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Density profile of the atomic Bose–Einstein condensation

Xue-Xi Yi†‡ and Jun-Chen Su†

† Department of Physics, Jilin University, Changchun 130023, People's Republic of China
‡ Institute of Theoretical Physics, Northeast Normal University, Changchun 130024, People's Republic of China

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Abstract. We study the density profile and the dynamics of atoms interacting with the quantized radiation field in a trap. The density profile is evaluated by using the Bogoliubov approximation. The calculated mean number of atoms at zero temperature appears to be a function of time which shows a damped oscillation. The shape of the lines for the light scattered from Bose–Einstein condensates are also discussed.

Evidence of Bose–Einstein condensation (BEC) in magnetically trapped gases of rubidium [1], lithium [2], and sodium [3] atoms has recently been reported. An urgent task now is to detect and diagnose the BEC of atoms in a trap. A direct method of detecting the BEC is to observe the light scattered from the BEC. Therefore, it is necessary to study optical properties of the BEC when it interacts with an external light field. Until now, this problem has only been investigated in some limiting cases. Javanainen [4] considered the case of an optically thin condensate with a size a of the order of the resonant wavelength. In such a case, the scattering takes place mainly in the forward direction, and the scattering cross section has a Lorentzian line shape. You *et al* [5] discussed the problem of scattering of the light field in another case in which an intense short laser pulse is used. They found that above the critical temperature of BEC, such a system scatters very weakly, while below the critical temperature, the number of scattered photons increases dramatically and the scattered light is emitted into a solid angle which is determined by the size of the condensate. The subject of the density profile has attracted much attention since the experimental achievement of BEC. The theoretical study of this problem was reported earlier by both groups, Goldman *et al* [6] and Huse and Siggia [7], who extended the Gross–Pitaevskii theory of the weakly interacting inhomogeneous Bose gas to finite temperatures. They obtained the density profile of magnetically confined polarized hydrogen $H_\downarrow$ by employing the Hartree–Fock and Bogoliubov approximation. Oliva [8] developed a general theory of the low-temperature density profile for a weakly non-ideal Bose gas trapped within an arbitrary potential well. In the absence of radiation field, Bagnato *et al* [9] presented theoretical studies of the density profile of atoms in a trap for cases of both with and without interaction among atoms, and found that the critical temperature of BEC, the condensate fraction, and the heat capacity vary markedly with the shape of the trap potential. Based on local density approximation [8], Chou *et al* [10] gave a quantitative result of atomic BEC which is easily checked by experiments.

It should be pointed out that all of the aforementioned studies of the density profile only concern the classical light field and hence rely on the semiclassical theory. The purpose of this paper is to try to calculate the density profile of atomic BEC in full quantum framework. The results obtained show that the mean number of atoms at zero temperature appears to be a function of time. For a fixed momentum p, the function is oscillatory with a period of $\pi/(\mu\sqrt{n_0}\sin 2\theta_p)$. If the momentum satisfies the Gaussian distribution, then the mean number of atoms becomes a damping-oscillatory function with damping rate depending on the number of condensate atoms. Using yet another method, the line shape for the light scattered from BEC is no longer of Lorentzian type, and exhibits a very narrow spike close to the resonance.

Let us start our discussion with a one-dimensional model and consider N atoms of mass, m, without mutual interaction which are localized in a trap $V(x)$. The second-quantized Hamiltonian for such a system given in the rotation-wave approximation (RWA) and the local density approximation (LDA) is

$$H = \sum_p \varepsilon_p^g(x) g_p^+ g_p + \sum_p \varepsilon_p^e(x) e_p^+ e_p + \sum_k \hbar\omega_k a_k^+ a_k + \hbar\mu \sum_{k,p} (e_{p+k}^+ g_p a_k + \mathrm{hc}) \tag{1}$$

