Expansion of a Bose-Einstein Condensate in an atomic waveguide

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The expansion of a Bose–Einstein condensate in an atomic waveguide is analyzed. We study different regimes of expansion, and identify a transient regime between one-dimensional and three-dimensional dynamics, in which the properties of the condensate and its further expansion can be well explained by reducing the transversal dynamics to a two–level system. The relevance of this regime in current experiments is discussed.

During the last years, the Bose–Einstein Condensation (BEC) has constituted one of the most active research fields in modern Atomic Physics. Several experiments have shown the coherent character of the outcoupled bosons from a condensate, i.e. a BEC constitutes a bright coherent matter–wave source, offering promising possibilities in the context of matter–wave optics. However, contrary to the extremely dilute non–condensed cold atomic clouds traditionally used in Atom Optics, the atom–atom interaction induces the BEC dynamics to be intrinsically nonlinear. In this sense, the BEC optics has also been called Nonlinear Atom Optics (NLAO). Remarkable experiments have investigated the resemblance between nonlinear optics phenomena and those in NLAO, as four–wave mixing and dark–solitons. The nonlinearity may deeply alter the dynamics of the wavefunction, and the straightforward validity of atom optics elements should be questioned. As a consequence, BEC optics should not be considered only as a trivial extension of atom optics, but an emerging discipline of its own.

The analysis of low–dimensional BEC has been recently a subject of active investigation. In these systems one or two spatial directions do not contribute to the dynamics, since the mean–field energy is smaller than the typical trapping energy in these directions. New effects have been predicted in low–dimensional BEC, as quasicondensates (for a recent experiment, see Ref. [9]), and Tonks gas [13, 14]. In addition, the physics of low–dimensional Bose gases is closely related with one of the most actual challenges of the modern Atom optics, namely the developing of atom optics micro-structures [15, 16]. In these devices, an integrated element should be designed to solve the fundamental problem of wiring, i.e. to allow for signal propagation between different parts of the structure, with negligible leaks. In this direction, current–carrying structures [16] or dipole–force confinement in light fields [17] constitute the most promising possibilities. Up to now, the majority of experiments with atomic waveguides have used cold non–condensed atomic clouds. However, recent experiments in which a BEC have been confined into an atomic waveguide open the interesting and timely question of how a BEC expands inside of an atomic waveguide. It is the aim of this paper, to characterize in detail the loading of a BEC into a waveguide by the expansion of an initially 3D trapped BEC. The BEC properties (both the initial chemical potential and the subsequent expansion dynamics) strongly depend on the dimensionality of the guiding, ranging from a purely 3D character to a fully 1D one. We shall show that due to the cylindrical symmetry of the guiding potential, there is an intermediate regime, significant for a large number of experimental situations, in which the BEC is well described by considering the radial degree of freedom as a two–level system, significantly departing from the 1D predictions, even when the excited radial states are scarcely populated. As a consequence, very large radial frequencies are necessary to neglect observable 3D effects on the dynamics, even for a small number of condensed particles.

In the following, we consider the guiding geometry currently used in experiments performed at the University of Hannover, although our study may be equally extended to similar geometries, as quantum wires. Typically, a BEC is initially created in a hybrid trap, produced by the overlapping of a cylindrical magnetic trap, and a blue–detuned TEM$_{01}$ (doughnut–mode) laser beam propagating along the axis of the magnetic trap. The corresponding potential exerted on the atoms can be written as $V(r) = V_i = m \omega_r^2 r^2/2 + m \omega_z^2 z^2/2$, where $\omega_r$ and $\omega_z$ are the radial and axial trapping frequency respectively. After the creation (at $t = 0$), the magnetic trap is switched off. The subsequent evolution corresponds, therefore, to a BEC confined radially by the laser field but free to move in the axial dimension, as in a waveguide. We shall assume that the radial frequency is kept unchanged after the releasing of the magnetic trap, and therefore for $t > 0$, $V(r) = V_f = m \omega_r^2 r^2/2$. To facilitate the discussion of our results, we shall take as a reference case a $^{87}$Rb BEC of $10^4$ atoms initially located in an hybrid trap of $\omega_r = 2\pi \times 450$Hz and $\omega_z = 2\pi \times 10$Hz. This is a typical situation in the ongoing experiments performed at the University of Hannover.

