# Expansion of a Bose-Einstein condensate in a harmonic potential

M. Holland and J. Cooper
*JILA and Department of Physics, University of Colorado, Boulder, Colorado 80309-0440*
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We analyze the three-dimensional dynamic expansion of a weakly interacting Bose-Einstein condensate in a harmonic trap when the spring constants of the confining potential are instantaneously reduced. Our results are compared with experimental observations from a condensate of $^{87}$Rb atoms.

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The recent demonstrations of Bose-Einstein condensation in magnetic alkali-metal vapor traps using rubidium [1], lithium [2], and sodium [3] are a result of the tremendous progress in magnetic and optical techniques for trapping and cooling neutral atoms over the last few years [4,5]. One reason that the observation of a condensate is a significant achievement in atomic physics is that it is one of the most interesting demonstrations of the wave nature of matter. Once a weakly interacting condensate is formed in a finite system, any dissipation, including background loss processes, will induce a symmetry breaking for the many-particle ground-state wave function and generate a well-defined phase for the condensate that diffuses slowly over time [6]. This is analogous to the coherence property of the laser in which photons are stimulated into a resonant mode of a cavity. The ability to evaporatively cool an atomic vapor into the regime of significant quantum degeneracy leads to the possibility for a number of new kinds of experiments designed to probe novel light scattering and atomic interference effects [7]. In order to model the condensate evolution, it is usually necessary to consider not only the quantum statistics, but also ground-state collisions that introduce an intrinsic nonlinearity into the dynamics. Photons do not usually interact directly so that this is one difference between a Bose-Einstein condensate and an optical laser. In addition the condensate energies are resonant in all three dimensions of the confining potential.

In the recent experiment, the spatial extent of the condensate arose from the interplay between two potentials. A magnetic trap was used to generate a time-averaged harmonic confining potential with equal spring constants in the two dimensions defining the horizontal plane, and a spring constant that was approximately eight times larger in the vertical direction. A second effective potential was formed from the intrinsic self-interaction due to ground-state collisions. This interaction energy is proportional to the local average density of the condensate wave function since the ground-state scattering length for the isotope of rubidium used is very much less than the characteristic de Broglie wavelength for the center-of-mass motion of the atom at the trap temperature. This allows a shape-independent approximation to be made for the interaction between ground-state atoms [6]. The steady-state wave function is then self-consistent and an iterative method can usually be used to find its form.

A procedure for deriving this self-consistent ground state in the case of one dimension and in the isotropic three-dimensional situation has been previously demonstrated using a time-dependent solution of the nonlinear Schrödinger equation [8]. In this calculation, the wave function was initialized to the ground state of the harmonic potential and the nonlinearity increased adiabatically. Although the experimental configuration in which condensation was observed is neither one dimensional nor isotropic, this approach may be extended to two dimensions to describe the expansion phase of the experiment by taking advantage of the rotational symmetry about the vertical axis. The light scattering properties of the condensate are predicted to be a sensitive function of the atomic density and so there is considerable motivation for determining the condensate number. The trap was opened by reducing the spring constants in all three dimensions before the probe field was introduced in order to reduce the density and increase the size of the cloud. The initial expansion rate would have depended on the number of atoms in the original condensate because of the self-consistent field. Modeling the ballistic expansion allows us to calculate this effect. It is also interesting to evaluate the relative size of the collisional nonlinearity from the experimental parameters since the interactions may strongly influence the spatial and temporal correlation functions for the condensate amplitude and therefore the diffusion of the macroscopic phase.

The evolution of the condensate wave function $\psi(\mathbf{r},t)$ may be described by the nonlinear Schrödinger equation known as the Ginzburg-Pitaevskii-Gross equation [9]

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)+V(\mathbf{r})\psi(\mathbf{r},t)+NU_0|\psi(\mathbf{r},t)|^2\psi(\mathbf{r},t), \tag{1}$$

where $\mathbf{r}=(x,y,z)$ is the displacement from the trap center and $m$ is the mass. The harmonic potential may be written as $V(\mathbf{r})=\frac{1}{2}m\omega^2(x^2+y^2+\epsilon z^2)$ where $\epsilon$ is the ratio of the vertical ($z$ direction) and horizontal spring constants. The nonlinearity is proportional to both the number of atoms $N$ and to $U_0=4\pi\hbar^2a/m$, which characterizes the interaction and is defined in terms of the ground-state scattering length $a$. Using the circular cylinder coordinate system $(r,\theta,z)$ with $x=r\cos\theta$ and $y=r\sin\theta$ we take the case in which the wave function is invariant with respect to changes in $\theta$. The spatial scale for the ground state of the trap in the horizontal plane is $l=\sqrt{\hbar/(2m\omega)}$, so we may scale the coordinates $\rho=r/l$ and $\zeta=z/l$ and rewrite Eq. (1) in the dimensionless form

