$, when BEC occurs. The quantity N_0 is the average number of particles occupying the zero momentum state and BEC means that this number becomes very large and macroscopic. Roughly speaking, this replacement is justified as follows: For BEC state, N_0 particles are in the zero momentum state. Thus the creation and annihilation operators for zero momentum state give

$$c_0^\dagger |N_0\rangle = \sqrt{N_0+1}\,|N_0+1\rangle$$
$$c_0 |N_0\rangle = \sqrt{N_0}\,|N_0-1\rangle. \tag{2}$$

Since the number N_0 is very large, $N_0+1 \approx N_0$, both the operations of $c_0^\dagger$ and c_0 on system states are similar, giving the result $\sqrt{N_0}$ as an eigenvalue. Thus we can treat both the operators $c_0^\dagger$ and c_0 as c-number $\sqrt{N_0}$.

To extend this idea to a trapped Bose gas, first let us introduce annihilation operators of particles a_n in the harmonic oscillator modes by expanding the field operator $\phi(x)$ in terms of a complete set of the harmonic oscillator wave functions $u_n(x)$:

$$\phi(x) = \sum_n a_n u_n(x), \tag{3}$$

where $u_n(x)$ satisfies

$$\left\{ -\frac{1}{2}\Delta + \frac{1}{2}\sum_{i=1}^{3} w_i^2 x_i^2 \right\} u_n(x) = \varepsilon_n u_n(x), \tag{4}$$

and $n = (n_1, n_2, n_3)$ with non-negative integers n_i.

In a condensed state, most particles are in the ground state of the harmonic oscillator, that is, the state for $n = (0, 0, 0)$. Therefore, the occupation number N_0 of this state is supposed to be very large. In typical experiments, the total particle number is of the order of $10^3 \sim 10^5$. Then we can apply the Bogoliubov replacement to the creation and annihilation operators, $a_0^\dagger$ and a_0:

$$a_0^\dagger \longrightarrow \sqrt{N_0}, \quad a_0 \longrightarrow \sqrt{N_0}. \tag{5}$$

Then the field operator $\phi(x)$ reads

$$\phi(x) = \sqrt{N_0}\,u_0(x) + \sum_n{}' a_n u_n(x), \tag{6}$$

where the prime in Σ_n' means to omit the term $n=(0, 0, 0)$.

Substituting the above expression of $\phi(x)$ into H_B in (1), we have

$$H_B = N_0\varepsilon_0 + \sum_n{}' \varepsilon_n a_n^\dagger a_n$$
$$+\frac{1}{2} gN_0^2 \int dx\, dx' u_0^2(x) V(x-x') u_0^2(x')$$
$$+gN_0^{3/2} \sum_n{}' (a_n^\dagger + a_n)$$
$$\times \int dx\, dx' u_n(x) u_0(x) V(x-x') u_0^2(x') + O(gN_0). \tag{7}$$

when $V(x)=V(-x)$ is assumed. Since N_0 is large, we shall retain only terms of order N_0^2 and $N_0^{3/2}$ in the interaction part. We remark the presence of the terms of order $N_0^{3/2}$. In the original Bogoliubov theory, the terms of order $N_0^{3/2}$ do not exist, which is due to momentum conservation. In the present case, however, we do not have such a conservation law, and the dominant q-number terms are linear in the creation and annihilation operators of excited states.

By defining operators $\alpha_n^\dagger$ and α_n by

$$\alpha_n = a_n + \sqrt{N_0}\gamma_n, \quad \alpha_n^\dagger = a_n^\dagger + \sqrt{N_0}\gamma_n \tag{8}$$

which satisfy the same commutation relations as $a_n^\dagger$ and a_n, we can diagonalize the approximated Hamiltonian thus obtained:

$$H_B = \sum_n{}' \varepsilon_n \alpha_n^\dagger \alpha_n + N_0\varepsilon_0 \left(1 + \frac{1}{2}\gamma_0 - \sum_n{}' \frac{\varepsilon_n}{\varepsilon_0}\gamma_n^2\right), \tag{9}$$

with the c-number coefficient

$$\gamma_n \equiv \frac{gN_0}{\varepsilon_n} \int dx\, dx' u_n(x) u_0(x) V(x-x') u_0^2(x'). \tag{10}$$

