Dynamics of a BEC bright soliton in an expulsive potential

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We theoretically investigate the dynamics of a matter-wave soliton created in a harmonic potential, which is attractive in the transverse direction but expulsive in the longitudinal direction. This Bose-Einstein-condensate (BEC) bright soliton made of $^7$Li atoms has been observed in a recent experiment (Science 296, 1290 (2002)). We show that the non-polynomial Schrödinger equation, an effective one-dimensional equation we derived from the three-dimensional Gross-Pitaevskii equation, is able to reproduce the main experimental features of this BEC soliton in an expulsive potential.

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I. INTRODUCTION

Bright and dark solitons are localized waves that travel over large distances without spreading. Bright solitons are local maxima in the field while dark solitons are local minima. Solitons are ubiquitous: they appear in systems as diverse as oceans, shallow waters in narrow channels, electric circuits and optical fibers [1]. Recently solitons have been experimentally produced in Bose-Einstein condensates (BECs) of alkali-metal atoms [2–5]. Dark solitons have been obtained with repulsive $^{87}$Rb atoms [2], while bright solitons have been observed with attractive $^7$Li atoms [3,4] and also in an optical lattice with $^{87}$Rb atoms (gap bright solitons) [5].

BEC solitons have been theoretically investigated in various papers but only in few of them there is a detailed comparison with experiments [6–8]. For instance, using the Gross-Pitaevskii equation [9], in Ref. [8] we have successfully simulated the formation and dynamics of the train of bright solitons observed in the experiment of the Rice University [3]. In this paper we consider instead the experiment of the Ecole Normale Supérieure [4], where Khaykovich et al. have produced and detected a single BEC bright soliton in an expulsive potential. The stable configurations of this BEC bright soliton have been analyzed by Carr and Castin [7] by means of an analytical variational method. Here we complete their theoretical investigation by studying numerically the full time-evolution of the bright soliton by using the non-polynomial Schrödinger equation (NPSE) [10], an effective one-dimensional (1D) equation we have recently derived from the 3D Gross-Pitaevskii equation [9]. We find that NPSE reproduces remarkably well the experimental data, in particular the center of mass dynamics of the BEC cloud and also the time dependence of its longitudinal width.

II. EXPULSIVE POTENTIAL AND NPSE

In the experiment of Khaykovich et al. [4] the Bose-Condensed $^7$Li atoms are confined in a trap that can be modelled by a harmonic potential

$$U(r) = \frac{1}{2}m\left[\omega_\perp^2(x^2 + y^2) + \omega_z^2z^2\right], \quad (1)$$

where $m$ is the atomic mass, $\omega_\perp = 2\pi \times 710$ Hz is the transverse frequency and $\omega_z = 2\pi i \times 78$ Hz is the imaginary longitudinal frequency. This imaginary frequency is due to an offset magnetic field that produces the slightly expulsive harmonic potential $-(m/2)|\omega_\perp|^2z^2$ in the longitudinal direction. The main effect of this expulsive term is that the center of mass of the BEC accelerates along the longitudinal direction [4].

The dynamics of a BEC at zero temperature can be described by the time-dependent 3D Gross-Pitaevskii equation (3D GPE), given by

$$i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi - U - gN|\psi|^2 \psi = 0, \quad (2)$$

where $\psi(r,t)$ is the macroscopic wave function (order parameter) of the Bose-Einstein condensate [9], $g = 4\pi\hbar^2a_s/m$ is the interatomic strength, $a_s$ is the s-wave scattering length, and $N$ is the number of condensed atoms.

In the case of strong cylindric radial confinement, i.e. when the BEC transverse energy $E_\perp$ of the BEC is equal to the transverse harmonic energy $\hbar\omega_\perp$, the 3D GPE reduces to a 1D GPE. This result can be easily obtained with a variational approach by using the following trial wave function $\psi(x,y,z,t) = f(z,t)\exp[-(x^2 + y^2)/(2\eta^2)]/\sqrt{\pi\eta^2}$, where $f(z,t)$ is the longitudinal wave function normalized to one and $\eta$ is the transverse width. Actually one finds

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} - \frac{\hbar\omega_\perp}{2} \left(\frac{\alpha^2}{\eta^2} + \frac{\eta^2}{\alpha^2_\perp}\right) - \frac{m}{2} \omega_z^2 z^2 - \frac{gN}{(2\pi\eta^2)|f|^2} \right] f = 0, \quad (3)$$

where $E_\perp = (\hbar\omega_\perp/2)(\alpha^2_\perp/\eta^2 + \eta^2/\alpha^2_\perp)$ is the transverse energy of the Bose condensate. In the 1D GPE one has $\eta = \alpha_\perp$ for which $E_\perp = \hbar\omega_\perp$. Instead, choosing a spacetime dependent $\eta$, one finds [10] that $\eta$ satisfies the equation...
\[ \eta(z,t) = a_\perp (1 + 2a_\perp N |f(z,t)|^2)^{1/4}. \] \hspace{1cm} (4)

