Self-induced density modulations in the free expansion of Bose-Einstein condensates

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PACS numbers: 03.75.Ss, 03.75.Hh, 64.75.+g

We simulate numerically the free expansion of a repulsive Bose-Einstein condensate with an initially Gaussian density profile. We find a self-similar expansion only for weak inter-atomic repulsion. In contrast, for strong repulsion we observe the spontaneous formation of a shock wave at the surface followed by a significant depletion inside the cloud. In the expansion, contrary to the case of a classical viscous gas, the quantum fluid can generate radial rarefaction density waves with several minima and maxima. These intriguing nonlinear effects, never observed yet in free-expansion experiments with ultra-cold alkali-metal atoms, can be detected with the available setups.

The anisotropic free expansion of a gas of \(^{87}\)Rb atoms was the first experimental evidence of Bose-Einstein condensation in ultra-cold gases\(^1\). The non-ballistic free expansion observed with \(^6\)Li atoms has been saluted as the first signature of superfluid behavior in a ultra-cold fermi vapor\(^2\). In both cases the atomic quantum gases can be described by the hydrodynamic equations of superfluids and, because the initial density profile is an inverted parabola, the free expansion is self-similar\(^3\)\(^,\)\(^4\)\(^,\)\(^5\)\(^,\)\(^6\)\(^,\)\(^7\).

The first theoretical investigations of the free expansion into vacuum of a classical gas sphere with constant initial density dates back to the 1960’s\(^8\)\(^,\)\(^9\); a numerical analysis was needed to analyze in detail the formation of a depletion at the center and of a shock wave at the surface\(^10\)\(^,\)\(^11\). More recently, rarefaction waves have been produced experimentally by the free expansion of an electron plasma\(^12\).

In this Letter we show that the free expansion of a bosonic superfluid into vacuum displays intriguing nonlinear phenomena. In particular, by integrating numerically\(^13\) the time-dependent Gross-Pitaevskii equation\(^14\) we prove that the expansion of a repulsive Bose-Einstein condensate (BEC) of initial Gaussian density profile gives rise to self-induced density modulations, i.e., self-induced rarefaction waves. In addition, we find that the bosonic cloud produces a shock wave at the surface, that is damped by the quantum pressure of the superfluid. These nonlinear effects, which can be observed experimentally with available techniques, are strongly suppressed if a harmonic confinement along two perpendicular directions is retained and free expansion is allowed in 1D only. Observe that the formation of shock and rarefaction waves induced by an \textit{ad hoc} external perturbation has been suggested\(^15\)\(^,\)\(^16\)\(^,\)\(^17\) and observed recently in BECs\(^18\)\(^,\)\(^19\) and also in non-dissipative nonlinear optics\(^20\).

We describe the collective motion of the BEC of \(N\) atoms in terms of a complex mean-field wavefunction \(\psi(\mathbf{r},t)\) normalized to unity and such that \(\rho(\mathbf{r},t) = N|\psi(\mathbf{r},t)|^2\) is the number-density distribution. The equation of motion that we assume for \(\psi(\mathbf{r},t)\) is the time-dependent Gross-Pitaevskii equation (GPE)\(^14\)

\[
\frac{i\hbar}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U + 4\pi\hbar^2a_sN|\psi|^2\right]\psi, \quad (1)
\]

where \(U(\mathbf{r},t)\) is a confining potential that we assume to vanish at \(t \geq 0\) (thus allowing free expansion) and \(m\) is the atomic mass. The nonlinear term represents the inter-atomic interaction at a mean-field level, where \(a_s\) is the s-wave scattering length, and we consider the repulsive regime \(a_s > 0\).

In traditional experiments with ultra-cold alkali-metal atoms\(^1\)\(^,\)\(^2\) expansion starts from an initial state coinciding with the ground state of the confined superfluid under the action of a (often anisotropic) harmonic potential. For robust interparticle interaction (large number of particles), the density profile in this initial state resembles closely a negative-curvature parabola\(^14\). When such density profile is taken as the initial state of a successive free non-ballistic expansion, to a very good degree of approximation it expands in a self-similar fashion, maintaining the same shape and only spreading out and scaling down its height proportionally, until a ballistic regime is reached when dilution leads to a fully non-interacting regime\(^3\)\(^,\)\(^4\)\(^,\)\(^5\)\(^,\)\(^6\)\(^,\)\(^7\).

In the present work we discuss the much more exciting...
All quantities are dimensionless: lengths in units of the initial Gaussian width $\sigma$ and time in units of $m\sigma^2/h$.