In terms of these α's, the particle number density operator $\hat{n}(x)$ is written as

$$\hat{n}(x) \equiv \phi^{\dagger}(x)\phi(x) = \sum_{m,n}{}' \alpha_n{}^{\dagger}\alpha_m u_n(x)u_m(x)$$

$$+\sqrt{N_0}\sum_n{}' (\alpha_n{}^{\dagger}+\alpha_n)u_n(x)\left\{u_0(x)-\sum_m{}' \gamma_m u_m(x)\right\}$$

$$+N_0\left(u_0(x)-\sum_n{}' \gamma_n u_n(x)\right)^2 \tag{11}$$

and its thermal average,

$$n(x) = Z^{-1}\,\mathbf{Tr}\,[e^{-\beta H_B}\hat{n}(x)] \tag{12}$$

with $Z=\mathbf{Tr}[e^{-\beta H_B}]$, can easily be calculated by making use of (9) to find

$$n(x) = N_0\left(u_0(x)-\sum_n{}' \gamma_n u_n(x)\right)^2 + \sum_n{}' \frac{1}{e^{\beta\varepsilon_n}-1}u_n{}^2(x). \tag{13}$$

In our approximation of taking only the linear terms in $a_n{}^{\dagger}$ and a_n, the energy spectrum of single particle states are not affected by the existence of interactions between particles. However the wave function of the ground state *does* change. This can be seen in the first term above.

The total particle number is also obtained by integrating the above $n(x)$ with respect to x:

$$N = N_0\left(1+\sum_n{}' \gamma_n{}^2\right) + \sum_n{}' \frac{1}{e^{\beta\varepsilon_n}-1}. \tag{14}$$

This equation gives the relation between the temperature and the condensate fraction $f_0 = N_0/N$. It shows that the interaction between particles lowers the fraction f_0.

Now we shall investigate how $n(x)$ evolves, if the trappingpotential is removed. Let us switch off the trapping potential at $t=0$, thereafter the system develops under the Hamiltonian,

$$H=\int dx\phi^{\dagger}(x)\left\{-\frac{1}{2}\Delta\right\}\phi(x)$$

$$+\frac{1}{2}g\int dx\,dx'\phi^{\dagger}(x)\phi^{\dagger}(x')V(x-x')\phi(x)\phi(x'). \tag{15}$$

For a while, however, the system must be still in BEC. Therefore we may be able to approximate the self-interaction term (the second term) in (15) by one in (7) (to neglect the terms of order gN_0). Hence we have

$$H\simeq\int dx\phi^{\dagger}(x)\left\{-\frac{1}{2}\Delta\right\}\phi(x)$$

$$+\sqrt{N_0}\sum_n{}'(a_n{}^{\dagger}+a_n)\varepsilon_n\gamma_n+N_0\varepsilon_0\left(1+\frac{1}{2}\gamma_0\right). \tag{16}$$

Here N_0, and hence γ_n, must become time dependent. In principle, this dependence will be determined self-consistently by the condition that the total particle number is conserved. In the following, however, our considerations are limited to the case of time-independent N_0 and γ_n, because we are interested in the short time evolution after switching off the trapping potential.

The quantum number n does not diagonalize the kinetic term in (15). It is convenient to introduce the creation and annihilation operators in momentum eigenstates $c_k{}^{\dagger}$ and c_k in the usual way:

$$\phi(x)=\frac{1}{(2\pi)^{3/2}}\int dkc_k\,e^{ik\cdot x}. \tag{17}$$

Inversely we get

$$c_k=\frac{1}{(2\pi)^{3/2}}\int dx\,e^{-ik\cdot x}\phi(x)$$

$$=\sqrt{N_0}\tilde{u}_0(k)+\sum_n{}'a_n\tilde{u}_n(k), \tag{18}$$

where we use the Bogoliubov replaced field operator (6).