 

$$i\frac{\partial\varphi(\rho,\zeta)}{\partial\tau}=\left(-\frac{\partial^2}{\partial\rho^2}-\frac{\partial^2}{\partial\zeta^2}+\frac{1}{4}(\rho^2+\epsilon\zeta^2-\rho^{-2})\right)\varphi(\rho,\zeta)$$
$$+8\pi N\alpha\rho^{-1}|\varphi(\rho,\zeta)|^2\varphi(\rho,\zeta), \quad (2)$$

where $\tau=\omega t$ is the time and $\alpha=a/l$ is the scattering length. This form is suitable for integration using an appropriate numerical method. The wave function $\varphi(\rho,\zeta)=l\sqrt{l\rho}\psi(\rho,\zeta)$ must be normalized at all times by satisfying the condition

$$2\pi\int|\varphi(\rho,\zeta)|^2 d\rho d\zeta=1, \quad (3)$$

since Eq. (2) contains a nonlinear term.

For small numbers of atoms, the self-consistent wave function may be found by inserting a time-dependent prefactor $f(\tau)=[1-\cos(\pi\tau/\tau_r)]/2$ in front of the term containing $N$ and choosing the ramp time $\tau_r$ to be long compared to the oscillation time of the ground state of the trap. At the start of the calculation, the wave function should be initialized to the ground energy eigenstate for the bare harmonic oscillator,

$$\varphi(\rho,\zeta)=\left(\frac{\sqrt{\epsilon}\rho^2}{8\pi^2}\right)^{1/4}e^{-(\rho^2+\sqrt{\epsilon}\zeta^2)/4}. \quad (4)$$

An alternative method suitable for larger numbers of atoms is to insert $f(\tau)$ in front of the terms $\partial^2/\partial^2\rho$, $\partial^2/\partial^2\zeta$, and $1/\rho^2$ in Eq. (2). This corresponds to increasing the kinetic energy contribution adiabatically. The appropriate initial wave function is then the energy eigenstate derived from considering the time-independent equation with only the harmonic potential and self-interaction terms [10]

$$\mu\varphi(\rho,\zeta)=\frac{1}{4}(\rho^2+\epsilon\zeta^2)\varphi(\rho,\zeta)$$
$$+8\pi N\alpha\rho^{-1}|\varphi(\rho,\zeta)|^2\varphi(\rho,\zeta). \quad (5)$$

This leads to the initial wave function

$$\varphi(\rho,\zeta)=\left(\frac{\rho(\mu-\frac{1}{4}(\rho^2+\epsilon\zeta^2))}{8\pi N\alpha}\right)^{1/2} \quad (6)$$

where

$$\mu=\left(\frac{15}{8}\sqrt{\epsilon}N\alpha\right)^{2/5} \quad (7)$$

is found from Eq. (3). The number of condensate atoms we have to consider in order to model the experiment turns out to be in the intermediate regime where both methods can be applied independently to provide a consistency check.

In order to expand the trap for probing, a nonadiabatic change in the spring constants of the harmonic potentials was made in the experiment. The resulting cloud increased in size and rapidly reached the region where the phase-space density decreased below the critical value required for the presence of a condensate. Evidence that a condensate had been created in the original trap was inferred from the size and shape of the expanded cloud. In order to compare with the experimental result, the initial evolution from the self-consistent wave function may be simulated by abruptly decreasing the oscillation frequencies in $V(\boldsymbol{r})$. The resulting cloud will then expand due to both the change in the confining force as well as the repulsive self-interaction.