where g_p, g_p^+ are the annihilation and creation operators of atomic ground state with momentum, p, and energy $\varepsilon_p^g(x) = \frac{p^2}{2m} + V(x)$, where e_p and e_p^+ denote the annihilation and creation operators of atomic excited state with momentum, p, and energy $\varepsilon_p^e(x) = \frac{p^2}{2m} + V(x) + \hbar\omega_0$. Here ω_0 is the bare Rabi frequency between ground and excited states of the atom, a_k, a_k^+ designate the annihilation and creation operators for photons with momentum k, and μ stands for the coupling constant. All operators fulfil the standard bosonic commutation relations. The local density approximation is an adaptation of the Thomas–Fermi method, and is reasonably good when $\hbar\omega/kT \ll 1$ (ω is the frequency of a harmonic trap potential) [10].

We consider a range of parameters describing the BEC of atoms [3]. The potential for the centre-of-mass motion of a single atom in the ground electronic state can be described by a harmonic oscillator potential of frequency $\omega \sim 410$ Hz. Although the potential forms a finite barrier, there are several thousand energy levels within the trap. By exploiting an evaporative cooling technique, the trap will store about 10^9 sodium atoms which will interact with the resonant light. At temperatures above 15 μK, the observed trapped atoms are of an elliptical shape with an aspect ratio of 2:1 due to the symmetry of the quadrupole field, and at temperatures below 15 μK, the atoms will be separated into two pockets at the two minima in the trap. Therefore, the RWA and LDA are good approximations for describing the BEC of atoms in a trap.

The condensate is modelled in the customary way by treating the creation and annihilation operators as a c number

$$g_0^+ \sim g_0 = \sqrt{n_0}$$

and hence the Hamiltonian can be written as

$$H = \sum_p \varepsilon_p^e(x) e_p^+ e_p + \sum_k \hbar\omega_k a_k^+ a_k + \hbar\mu\sqrt{n_0} \sum_p (e_p^+ a_p + \mathrm{hc}) \tag{2}$$

where we ignore the term

$$\sum_p \varepsilon_p^g g_p^+ g_p = \varepsilon_0^g n_0 + \sum_{p\neq 0} \varepsilon_p^g(x) g_p^+ g_p \sim \varepsilon_0^g n_0 = \text{constant}.$$

Through the Bogoliubov transformation

$$\begin{aligned} e_k &= \sin\theta_k c_k + \cos\theta_k d_k \\ a_k &= \cos\theta_k c_k - \sin\theta_k d_k \end{aligned} \tag{3}$$

where

$$\theta_k = 0.5 \arctan \frac{\varepsilon_k^e - \hbar\omega_k}{2\hbar\mu\sqrt{n_0}}$$

the Hamiltonian can be diagonalized:

$$H = \sum_k \varepsilon_k^c(x) c_k^+ c_k + \sum_k \varepsilon_k^d(x) d_k^+ d_k \tag{4}$$

and the energy of quasiparticles are

$$\begin{aligned} \varepsilon_k^c(x) &= \varepsilon_k^e(x)\cos^2\theta_k + \hbar\omega_k \sin^2\theta_k + \hbar\mu\sqrt{n_0}\sin(2\theta_k) \\ \varepsilon_k^d(x) &= \varepsilon_k^e(x)\sin^2\theta_k + \hbar\omega_k \cos^2\theta_k - \hbar\mu\sqrt{n_0}\sin(2\theta_k). \end{aligned} \tag{5}$$

Equations (4) and (5) show that the occurrence of BEC of trapped atoms causes a fundamental change in the system of the atoms and radiation field. Especially the coherent interaction between the radiation field and excited atoms in the condensate gives rise to quasiparticles in the system, each of which appears as the superposition of a photon and an excited atom. This analysis is meaningful if the rate of the spontaneous emission of the excited atom is small in comparison with the characteristic value of the excited atom energy $\varepsilon_p^e(x)$. The spontaneous emission of the excited atom can be analysed by incorporating in the Hamiltonian (1) an interaction between the atom and a bath (such as a multimode radiation field).