The operators a_n and c_k are related as,

$$a_n=\int dx u_n(x)\phi(x)=\int dk c_k \tilde{u}_n{}^*(k), \tag{19}$$

where $\tilde{u}$ means the Fourier transform of u defined by

$$\tilde{f}(k)=\frac{1}{(2\pi)^{3/2}}\int dx f(x)\, e^{-ik\cdot x}. \tag{20}$$

Putting (17) and (19) into (16), we have an expression of H written by $c_k^\dagger$ and c_k as

$$H=\int dk\varepsilon_k c_k^\dagger c_k+\sqrt{N_0}\int dk\left\{c_k^\dagger \sum_n{}' \tilde{u}_n(k)\varepsilon_n\gamma_n+\text{h.c.}\right\}$$

$$+N_0\varepsilon_0\left(1+\frac{1}{2}\gamma_0\right) \tag{21}$$

with $\varepsilon_k=\boldsymbol{k}^2/2$.

The Heisenberg operator for $t>0$,

$$c_k(t)=e^{itH}c_k\, e^{-itH} \tag{22}$$

satisfies the equation of motion

$$i\dot{c}_k(t)=e^{itH}[c_k, H]\, e^{-itH}$$

$$=\varepsilon_k c_k(t)+\sqrt{N_0}\sum_n{}' \varepsilon_n\gamma_n\tilde{u}_n(k). \tag{23}$$

We can solve this equation with the condition $c_k(0)=c_k$ to get

$$c_k(t)=c_k\, e^{-i\varepsilon_k t}+\frac{e^{-i\varepsilon_k t}-1}{\varepsilon_k}\sqrt{N_0}\sum_n{}' \varepsilon_n\gamma_n\tilde{u}_n(k). \tag{24}$$

Substituting (18) into the first term above, we have

$$c_k(t)=\sum_n{}' a_n\tilde{u}_n(k)\, e^{-i\varepsilon_k t}+\sqrt{N_0}\tilde{u}_0(k)\, e^{-i\varepsilon_k t}$$

$$+\frac{e^{-i\varepsilon_k t}-1}{\varepsilon_k}\sqrt{N_0}\sum_n{}' \varepsilon_n\gamma_n\tilde{u}_n(k). \tag{25}$$

The field operator in the Heisenberg picture is written as

$$\phi(x, t) = e^{itH}\phi(x)\, e^{-itH} = \frac{1}{(2\pi)^{3/2}}\int dk c_k(t)\, e^{ik\cdot x}$$

$$= \sum_n{}' a_n u_n(x, t) + \sqrt{N_0} u_0(x, t)$$

$$- i\sqrt{N_0}\, \sum_n{}' \varepsilon_n \gamma_n \int_0^t d\lambda u_n(x, \lambda), \tag{26}$$

where we denote

$$u_n(x, t) = \frac{1}{(2\pi)^{3/2}}\int dk \tilde{u}_n(k)\, e^{ik\cdot x - i\varepsilon_k t}. \tag{27}$$

In terms of α_n's, (26) can be rewritten as

$$\phi(x, t) = \sum_n{}' \alpha_n u_n(x, t) + \sqrt{N_0} u_n(x, t)$$

$$- \sqrt{N_0}\, \sum_n{}' \gamma_n u_n(x, t)$$

$$- i\sqrt{N_0}\, \sum_n{}' \varepsilon_n \gamma_n \int_0^t d\lambda u_n(x, \lambda) \tag{28}$$

and the number density operator in the Heisenberg picture is given by

$$\hat{n}(x, t) = \phi^\dagger(x, t)\phi(x, t)$$

$$= \sum_{n, m}{}' \alpha_n{}^\dagger \alpha_m u_n{}^*(x, t) u_m(x, t)$$

$$+ \sqrt{N_0}\, \sum_n{}' \{\alpha_n{}^\dagger u_n{}^*(x, t) f(x, t) + \text{h.c.}\}$$

$$+ N_0 |f(x, t)|^2, \tag{29}$$

where

$$f(x, t) = u_0(x, t) - \sum_n{}' \gamma_n \left\{ u_n(x, t) + i\varepsilon_n \int_0^t d\lambda u_n(x, \lambda) \right\}. \tag{30}$$