For sufficiently low temperature, the BEC dynamics can be accurately described by the corresponding Gross–
Pitaevskii equation (GPE) [18]

$$i\hbar \frac{\partial}{\partial t} \psi = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V + g |\psi(r,t)|^2 \right\} \psi,$$  

(1)

where the potential term $V(r,t)$ is defined above, and $g = 4\pi\hbar^2 a N/m$ is the coupling constant, with $a$ the $s$-wave scattering length ($5.8 nm$ for $^{87}$Rb), and $m$ the atomic mass, while $N$ is the number of condensed atoms. With this choice, $\psi(r,t)$ is normalized to 1.

The BEC expansion in the waveguide after releasing the axial trap is a particular case of an anisotropic harmonic trap with time-dependent frequencies. For sufficiently shallow traps, the BEC can be considered at any time to possess a self-similar 3D Thomas–Fermi (TF) wavefunction [19,20]:

$$\psi(r,t) = b_z^{-1} b_0^{-1/2} \chi(r/b_z, z/b_z) e^{-i\mu_0 \tau(t)/\hbar} e^{-i\phi(r,z,t)},$$  

(2)

where $\phi(r,z,t) = (m/2\hbar) (r^2 b_z^2 + z^2 b_z^2)$, $\chi(r,z) = (\mu - V(r))/g$, $b_z(t)$ and $b_0(r)$ are scaling factors which evolve in time according to $b_z(t)$ and $b_0(r) = \omega_0^2 b_z(t)/b_z^3(t)$ and $b_0(t) = \omega_0^2 b_z^3(t)/b_z^2(t)$, and $\tau(t) = \int dt' \sqrt{b_z^2(t') b_z^2(t')}$. We shall define the loose-guiding (LG) regime the situations in which the 3D TF approximation is valid. In this regime, the initial BEC in the hybrid trap is characterized by the corresponding chemical potential

$$\mu_t = \frac{1}{2} \left( 15Na\hbar^2 m^{1/2} \omega_z^{3/2} \right)^{2/5}.$$  

(3)

The TF approximation, which neglects the kinetic energy term, is roughly correct for trapping energies smaller than the corresponding self-interaction. Since the trapping geometry used in the guiding experiments is strongly cigar-shaped, the TF approximation may become invalid in the transversal directions, while still being accurate axially. We shall refer to this situations as tight-guiding regime. An extreme case of this regime occurs when the radial binding is strong enough to dominate completely the transversal dynamics, which can therefore be considered as frozen. In this case, the dynamics becomes 1D in the axial direction, and the wavefunction can be factorized as $\psi(r,t) = \psi_{1D}(z,t) \Phi_0(r)$, where $\Phi_0(r)$ is the ground-state wavefunction of the transversal harmonic oscillator. Provided the TF approximation is valid in the axial coordinate, the dynamics of the BEC in the 1D guiding limit can be accurately described by a self-similar TF solution in the axial direction,

$$\psi_{1D} = b_z^{-1/2} \chi_{1D}(z/b_z(t)) e^{-i(\mu_{1D} \tau(t)/\hbar + \omega_z t)} e^{-i\phi(z,t)},$$  

