Free expansion of a Bose–Einstein condensate in the presence of a thermal cloud

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Abstract

We investigate numerically the free-fall expansion of a ⁸⁷Rb atom condensate at nonzero temperatures. The classical field approximation is used to separate the condensate and the thermal cloud during the expansion. We calculate the radial and axial widths of the expanding condensate and find clear evidence that the thermal component changes the dynamics of the condensate. Our results are contrasted with the experimental data.

(Some figures in this article are in colour only in the electronic version)

Since the first experimental realization of Bose–Einstein condensation in dilute atomic gases [1], the measurement techniques based on time-of-flight expansion became a powerful method to study ultracold atomic systems. In fact, this kind of measurement was used to prove the existence of a condensate. Starting from an axially (cigar- or disc-shaped) symmetric atomic cloud, it happened that after its release from a trap the ratio of both the axial and radial condensates and thermal cloud widths systematically changed during the expansion. Eventually the anisotropy inversion for a condensate was observed which was a crucial distinction from the behaviour of a thermal cloud. The thermal part, in agreement with the classical Maxwell distribution of velocities, eventually takes a spherical shape. For a small condensate (like the very first rubidium condensate consisting of some 2000 atoms only) the anisotropy inversion is just a direct manifestation of the Heisenberg uncertainty principle—more spatial squeeze—higher momenta. For larger samples a similar inversion is a result of the interaction energy stored anisotropically in the trapped condensate. It is worth adding that the free expansion technique was also used for degenerate fermionic gases, for instance to probe the superfluidity of strongly interacting atomic Fermi mixtures [2] or to measure the p-wave Feshbach resonances for fermionic atoms [3].

The main purpose of this work is to investigate an influence of a thermal cloud on the dynamics of an expanding condensate. If such an impact exists, another question is whether it is restricted only to times just after the release or is continued over the whole expansion time. Finally, it would be interesting to know how the influence during the expansion compares to the influence while the system is confined.

To investigate the mutual interaction between the condensed and thermal components during the expansion we employ the classical field approximation in a version described in [4]. So, we start with the N-particle Hamiltonian written in terms of the field operator \( \hat{\Psi}(\mathbf{r}, t) \) satisfying the bosonic commutation relations. Assuming the usual contact interaction potential for colliding atoms the Hamiltonian takes the form

\[
H = \int d^3r \left[ \frac{\hbar^2}{2m} \nabla^2 + V_{tr}(\mathbf{r}, t) \right] \hat{\Psi}(\mathbf{r}, t) + \frac{g}{2} \int d^3r \hat{\Psi}^*(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t),
\]

where the interaction strength \( g = 4\pi\hbar^2a/m \) and \( a \) is the s-wave scattering length. The trapping potential \( V_{tr}(\mathbf{r}, t) \) is time dependent and is switched off instantaneously to trigger the expansion. The main equation of the classical field
approximation reads

\[
\frac{i\hbar}{\partial t} \Psi(r, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r, t) \right] \Psi(r, t) + g \Psi^*(r, t) \Psi(r, t) \Psi(r, t)
\]  

(2)

and is just the Heisenberg equation of motion for the field operator stripped of its operator character. The complex wavefunction \( \Psi(r, t) \), which we call the classical field, describes both condensed and noncondensed atoms. The use of the classical field instead of the field operator is justified when only macroscopically occupied modes are taken into consideration. This reasoning remains in analogy with the treatment of an intense light beam which, although consisting of single photons, may be described by the electric and magnetic fields.