Transformation (3) permits us to establish a relation between the quasiparticle states (QS) and the states of photon–atom (PA) system. First of all, it follows from equation (3) that the QS vacuum state $|0\rangle_{QS}$ defined by the stability condition

$$\forall k c_k |0\rangle_{QS} = d_k |0\rangle_{QS} = 0$$

exactly coincides with the photon–atom vacuum state

$$|0\rangle_{AP} \equiv |0\rangle_{a_p} \otimes |0\rangle_{e_p}.$$

Noticing this fact, one may easily derive the eigenstates or the quasiparticle number states of such a system as given by

$$\begin{aligned} |n_p^c, n_p^d\rangle_{QS} &= \frac{(c_p^+)^{n^c}}{\sqrt{n^c!}} \frac{(d_p^+)^{m^d}}{\sqrt{m^d!}} |0\rangle_{AP} = \sum_{k=0}^{n^c} \sum_{j=0}^{m^d} \binom{n^c}{k} \binom{m^d}{j} \\ &\times (-1)^{m^d - j} (\sin\theta_p)^{m^d + k - j} (\cos\theta_p)^{n^c + j - k} \\ &\times \sqrt{\frac{(k+j)!(m^d + n^c - k - j)!}{m^d! m^c!}} |k + j, m^d + n^c - k - j\rangle_{AP} \end{aligned} \tag{6}$$

and the corresponding eigenvalues as shown in the following:

$$E(n_p^c, m_p^d) = n_p^c \varepsilon_p^c(x) + m_p^d \varepsilon_p^d(x).$$

Equation (6) indicates that the quasiparticle number states is a linear combination of a finite number of photon–atom number states with weights representing the correlations between photons and atoms. Relation (6) is rather complicated. However, the coherent state of quasiparticles are related to the coherent states of photons and atoms in a simple way. The connection between the parameters of two different coherent states are

$$\alpha_{a_p} = \cos\theta_p \alpha_{c_p} - \sin\theta_p \alpha_{d_p}$$

and

$$\alpha_{e_p} = \sin\theta_p \alpha_{c_p} + \cos\theta_p \alpha_{d_p}$$

where α_{c_p} and α_{d_p} are the parameters of the quasiparticle coherent states and α_{ap} and α_{ep} are those of the photon and atom coherent states.

In the following, we study the dynamics of the system at zero temperature. For clarity, we set $V(x) = 0$. In this case, the time-dependent number of atoms with fixed momentum p (in excited state with $p \neq 0$) is found to be

$$\langle e_p^+ e_p \rangle_t = \sin^2\theta_p \langle c_p^+ c_p \rangle_t + \cos^2\theta_p \langle d_p^+ d_p \rangle_t - 2\sin\theta_p \cos\theta_p \,\mathrm{Re}(\langle c_p^+ d_p \rangle_t). \tag{7}$$

One can easily see that different initial conditions lead to different results. If the atom and the quantized radiation field are initially in coherent states $|\alpha_p^A\rangle$ and $|\alpha_p^P\rangle$, respectively, the initial conditions will be

$$\langle e_p^+ e_p \rangle_{t=0} = |\alpha_p^A|^2 \qquad \langle a_p^+ a_p \rangle_{t=0} = |\alpha_p^P|^2$$

or

$$\begin{aligned} \langle c_p^+ c_p \rangle_{t=0} &= |\sin\theta_p \alpha_p^A - \cos\theta_p \alpha_p^P|^2 \\ \langle d_p^+ d_p \rangle_{t=0} &= |\sin\theta_p \alpha_p^P + \cos\theta_p \alpha_p^A|^2. \end{aligned} \tag{8}$$