The isotropic case $\sigma_x = \sigma_y = \sigma_z = \sigma$ is conceptually advantageous, as the expansion can be studied within the GPE model in its full generality as a function of a single parameter. Consider rescaling the variables of Eq. (1) as follows: $\mathbf{r} \rightarrow \mathbf{r}/\sigma$, $t \rightarrow t \hbar/(m\sigma^2)$, and $\psi \rightarrow \psi \sigma^{3/2}$, to produce a dimensionless form

$$i \frac{\partial}{\partial t} \psi = \left[ -\frac{1}{2} \nabla^2 + g|\psi|^2 \right] \psi ,$$

of the equation for the free expansion of a condensate starting off from a Gaussian initial state of unit width. The dimensionless interaction strength $g = 4\pi N a_s/\sigma$ is the one free parameter determining the properties of the free expansion. A gas of non interacting ($g = 0$) bosons starting from the Gaussian state expands self similarly according to the formula

$$\psi(\mathbf{r}, t) = \frac{1}{\pi^{3/2}(1 + t^2)^{3/2}} \exp \left( -\frac{r^2(1 + it)}{2(1 + t^2)} \right) .$$

By using an efficient finite-difference Crank-Nicolson algorithm we have verified that little changes affect the expansion as long as the interaction is small. $g < 1$ tracks the weak-coupling limit where interaction only accelerates slightly the free expansion, while $g \gg 1$ represents the strong-coupling regime, where the mean-field self-interaction term in Eq. (3) dominates the expansion for long enough to produce substantial nonlinear effects such as those sketched in Fig. 1. In particular we observe the rapid build-up of a sharp expanding spherical density wave which leaves behind a central region of depleted density. New successively formed radial ripples cross this density-depleted region. Eventually, at very long times, when the overall density has decayed enough for the nonlinear term in Eq. (3) to become negligible everywhere, the expansion recovers a bell-shaped profile.

More quantitatively, for increasing $g$, the rarefaction starts to be evidenced by a local minimum at the droplet center for $g \gtrsim 48.3$, and becomes more and more pronounced and long lived for larger interaction strength $g$. 

FIG. 1: (Color on line). Four successive frames of the radial density profile (solid line) for the expansion of a strongly interacting condensate, characterized by dimensionless interaction parameter $g = 2000$. The “opacity” of the expanding cloud (dashed line) given by the density $\rho_1(\mathbf{r})$ integrated along lines at a distance $r$ from the center (rescaled by a factor 0.036). 

FIG. 2: (Color on line). Characteristic times of the free expansion as a function of the interaction strength $g$. For $g \gtrsim 48.7$, a first minimum in the radial density profile appears at the center $r = 0$ at time $t_{\text{im}}$ (dashed) and fills in at $t_{\text{im}}$ (dot-dashed). For $g \gtrsim 363$, a local maximum re-forms at the center at time $t_{\text{im}}$ (solid) and disappears at time $t_{\text{IM}}$. A density maximum appears within the rarefaction region at time $t_{\text{IM}}$ (dot-dot-dashed). Inset: the time of appearance $t_a$ and disappearance $t_d$ of a denser ring (sketched in the small square for $g = 1200$, $t = 1.8$) of visibility $h$ (defined in Fig. 1) 1% (solid) and 5% (dashed) in the opacity profile (dashed lines of Fig. 1), as a function of $g$. Units as in Fig. 1.
In the highly nonlinear regime, the free expansion of the bosonic cloud into vacuum develops sequences of radial density waves with minima and maxima, each starting at a characteristic time and disappearing at a later time. Figure 2 tracks a few early times in this class, as a function of time and density, as Fig. 3 illustrates: for a strongly interacting BEC, at a fixed time \( t \) the ratio \( v/r \) of the sound velocity to the local phase velocity, given by

\[
v = \frac{r}{2} \frac{t}{1 + t^2}.
\]  

This velocity can be written as \( v(r, t) = \nabla \theta(r, t) \), where \( \theta(r, t) \) is the phase of the macroscopic wave function \( \psi(r, t) \). From Eq. (4) one finds immediately the radial phase velocity of a spherical non-interacting Bose gas \( (g = 0) \):

\[
v = \frac{r}{2} \frac{t}{1 + t^2}.
\]  