The important question of how to extract from the classical field the information on a condensate and a thermal cloud is resolved using the Penrose and Onsager definition of Bose–Einstein condensation [5] and by taking into consideration the measurement process. Since any detector has a limited spatial and temporal resolution, a complicated (both in space and time) behaviour of the high-energy classical field is smoothed out during the measurement. Therefore, the quantity which is physically important is a time and/or space averaged one-particle density matrix. According to the Penrose and Onsager definition the condensate wavefunction is an eigenvector corresponding to the dominant eigenvalue of a one-particle coarse-grained (i.e. averaged over time and/or space) density matrix. We closely follow the experiment and realize the averaging as a column integration along one of the radial directions. The physically important (averaged along the y direction) one-particle density matrix is given by

\[
\bar{\rho}(x, z, x', z'; t) = \int dy \Psi(x, y, z, t) \Psi^*(x', y, z', t)
\]  

(3)

and the splitting procedure requires the diagonalization of (3). This kind of averaging was already used to investigate a decay of multiply charged vortices [6]. The splitting procedure is then summarized as

\[
\bar{\rho} = \sum_k N_k \phi_k(x, z, t) \phi_k^*(x', z', t)
\]  

(4)

\[
\psi_0(x, z, t) = \sqrt{N_0} \phi_0(x, z, t)
\]  

(5)

\[
\rho_T(x, z, t) = \bar{\rho}(x, z, x, z; t) - |\psi_0(x, z, t)|^2
\]  

(6)

Here, \( \phi_k \) are the macroscopically occupied modes, \( N_0 \) is the dominant eigenvalue, \( \psi_0 \) is the condensate wavefunction and \( \rho_T \) is the density of thermal cloud.

Having introduced the classical field approximation we now describe our numerical procedure. First, we find the classical field corresponding to the \(^{87}\text{Rb} \) Bose gas (with a scattering length \( a = 5.82 \) nm) at equilibrium confined in a harmonic trap with frequencies \( \omega_x, \omega_y = \frac{2\pi}{137.4} \) Hz and \( \omega_z = 2\pi \times 12.6 \) Hz. Details on how to obtain an equilibrium state for a given number of atoms and at particular temperature are explained in [7]. Here, we just briefly outline our procedure. First, we solve iteratively the equations of the self-consistent Hartree–Fock method [8] and obtain in this way the densities of the condensed, \( n_c(r) \), and the thermal, \( n_{th}(r) \), fractions corresponding to the system with the total number of \( N \) atoms being at the equilibrium at a given temperature \( T \). Next, we built an initial classical field:

\[
\Psi(r, t = 0) = \sqrt{n_c(r)} + \sqrt{n_{th}(r)} e^{i\varphi(r)},
\]  

(7)

and randomize both the phase \( \varphi(r) \) and the density \( n_{th}(r) \) in such a way that the total energy per atom in the classical field equals the corresponding energy in the Hartree–Fock model. The presence of the phase factor in the second term in (7) is necessary; otherwise the classical field suffers from a lack of kinetic energy in comparison with the Hartree–Fock method. Then we let the field thermalize by evolving it according to equation (2). However, equation (2) is solved on a grid with a particular value of the spatial step for which the condensate fraction \( N_0/N \) does not change in time. The optimal spatial step \( \Delta x \) is approximately related to temperature by \( \frac{\Delta x^2}{2m} \approx k_B T \), where \( \Delta x_{\text{max}} = \pi/\Delta x \).

Since we intend to investigate the influence of thermal atoms on the condensate expansion, we generate numerically various equilibrium states, all having the same number of condensed atoms (\( N_0 = 30000 \) or \( N_0 = 90000 \)). Next, we suddenly turn off the trapping potential and allow the atomic cloud to expand. Technically speaking, we solve equation (2) on a larger grid (but having the same spatial step) and without any trap. We monitor the momentum distribution (i.e. the Fourier transform of the classical field) during the expansion and find that it changes for the first few milliseconds only. In other words, a few milliseconds are required to convert fully the interaction energy into the kinetic energy. Afterwards, the classical field evolves freely and can be found with the help of the propagator of the free Schrödinger equation. Finally, at a desired time the splitting of the classical field into the condensed and noncondensed components is performed. We have also investigated the case of switching off the trapping potential in a finite time of a few hundreds of microseconds as is done in the experiment, but the procedure just outlined showed no differences in the results.

In figure 1 we plot the radial and axial densities of an expanding atomic cloud at 22 ms. Initially the condensate is cigar shaped like a trap. Its aspect ratio in the Thomas–Fermi approximation is given by \( R_z/R_x = \omega_z/\omega_x \) [8] which equals approximately 1/10. After 22 ms, as can be seen in figure 1, the initial anisotropy is actually inverted. The radial size gets larger than the axial one. This, of course, is not true for the thermal cloud, in which case the final density becomes spherical.