(4)

where $\chi_{1D}(z)^2 = (\mu_{1D} - V(z))/g_{1D}$, $\phi(z,t) = m b_z z^2/2 h_\omega^2$, $b_z(t) = \omega_z^2/b_z^2(t)$, $\tau(t) = \int dt' b_z(t')$, and $V(z) = m \omega_z^2 z^2/2$. After integrating over the transversal direction, one can find the effective nonlinear energy term, is roughly correct for trapping energies smaller than the corresponding self-interaction. Since the TF condition is violated in the radial direction. The value of the chemical potential can be found easily by graphical methods. For $\tilde{\mu} = \mu_t - \hbar \omega_r$, with $\mu_t$ is the chemical potential in the tight-guiding regime. Keeping only first order terms in $|C_1|/|C_0|$, we find that the axil profile $n(z) = \int dx dy |\psi(x,y,z)|^2$ can be written in the form

$$n(z) \simeq n_{1D}(z) \left[ 1 + \frac{3}{4} \left( \frac{n_{1D}(z)}{2\hbar \omega_r / g_{1D} - n_{1D}(z)} \right) \right].$$  

(9)

where $n_{1D}(z) = |\chi_{1D}(z)|^2$ is the the axial density in the 1D limit, while the second term within the brackets introduces the correction coming from the transversal dynamics. The value of the chemical potential can be found by imposing normalization to the wavefunction:

$$1 = \int n(z) dz = \frac{2^{5/2}}{3} \tilde{\mu}^{3/2} g_{1D} m^{1/2} \omega_z \times$$

$$\left\{ 1 + \frac{9}{16} \left[ \frac{2}{\sqrt{\beta}} (\beta + 1)^2 \arctan \sqrt{\frac{\beta}{\beta - 2 - \frac{10}{3}}} \right] \right\}.$$  

(10)

where $\beta = 2 \hbar \omega_r / \mu_{1D} - 1$. The root $\tilde{\mu}$ of this equation can be found easily by graphical methods. For $\tilde{\mu}/2\hbar \omega_r \ll 1$ one can find the analytic correction to the 1D solution:

$$\tilde{\mu} \simeq \mu_{1D} \left( 1 - \frac{\mu_{1D}}{5 \mu_{1D}} \right).$$  

(11)

In order to test the above discussion, we have numerically solved the 3D GPE by means of a Crank–Nicholson method. After obtaining the ground–state of the hybrid trap using imaginary time evolution, we have calculated

$$\mu_{1D} = \frac{1}{2} \left( \frac{3}{7} g_{1D} m^{1/2} \omega_z \right)^{2/3}.$$  

(5)

However, in a general tight-guiding situation, the transversal dynamics cannot be considered as frozen, even though the TF condition is violated in the radial direction. Since $\hbar \omega_r > g |\psi|^2$, only a few number of radial excited states is occupied. In particular, for a cylindrically symmetric trap only excited states of zero polar angular momentum are possible, i.e. only one excited state $\Phi_n$ is possible within the $2n$-th radial energy shell. This produces that for a large number of cases of tight–guiding waveguides (even for $\mu \sim 2 \hbar \omega_r$), only the first excited state $\Phi_1$ is significantly populated before the opening of the hybrid trap. In that case the transversal degree of freedom can be well described by a two-level system formed by the first two radial eigenstates:

$$\psi(r,t) = C_0(z,t) \Phi_0 + C_1(z,t) \Phi_1.$$  

(6)

Due to the tight–guiding, $|C_1|/|C_0| \ll 1$. Expanding up to first order in this small parameter, and assuming TF axial profile, the GPE at $t = 0$ can be cast to the form

$$\dot{\mu}_t C_0 = V(z) C_0 + g_{1D} C_3 - \frac{3 g_{1D}}{2} C_0^3 C_1,$$  

(7)

$$\dot{\mu}_t C_1 = (2 \hbar \omega_r + V(z)) C_1 - \frac{g_{1D}}{2} C_0^3 + \frac{3 g_{1D}}{2} C_0^3 C_1.$$  

(8)