The Ginzburg-Pitaevskii-Gross equation for the mean field can only be used when particle fluctuations do not significantly affect the macroscopic dynamics. The effect of fluctuations at zero temperature can be characterized by the populations of the fundamental excitations about the mean-field solution that scale with the parameter $na^3$ where $n$ is the atomic density [11]. Although in the case of liquid helium this parameter may approach unity, in the magnetic trapping of a dilute vapor it is typically small and for our situation is of order $10^{-5}$. Fluctuations can therefore be neglected in the establishment of the condensate density distribution. Alternative arguments based on a cluster expansion and the smallness of the collision frequency relative to frequencies associated with the mean field and the trap give comparable results. The same applies to the expansion phase when the trapping potential is reduced, since in this case the density decreases rapidly and the dynamics are dominated by free-particle trajectories. The temperature of the cloud we analyze prior to expansion is very close to zero and much less than the critical temperature at which the condensate starts to form since the noncondensed part has been mostly evaporated away. We are therefore not concerned with critical fluctuations at the phase transition temperature [11]. The condensate fraction is near unity and dissipation, arising from collisions with above condensate atoms, is strongly suppressed. The validity of the expansion model is limited to the initial transient regime where it is applied since dissipation in the expanded trap is not included. Eventually the cloud will thermalize in the new potential, but this occurs on a long time scale (set by the time between collisions in the very low density cloud and inelastic collisions with the background gas).

The spatial distribution in the $(x,z)$ plane was recorded after a time corresponding to approximately a quarter cycle of the oscillation in the horizontal dimension of the expanded trap. The absorption of a weak probe pulse propagating in the $y$ direction was observed through a telescope with a camera. The camera pixel resolution corresponded to approximately 4.2 $\mu$m in the original cloud. We model the detection process by integrating the wave-function density we calculate through the $y$ direction,

$$\mathcal{F}(x,z)=\int_{-\infty}^{\infty}dy|\psi(x,y,z)|^2. \quad (8)$$

The distribution $\mathcal{F}(x,z)$ can be compared with the camera image in which each pixel is a measure of the integrated

TABLE I. Values of the model parameters.

| | Original trap | Expanded trap |
|---|---|---|
| $\epsilon$ | 8 | 0.25 |
| $\omega$ | 51 $s^{-1}$ | 26 $s^{-1}$ |
| $l$ | 2.7 $\mu$m | 3.7 $\mu$m |
| $N$ | 2000 | 2000 |
| $a$ | 5.2 nm | 5.2 nm |

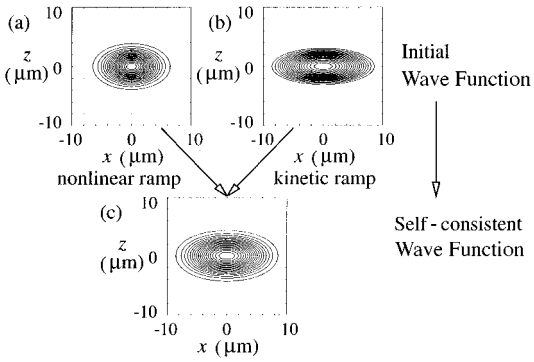


FIG. 1. The two ways of deriving the self-consistent wave function.

column density through the atomic cloud. The experimental parameters that enter into the model are indicated in Table I. The number of atoms is estimated from the optical density associated with the amount of probe absorption. The ground-state scattering length for spin-polarized $^{87}$Rb atoms has recently been measured and is believed to be accurate to $\pm 15\%$ [12].

In Fig. 1, we illustrate the application of the two methods for deriving the self-consistent wave function. The wave function may be initialized to the distribution given in Eq. (4) as illustrated in Fig. 1(a) and the nonlinear term adiabatically increased to produce the wave function shown in Fig. 1(c). Alternatively, we may initialize the wave function to the distribution given in Eq. (5) as shown in Fig. 1(b) and increase the kinetic energy terms. This produces the same wave function given in Fig. 1(c) to good numerical agreement. From this result it is evident that the kinetic energy terms, harmonic potential terms, and the self-interaction potential, are all important in establishing the self-consistent wave function for these parameters. Tests of the numerical method are provided by checking that the final distribution is not sensitive to the grid spacing on which the wave function is stored, to the time step used for the integration, or to the adiabatic ramp time. The number of grid points was $256\times 512$ with equal grid spacing in the two dimensions, and 40 000 equal time steps were taken giving a computation time of a few hours on a workstation. The propagation algorithm used was the Crank-Nicholson differencing method in which an alternating direction implicit algorithm was used to

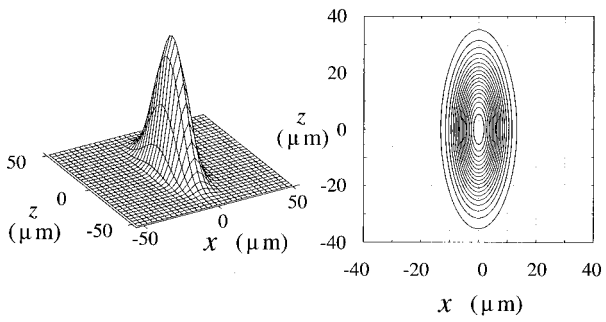


FIG. 2. The evolved density distribution $\mathcal{F}(x,z)$ found by evaluating the self-consistent wave function for 2000 atoms, abruptly reducing the spring constants for the harmonic potential, and expanding for 60 ms.