From the Heisenberg equation $\mathrm{i}\hbar \frac{\partial b}{\partial t} = [b, H]$ and the above initial conditions, the expression for the mean number of atoms with momentum p can be derived and is of the form

$$\begin{aligned} \langle e_p^+ e_p \rangle_t = {} & [\sin^4\theta_p + \cos^4\theta_p + 2\sin^2\theta_p \cos^2\theta_p \cos[(2\mu\sqrt{n_0}\sin 2\theta_p)t]]|\alpha_p^A|^2 \\ & + 2\sin^2\theta_p \cos^2\theta_p (1 - \cos[(2\mu\sqrt{n_0}\sin 2\theta_p)t])|\alpha_p^P|^2 \\ & + (1 - \cos[(2\mu\sqrt{n_0}\sin 2\theta_p)t])(-2\sin^3\theta_p \cos\theta_p + 2\sin\theta \cos^3\theta_p)\alpha_p^A \alpha_p^P. \end{aligned} \tag{9}$$

As we see, the number of atoms in the excited state with a fixed momentum, p, is an oscillatory function of time with the period of $\pi/(\mu\sqrt{n_0}\sin 2\theta_p)$. The larger the momentum $|p|$, the shorter the period of oscillation. Particularly, the mean number of atoms in the excited state is close to a constant when $|p| \to 0$. If the momentum of atoms initially distributes like a Gaussian wavepacket, then the total number of atoms (in the excited state) reads

$$N_e = \sum_p |c(p)|^2 \langle e_p^+ e_p \rangle_t \tag{10}$$

where

$$|c(p)|^2 = \sqrt{2W^2/\pi}\, \exp(-2W^2(p - p_0)^2/\hbar^2).$$

The numerical result is displayed in figure 1. From the figure, we see that the mean number of atoms varies with time as a damped oscillation with a damping rate and a quasiperiod depending on the number of condensate atoms. This property might be used to detect the BEC.

For the case of finite temperature, the normal part of density function can be written as

$$\rho_n(x) = \sum_k (\sin^2\theta_k n_k^c + \cos^2\theta_k n_k^d) \tag{11}$$

where n_k^c and n_k^d are the occupation number of quasiparticles c and d at the energy level k, respectively, which are given by Bose–Einstein distribution

$$n_k^{c(d)} = \left(\exp\left(-\frac{\varepsilon_k^{c(d)}}{k_B T} \right) - 1 \right)^{-1}$$

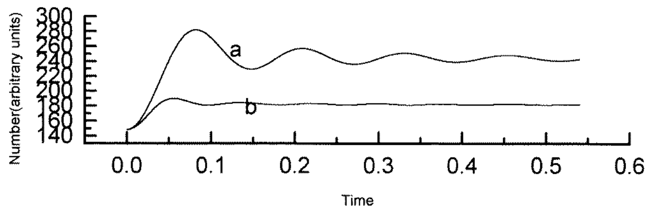

Figure 1. The mean number of atoms versus time. The parameters $\alpha_p^A = 3$, $\alpha_p^P = 4$. In (*a*), we take $n_0 = 1000$, in (*b*), $n_0 = 10\,000$.

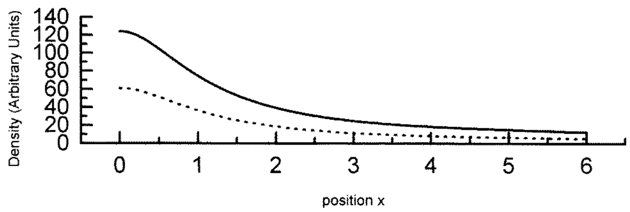

Figure 2. The normal density profile of trapped atoms for several temperatures, the parameter $n_0 = 1000$. For the full curve $T = 100$, for the dotted curve $T = 10$.