$C_0$ and $C_1$ are taken as real functions, and $\mu_t = \mu_t - \hbar \omega_r$, with $\mu_t$ is the chemical potential in the tight-guiding regime. Keeping only first order terms in $|C_1|/|C_0|$, we find that the axil profile $n(z) = \int dx dy |\psi(x,y,z)|^2$ can be written in the form

$$n(z) \simeq n_{1D}(z) \left[ 1 + \frac{3}{4} \left( \frac{n_{1D}(z)}{2\hbar \omega_r / g_{1D} - n_{1D}(z)} \right) \right].$$  

(9)

where $n_{1D}(z) = |\chi_{1D}(z)|^2$ is the the axial density in the 1D limit, while the second term within the brackets introduces the correction coming from the transversal dynamics. The value of the chemical potential can be found by imposing normalization to the wavefunction:
the corresponding chemical potential $\mu$ and compared it with the analytical predictions for the different guiding regimes (Eqs. (B1, B2, and B3)), for different trapping parameters and number of condensed atoms. Fig. 3 shows the dependence of $\mu$ with respect to the radial trap frequencies, for the reference experiment discussed above. As expected, (B1) becomes inaccurate in the tight–guiding regime, and vice versa (B3) provides wrong results for the LG region (shaded region). It becomes clear from the figures that the corrected chemical potential, which accounts for the two–level transversal dynamics, describes very well the results obtained by direct numerical integration of the 3D GPE out of the LG region. In particular, it accounts very well for the transition region between the 3D and the 1D regime, and it will merge with the 1D result for low chemical potentials. It is particularly interesting that a radial compression does not easily lead to a fully 1D behavior (even for $10^4$ atoms), unless very large compressions ($\omega_r > 2 \pi \times 10^4$ Hz) are applied. On the contrary, there is a large regime of trap aspect ratios ($\omega_r = 2 \pi \times 500$ Hz–$2 \pi \times 10^4$ Hz) for which Eq. (B3) describes the actual chemical potential of the BEC. We should note that the 1D prediction can significantly overestimate the chemical potential. As an example, for $\omega_r = 2 \pi \times 1.35$kHz, $\mu_{1D}$ is 10% larger than the actual one, even taking into account that more than 95% of the atoms are in the radial ground state. This difference will have significant consequences in the BEC expansion after the releasing of the axial trap, as discussed below.

When the magnetic trap is released, the BEC expands axially within the waveguide produced by the doughnut laser, until reaching a stationary mean velocity. We have numerically simulated this process by solving equation (13) in real time. We shall concentrate in the dynamics of the BEC variance, defined as $\sigma = \sqrt{\langle z^2 \rangle}$. For the LG regime: $\sigma(t) = \sigma(0) b_z(t) / \sqrt{7}$, where $\sigma(0) = a_z (15 N (a/a_z) (\omega_r / \omega_z)^2)^{1/5}$, with $a_z = \sqrt{\hbar / m \omega_z}$, whereas for the 1D regime: $\sigma_{1D}(t) = \sigma_{1D}(0) b_z(t) / \sqrt{5}$, with $\sigma_{1D}(0) = a_z (3N (a/a_z) (\omega_r / \omega_z))^{1/3}$. Therefore, at a given time, $v = \frac{d \sigma_z}{d t}$ has different laws for the different regimes: $v_1 \sim N^{1/5} \omega_r^{2/5}$ and $v_{1D} \sim N^{1/3} \omega_r^{1/3}$. Fig. 2 shows the variation of $v$ at 50 ms, for the cases considered in Fig. 1. At this $t$, $v$ has reached an almost stationary value. From the figure, it becomes clear the transition between the 3D behavior and the 1D one. However, as in Fig. 2 the regime for which the 3D effects on the dynamics become unobservable is not easily achievable by increasing $\omega_r$. This point becomes clear in the inset of Fig. 2, where the numerical results are shown to be parallel to the 1D ones for a large range of radial trap frequencies. In particular, $v$ can be significantly lower than $v_{1D}$ even for large compressions. From the results of the previous section, this effect can be explained by (i) the reduction of the initial chemical potential due to the non–negligible influence of the population of the first transversal state, and (ii) the departure from the TF profile due to the same reason. As an example, for $\omega_r = 2 \pi \times 1.35$kHz, at 50 ms $v_{1D} - v \simeq 0.15$ mm/s, which determines that the condensate variance becomes approximately 7$\mu$m smaller than that expected from a 1D solution. Such difference is experimentally observable with the current imaging techniques. In the two–level regime, Eq. (13) is equivalent to the system of time–dependent differential equations:

$$i \hbar \dot{C}_0 = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V(z) - \tilde{\mu} + g_{1D} |C_0|^2 \right) C_0$$

$$- g_{1D} |C_0|^2 C_1 - \frac{1}{2} g_{1D} C_0^2 C_1^*,$$

$$i \hbar \dot{C}_1 = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V(z) + 2\hbar \omega_r - \tilde{\mu} + g_{1D} |C_0|^2 \right) C_1 - \frac{1}{2} g_{1D} |C_0|^2 C_1^* + \frac{1}{2} g_{1D} C_0^2 C_1^*.$$

(12)

The numerical simulation of the previous equations, also depicted in Fig. 2, shows an excellent agreement with the direct integration of Eq. (13). Therefore, the numerically hard task of calculating the 3D corrections by solving the 3D GPE, can be performed in a much simpler way, by simply solving a set of 4 1D coupled differential equations ($\dot{C}_0$, $\dot{C}_1$, $\dot{C}_0^*$, $\dot{C}_1^*$).

Finally we shall analyze the acceleration of the expa-
sion. It is easy to find that for the 1D regime
\[ \tilde{\sigma}_{1D} = \frac{3}{5/2} \frac{\hbar \omega_r a N}{m} \frac{1}{\sigma_{1D}^2}. \] (14)

On the other hand, since \( \omega_r > \omega_z \) in a general guiding situation, we may consider \( b_r \) to follow adiabatically \( b_z \), and in the LG regime \( b_r(t) = b_z(t)^{-1/4} \). Then,
\[ \tilde{\sigma}_t = \frac{1}{7^{5/4}} \frac{(15 \hbar^2 \omega_r^2 a N)^{1/2}}{m} \frac{1}{\sigma_t^{1/2}}. \] (15)

Therefore, in general, the acceleration decreases as \( \tilde{\sigma}(t) \sim 1/\sigma^n(t) \), with \( n \) ranging from \( n = 3/2 \) in the LG condition and \( n = 2 \) in the 1D regime. Fig. 3 shows \( n \) obtained from the 3D GPE, for the cases of Fig. 2.

![Coefficient n (see text) as a function of the radial frequency, \( \omega_r/2\pi \). The LG region is shaded.](image)

FIG. 3. Coefficient \( n \) (see text) as a function of the radial frequency, \( \omega_r/2\pi \). The LG region is shaded.

In the present paper, we have analyzed the chemical potential, and characterized the expansion dynamics of a BEC within a waveguide. We have numerically investigated the transition between a 3D situation (loose guiding) and a 1D one. Although the extreme 3D and 1D situations are well described by the corresponding TF self-similar solutions, there is a broad region of intermediate parameters which is not well accounted by these solutions. Due to the cylindrical symmetry of the guiding potential, we have shown that in this region the transversal dynamics of the BEC can be modeled as a two-level system, formed by the ground and first excited state of the radial trapping potential. This model is in good agreement with the direct numerical simulation of the corresponding 3D GPE. As we demonstrate, even a small population in the first radial excited state can introduce observable differences between the actual situation and the 1D one, in the resulting chemical potential, and in the subsequent expansion of the BEC after releasing of the axial trap. From our results, we can predict that a very tight transverse confinement is needed to neglect observable 3D effects determined by the transversal two-level system. In particular, this two-level structure could have important effects in the reflection and beam-splitting of BEC in waveguides, due to the enhancement of the nonlinearity at the edge of the optical elements, which could re-couple the transversal levels. The properties of a BEC under such conditions will be the subject of further investigations.

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