The thermal average of $\hat{n}(x, t)$ is given by

$$n(x, t) = Z^{-1}\,\mathbf{Tr}\,[e^{-\beta H_B}\hat{n}(x, t)], \tag{31}$$

since the density matrix does not change in time in the Heisenberg picture. Making use of the eqs. (9) and (29), finally we find

$$n(x, t) = N_0 \left| u_0(x, t) - \sum_n{}' \gamma_n \left\{ u_n(x, t) + i\varepsilon_n \int_0^t d\lambda u_n(x, \lambda) \right\} \right|^2 + \sum_n{}' \frac{1}{e^{\beta\varepsilon_n} - 1} |u_n(x, t)|^2. \tag{32}$$

As seen in the definition (27), the functions $u_n(x, t)$ represent the wave functions of free motion started from the harmonic oscillator eigenfunctions. Comparing the above $n(x, t)$ with $n(x)$ given in (13), we can see that $n(x, t)$ is the result of free evolution of $n(x)$, except for the term $i\varepsilon_n \int_0^t d\lambda u_n(x, \lambda)$. This term gives the effect of the interaction between particles. If we drop this term, the integration of $n(x, t)$ with respect to x becomes the same as N in eq. (14), because of the orthogonality of $\{u_n(x, t)\}$:

$$\int dx u_n{}^*(x, t) u_m(x, t) = \delta_{nm}. \tag{33}$$

This means that, in our approximation, the time dependence of the fraction f_0 stems from the interaction between particles.

In summary, the two main results of this work are as follows: (I) The ground state particle distribution in a Bose condensate under the trapping potential, seen from the first term in (13), is different from the noninteracting case, where the distribution is expected to be $|u_0(x)|^2$. (II) The time evolution of the particle distribution of a condensed Bose gas immediately after switching off the trapping potential suddenly can be calculated analytically as in (32). In (13) and (32) the parameter γ_n, representing the interaction effect, is crucial quantitatively. Simple manipulations of (10) lead to

$$\gamma_n = \begin{cases} \dfrac{4\pi a}{(2\pi)^{3/2}\varepsilon_n} N_0 \prod_{i=1}^{3} w_i^{1/2} \left(-\dfrac{1}{2}\right)^{n_i/2} \sqrt{\dfrac{(n_i-1)!!}{n_i!!}} & \text{for all even } n_i \\ 0 & \text{otherwise} \end{cases} \tag{34}$$

where we put $g=4\pi a$ and a is the s-wave scattering length. To estimate the numerical order of the interaction effects in our calculations, let us see the values of the parameters in the experiment[1]using Rb atoms. There we have $N_0=2\times10^3$, $a=110a_0$(a_0: Bohr radius), $\omega_3=\sqrt{8}\,\omega_1=\sqrt{8}\,\omega_2=200\pi$ Hz, then the leading γ_n for $n=(2, 0, 0)$ or $(0, 2, 0)$ and the next-leading one for $n=(2, 2, 0)$ become -0.23 and 0.06, respectively.

Our calculations are based on the Bogoliubov theory, adapted to a system trapped by a harmonic oscillator potential. Our approximation scheme is to take only the dominant terms in $N_0^{-1/2}$ expansion, but is still nonperturbative with respect to g (the interaction between particles). Higher order calculation in $N_0^{-1/2}$ expansion is under study. The future task is to combine this field theoretical approach with nonequilibrium Thermo Field Dynamics[4,5].

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