Figure 2 reveals some technical details related to the read-out procedure. After the splitting of the classical field is concluded and the two-dimensional condensate density is known, this density is fitted by a two-dimensional inverted parabola (since according to the large number of atoms in the condensate the Thomas–Fermi approximation is valid). The fit is performed based on the least-squares method. In fact, fits depend on the realization and, as will be shown later, the aspect ratio is a quantity which is most sensitive to the realization.

The main result of this work is presented in figure 3. It shows the radial and axial condensate widths after 22 ms of
Figure 1. Axial (upper frame) and radial (lower frame) cuts of the total (thick solid line), condensate (dashed line) and thermal (thin solid line) densities as obtained by splitting the free expanding classical field at 22 ms as described in the text. The condensate fraction is equal to 0.3 and the number of condensed atoms \( N_0 = 90000 \). The oscillatory unit of length is defined based on the axial trap frequency: \( \sqrt{\frac{2}{m\omega_z}} \) and equals 3.0 \( \mu \text{m} \).

Figure 2. Condensate axial (left frame, dashed line) and radial (right frame, dashed line) densities for two single realizations (upper and lower frames, respectively) at 22 ms. Condensate density is extracted from the classical field by the splitting procedure and is fitted to a two-dimensional inverse parabola. The black lines show axial (left frame) and radial (right frame) cuts of such a fit. The parameters are the same as in figure 1.

Figure 3. Radial (squares and stars) and axial (circles and triangles) condensate radii as a function of the condensate fraction after 22 ms of ballistic expansion. Two sets of points marked by squares and circles correspond to the systems with the number of condensed atoms \( N_0 = 90000 \) whereas two other sets (marked by stars and triangles) represent the systems with \( N_0 = 30000 \) condensed atoms. The solid lines are shown to guide the eye. The horizontal dashed lines denote the Thomas–Fermi values for the radial lengths (two upper lines, the upper line for \( N_0 = 90000 \) and the lower line for \( N_0 = 30000 \)) and the axial lengths (two lower lines, the upper line for \( N_0 = 90000 \) and the lower line for \( N_0 = 30000 \)). Note that both radial and axial widths get shorter in comparison with the size of a pure condensate of the same number of atoms.

The authors claim that their experiment is performed in the Thomas–Fermi limit. Our data suggest that thermal atoms somehow temper the expansion of the condensate.

There are three experimental papers discussing the temperature effects having influence on the ballistic expansion of a condensate [10–12]. All of these papers claim that the behaviour of the condensed cloud measured in terms of its size during the expansion depends on the temperature of the system before the expansion. So, the quantitative comparison between the numerical calculations and the experiment is possible.

Since our numerical parameters were taken in a way to match the parameters of the experiment of [11] we started with that paper. In that experiment the authors attempted to keep constant the number of condensed atoms while expanding the atomic samples at various temperatures. They found the increase of radial and axial condensate lengths when the temperature gets higher (see figure 4 in [11]). The measured widths are larger than the corresponding Castin–Dum values.

So, the authors claim that their experiment is performed in the non-Thomas–Fermi regime. An increase of radial and axial widths with temperature is explained by an assumption that at equilibrium in a trap the thermal atoms exert a force on condensed atoms towards the centre of a trap thus compressing the condensate cloud. This compression results in a faster expansion in all directions after the trap is released. However, our calculations within the classical field approximation show that, actually, no compression of a condensate cloud occurs in a trap. We stress that this statement is also true within the self-consistent Hartree–Fock model [8]. In figure 4 we plot the axial and radial condensate densities obtained by solving self-consistently the equations of the Hartree–Fock model for a particular number of condensed atoms \( N_0 = 90000 \) but at various temperatures (solid lines which correspond to the condensate fractions 0.15, 0.30 and 0.60). We also added to the figure the densities of a pure condensate consisting...
of 90,000 atoms calculated by solving the Gross–Pitaevskii equation in imaginary time (dotted line) as well as by the Thomas–Fermi formula (dashed line). Clearly, figure 4 shows no compression due to the presence of a thermal cloud.