In the interacting case \( (g > 0) \) the nonlinear term acts as the chemical potential of a fluid of classical pressure \( P = g|\psi|^2/2 \) and sound velocity \( c_s = \sqrt{g|\psi|^2} \). For \( g \ll 1 \) the gas velocity follows Eq. (4) closely, while for large \( g \) deviations from Eq. (4) are substantial, as mainly the interaction term, rather than the quantum tendency to delocalization, drives the expansion. The ratio \( v/r \), a constant as a function of \( r \) according to Eq. (6), in a non-interacting expansion, shows strong deviations induced by the nonlinear term \( g|\psi|^2 \). In practice, the phase velocity of a strongly interacting BEC approaches the local sound velocity, with larger densities implying higher velocities. Accordingly, initially the central part of the strongly repulsive bosonic superfluid accelerates and propagates faster than the periferic part: the ensuing mass flow is responsible for the formation of the rarefaction region inside the cloud, shown in Fig. 1. The matter flowing quickly out of the central region accumulates near the profile edge on top of the slower external tail, thus tending to produce a shock wave \[ \text{[16, 14, 20]} \], with a BEC density profile extremely steep at the surface, approaching a step function: this is illustrated by the \( t = 0.24 \) panel of Fig. 1. This steep wave front survives for a brief period, after which density oscillations shoot backwards and the surface profile rapidly smoothens its density gradient. At this point, the expansion dynamics is strongly affected by these backward density oscillations, which induce an inverted relation between local velocity and density, as Fig. 3 illustrates: for a strongly interacting BEC, at a fixed time \( t \) the ratio \( v/r \) finds local maxima (minima) in correspondence to the local minimum (maximum) of the density profile \( \rho_1 \). This inversion demonstrates the inward motion of the density ripples. These local minima represent the rarefaction waves produced by the surface step smoothing: this smoothing is driven by the quantum pressure term \[ \text{[16]} \].

The quantum pressure \( -\langle (\nabla \psi)^2 \rangle/(2\rho_1) \), which plays a negligible role in the self-similar non-ballistic expansion \[ \text{[7]} \] of both Fermi and Bose superfluids with an inverted-parabola initial profile \[ \text{[23]} \], becomes relevant in regularizing the shock-wave singularity, like the dissipative term in classical hydrodynamics \[ \text{[19]} \]. Analogous depletion and shock-wave phenomena are indeed observed in the hydrodynamical expansion of hot classical fluids, and can
be simulated e.g. by means of the Navier-Stokes equations (NSE), which depend on the (dissipative) coefficient of shear viscosity \( \eta \). For \( \eta = 0 \) the irrotational (\( \nabla \times v = 0 \)) NSE reduce to the Euler equations of an ideal (non-viscous) fluid. By using \( P(\rho) = g\rho^4/2 \) as the equation of state, the Euler equations are exactly equivalent to the GPE without the quantum pressure term [14]. In Fig. 4 we compare the expanding BEC (GPE, Eq. (3)) and classical gas (NSE), for \( g = 10000 \). The NSE are solved by means of a Lagrangian finite-difference method [24]. The four successive frames displayed in Fig. 4 show that, while expanding, the BEC and the classical gas produce a remarkably similar self-depletion of the central region. On the other hand, the multi-peak rarefaction structures predicted by the GPE are not reproduced by the NSE. Thus the novelty of the free expansion of a BEC with respect to that of a weakly viscous classical fluid, stands mainly in the distinct large-amplitude rarefaction waves moving inside the depletion region, which are supported by the nondissipative nature of quantum pressure.

The expansion of the BEC in an anisotropic context is also interesting. In particular, we find that a 1D expansion starting from a Gaussian state produces no shock wave and no central depletion. This applies both for an idealized 1D BEC, represented by a purely 1D GPE, and for the 3D expansion of a Gaussian wavepacket to which an harmonic confining potential is kept along two orthogonal space directions. Interestingly, if for the initial state of the 3D geometry a spherical Gaussian [2] of width equal to the confining-potential harmonic length \( [h/(m \omega)]^{1/2} \) is taken, the strongly-interacting BEC shoots out rapidly in all directions, thus producing a shock wave, depletion, and rarefaction waves around the cylindrical symmetry axis. However, the total density, integrated in the directions perpendicular to the symmetry axis, always retains a bell shape, even for very large interaction.

In conclusion, we have shown that the free expansion of a Bose-Einstein condensate reveals novel and interesting nonlinear effects, not achievable with classical viscous fluids, and which are awaiting experimental investigations.

The authors thank Paolo Di Trapani, Luciano Reatto and Flavio Toigo for useful suggestions.
(2005).

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