where T is the temperature, and k_B is Boltzmann's constant. Now we turn to the case of $T \sim 0$. In this case, the term $\cos^2\theta_k n_k^d$ in equation (11) and the detuning term $\delta_k = \omega_0 - \omega_k$ in the quasiparticle energy can be negligible. Thus, we obtain

$$\rho_n(x) = \sum_k \left(\exp\left(\frac{k^2/2m + V(x)}{k_B T} \right) - 1 \right)^{-1} = \lambda^{-3} g_{3/2}(e^{-\beta V(x)}). \tag{12}$$

This is just the LDA result that is obtained by replacing the fugacity in [11, 12] with $z\exp(-\beta V)$. The numerical result of equation (11) is depicted in figure 2, where the curve is for a harmonic trap $V(x) = \frac{m}{2}\omega^2 x^2$. The condensate part $\rho_s(x)$ of total density $\rho(x)$ can be calculated by using the Mayer cluster expansion theory [10, 11]

$$\rho_s(x) = \frac{z_1}{1 - z_1} |\psi_0(x)|^2 \tag{13}$$

where $z_1 = \exp(-\beta V(x))$ and $\psi_0(x)$ is the ground state of a particle in the harmonic oscillator potential.

In equilibrium, the expectation number of photons with frequency ω_k may be given as

$$\langle a_k^+ a_k \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, [\cos^2\theta_k \langle c_k^+ c_k \rangle + \sin^2\theta_k \langle d_k^+ d_k \rangle]. \tag{14}$$

It is well known that the quasiparticle occupation number can be expressed as a Bose–Einstein distribution function. Therefore, we can write

$$\langle a_k^+ a_k \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, [\sin^2\theta_k (\exp(-\varepsilon_k^c/k_B T) - 1) + \cos^2\theta_k (\exp(-\varepsilon_k^d/k_B T) - 1)]. \tag{15}$$

From this expression and the fact that the rate $S(k)$ of photon scattering from the condensate is proportional to $\langle a_k^+ a_k \rangle$, we see that the line shape is non-Lorentzian, and exhibits a very narrow spike close to the resonance (see figure 3), the larger the number of condensate

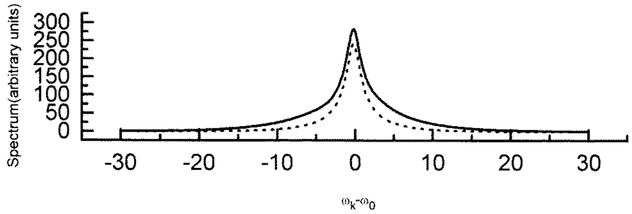

Figure 3. The spectrum scattered form BEC of trapped atoms for different n_0. For the dotted curve $n_0 = 1000$, for the full curve $n_0 = 100$. The temperature is commonly taken to be $T = 100$.

atoms, the narrower the shape of the spectrum scattered from the BEC of atoms. The situation will change somewhat when the interaction among the atoms

$$H_i = \sum_{p_1, p_2, p_1', p_2'} V_{p_1, p_2, p_1', p_2'} g_{p_1}^{+} e_{p_2}^{+} e_{p_2'} g_{p_1'}$$

is included. However, for the Bogoliubov approximation considered here, the inclusion of the interaction between the ground and excited atoms only causes a change of a parameter in the $\varepsilon_p^e(x)$, which does not change the shape of the spectrum. In fact, as argued in [13], our model includes all the effects of atom–atom interactions due to the exchange of transverse photons.

In summary, we conclude that when Bogoliubov approximation is used to simplify the Hamiltonian of the atom-quantized radiation field system, the mean number of atoms appears to be a function of time, which behaves as a damped oscillation. The damping rate and the period of quasioscillation depend on both the coupling constant μ and the number of condensate atoms n_0, whereas the density profile of the normal part of trapped atoms depends weakly on the number of condensate atoms. Particularly, the line shape of the spectrum scattered from BEC is non-Lorentzian and closely related to the number of condensate atoms. The narrow feature of the spectrum at $\omega_k \sim \omega_0$ exhibits interesting and feasible applications for precision spectroscopy.

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