A qualitative difference between numerical results and the experimental data of [11] motivated us to make a comparison with other experimental works. For example, in [10] a deviation from the ballistic expansion is also reported. In figure 5(a) of that paper the authors plot the aspect ratio of the condensed component after 22.3 ms of free expansion as a function of reduced temperature. It is clear from this figure that for higher temperatures the results are different than the Castin–Dum limit [9] (the aspect ratio shows a deviation from the Castin–Dum values also in [11]). Therefore, we look separately at the axial and radial sizes of the expanding condensate in the case of the Orsay experiment. The results are presented in figure 5. Here, the experimental data are compared with the Castin–Dum values. This figure clearly shows that the experimental data stay close to the Castin–Dum values. In the axial direction the thermal cloud seems to temper the expansion of a condensate whereas the interplay between the condensate and the thermal component in the radial direction gets more complicated. Differences are on the level of a few per cent similar to what we obtain from our numerics (although for a different trap geometry) and opposite to what is reported in paper [11].

In other experimental work [12], the authors find a finite temperature correction to the Thomas–Fermi approximation as a function of the condensate fraction by measuring the ratio \( R^2 / N_0 \), where \( R \) is the condensate radius defined as \( R = (R_\perp R_\|)^{1/3} \) and \( N_0 \) is the number of condensed atoms. There is an agreement with Castin–Dum predictions [9] for low temperatures; however, when the temperature gets higher, the ratio \( R^2 / N_0 \) departs from the Castin–Dum value, getting larger (see figure 4 of [12]). The authors explain this behaviour using a combination of a modified Hartree–Fock model to describe the condensed and thermal fractions in a trap and an expansion model formulated by Castin and Dum [9]. They conclude that the influence of the thermal cloud on the condensate during the expansion is negligible which seems to be in opposition to what is claimed in [10] and [11]. It also contradicts our findings. Therefore, we decided to compare all experiments and our numerical results on a graph where we plot \( R / N_0 \) (actually, normalized to the value given by the Castin–Dum approach to make the comparison feasible) as a function of the condensate fraction. In the Castin–Dum formulation one has

\[
R^2(t) / N_0 = 15a^2 \lambda_{\perp}(t) \lambda_{\|}(t)^{5/3}
\]

where

\[
\lambda_{\perp}(t) = \sqrt{1 + t^2}
\]

\[
\lambda_{\|}(t) = 1 + \beta^2 (t \arctan t - \ln \sqrt{1 + t^2}),
\]

\[
\beta = \omega_{\|} / \omega_{\perp}
\]

and the time \( t \) is expressed in units of \( 1/\omega_{\perp} \) whereas \( a \) is an oscillatory unit length calculated based on the geometric mean of all angular frequencies. Figure 6 shows that our results (solid squares for \( N_0 = 90,000 \) and open squares for \( N_0 = 30,000 \)) remain in a quite good agreement with the Orsay experimental data.

Certainly, further experimental and theoretical effort is required to gain more insight to what indeed is happening during the expansion of condensate and thermal cloud.

Finally, in figure 7 we plot the aspect ratio for a condensate for various condensate fractions. The aspect ratio seems to be a quantity which is most sensitive to the interplay between the thermal cloud and the condensate. For low temperatures...
In conclusion, we have studied the expansion of the Bose–Einstein condensate in the presence of thermal atoms. Using the classical field approximation we have shown that thermal atoms change the dynamics of a condensate in such a way that both radial and axial condensate widths get smaller in comparison with the case when there is no thermal cloud. This results in a change in the condensate aspect ratio which becomes larger for a smaller condensate fraction (i.e., larger thermal cloud). While all papers agree that the thermal cloud does play a role in the expansion of the condensate, the details remain unclear. The three experimental papers are not mutually in agreement and also our results do not coincide with some measurements. Clearly more work is needed to clarify this somewhat confusing situation.

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