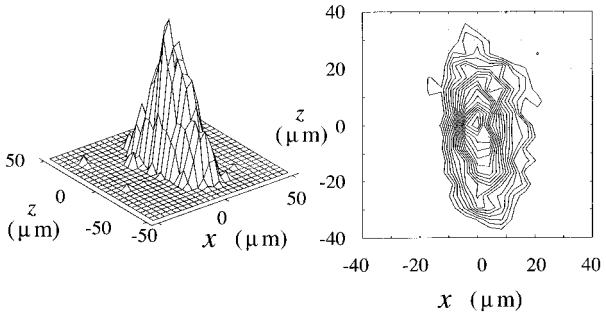


FIG. 3. The experimental image of the rubidium condensate observed on the camera after an expansion time of 60 ms.

switch between the two dimensions [13]. In all of the contour diagrams in this paper, we have drawn 20 equally spaced contours from the minimum up to the maximum value.

In Fig. 2 we show the result of evolving the wave function in Fig. 1(c) for a time $\tau = 3.07$ corresponding to 60 ms in the expanded trap. The numerical result may be compared with the experimentally observed condensate distribution shown in Fig. 3. The evaporative cooling process in this case was continued to the point at which the cloud contained almost no isotropic thermal component and was almost purely condensate atoms. The spring constants were then reduced to the same values used in the simulation and the image recorded after the same expansion time.

The comparison between the wave function derived from the nonlinear Schrödinger equation and the experimental result shows a number of notable features. The aspect ratio found by dividing the width of the density distribution in the $x$ direction by that in the $z$ direction is almost the same in both cases. This ratio is a property of the ground state of the quantized harmonic oscillator perturbed by the self-field and provides good evidence that the observed cloud evolved from a condensate. In contrast, the thermal component which was recorded in other images [1,14] gives a density feature at larger distances that is circular. The overall spatial extent of the expanded wave function for 2000 atoms is also consistent with the observed condensate. In Table II we indicate the full widths at half maximum in the two dimensions calculated for different numbers of condensate atoms. The zero atom simulation corresponds to the limit in which the mean field can be neglected. The tighter confinement in the vertical direction of the original trap corresponds to a higher zero point energy in that direction. Consequently, the ground state contains a range of momentum components that is larger vertically than horizontally. This translates to an increased vertical spread-

TABLE II. Full width at half maximum for the experimental results and simulated data showing the dependence of the expansion on the condensate number. The experimental widths have an uncertainty of order 3 $\mu$m.

| | $\Delta z$ ($\mu$m) | $\Delta x$ ($\mu$m) |
|---|---|---|
| Experiment | 36 | 15 |
| 0 atom simulation | 29.3 | 12.3 |
| 1000 atom simulation | 35.6 | 12.6 |
| 2000 atom simulation | 38.4 | 13.1 |
| 3000 atom simulation | 40.4 | 13.6 |

ing in the evolved density distribution even in the absence of particle interactions. However, the aspect ratio for the calculation omitting the mean field is less than that observed in the experiment. The effect of the mean field on establishing the self-consistent ground state can clearly be seen even for this relatively small condensate.

The spatial and temporal diffusion properties of the condensate phase are dependent on the strength of the interaction between condensate atoms. For 2000 rubidium atoms, our model gives the maximum of the interaction energy at the peak density to be only 20% larger than the zero-point energy for the harmonic confining potential. This result is significant because it indicates that it may be possible to access different kinds of parameter regimes from the standard trap geometries. Adiabatically expanding the trap by reducing the spring constants would lead to a regime in which the spatial coherence of the condensate is determined almost entirely by the ground-state size. This linear regime is required for proposals for an atom laser designed to generate a coherent beam of atoms in analogy with the normal laser for photons [15]. Alternatively, by ramping up the trap, as was actually done in the experiment, the effect of the nonlinearity can be increased until the spatial coherence of the condensate is determined primarily by collisions. The situation is then much closer to that of an infinite homogeneous system since the confining potential may play an important role only at the boundaries.

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