By inserting this formula in the previous differential equation one gets a nonpolynomial Schrödinger equation (NPSE) [10], that reduces to the 1D GPE in the weakly-interacting limit \( a_\perp N |f|^2 << 1 \). The NPSE has been found to be very accurate in the description of BECs under transverse harmonic confinement and a generic longitudinal external potential. The NPSE is accurate with both repulsive and attractive scattering length [8,10,11]. In our last paper [12] we have extended the NPSE to include also beyond mean-field effects, like the formation of a gas of impenetrable bosons in the Tonks-Girardeau regime.

**III. BEC BRIGHT SOLITONS**

For simplicity we consider first the case with \( \omega_z = 0 \) in Eq. (3). In this case, it is well known that the 1D GPE (namely the Eq. (3) with \( \eta = a_\perp \)) with negative scattering length \( (a_s < 0) \) admits bright soliton solutions [1], that set up when the negative inter-atomic energy of the BEC compensates the positive kinetic energy such that the BEC is self-trapped. Scaling \( z \) in units of \( a_\perp \) and \( t \) in units of \( \omega_\perp^{-1} \), with the position

\[ f(z,t) = \Phi(z-vt)e^{i\nu(z-vt)}e^{i(v^2/2-\mu)t}, \] \hspace{1cm} (5)

from 1D GPE one finds the text-book bright soliton

\[ \Phi(z-vt) = \left(\frac{\gamma}{2}\right) sech \left[ \gamma(z-vt) \right], \] \hspace{1cm} (6)

where \( \gamma = |a_s|N/a_\perp \) and the chemical potential \( \mu \) is given by \( \mu = 1 - \gamma^2/2 \), while the velocity \( v \) of the bright soliton remains arbitrary. Given a value of the scattering length \( a_s \), the number \( N \) of condensed atoms fixes the chemical potential \( \mu \) of the bright soliton.

The solitary wave solution of Eq. (6), that we call 1D bright soliton, exists for any positive value of \( \gamma \). On the other hand, it has been theoretically predicted [10,13] and experimentally shown [3,4] that above a critical interaction strength the BEC bright soliton, that we call 3D bright soliton, will collapse. To study the properties of a 3D bright soliton it is not necessary to solve the full 3D GPE; in fact, the 3D bright solitons can be very accurately described by NPSE [8,10]. In particular, from the NPSE (namely the Eq. (3) with \( \eta \) given by Eq. (4)) one finds the 3D bright soliton written in implicit form

\[ z-vt = \frac{1}{\sqrt{2}} \sqrt{1-\mu} \ \text{arcth} \left[ \frac{\sqrt{1-2\gamma\Phi^2-\mu}}{1-\mu} \right] - \frac{1}{\sqrt{2}} \sqrt{1+\mu} \ \text{arctg} \left[ \frac{\sqrt{1-2\gamma\Phi^2-\mu}}{1+\mu} \right]. \] \hspace{1cm} (7)

It is important to observe that this equation is well defined only for \( \gamma\Phi^2 < 1/2 \); at \( \Phi^2 = 1/(2\gamma) \) the transverse width \( \eta \) becomes zero. Moreover, by imposing the normalization condition, one finds

\[ (1-\mu)^{3/2} - \frac{3}{2}(1-\mu)^{1/2} + \frac{3}{2\sqrt{2}}\gamma = 0, \] \hspace{1cm} (8)

which admits solutions only for \( 0 < \gamma < 2/3 \).

There are thus two kind of collapse: the transverse collapse, when the condensate probability density \( \rho = |\Phi|^2 \) exceeds \( \rho_c = 1/(2\gamma) \), and the 3D collapse, when \( \gamma \) reaches the value 2/3. Note that for a single 3D bright soliton at \( \gamma_c = 2/3 \) the transverse size of the condensate soliton is not yet zero, in fact \( \gamma_c\mu < 1/2 \). Nevertheless, if we consider two colliding 3D bright solitons with \( \gamma < 2/3 \), at the impact the total density of the cloud can become equal to \( \rho_c \) and the system will collapse.

In Figure 1 we show the maximum probability density \( \rho_M \) of bright solitons as a function of the nonlinear strength \( \gamma = |a_s|N/a_\perp \). Length \( z \) in units \( a_s = (\hbar/m\omega_z)^{1/2} \), density \( \rho \) in units \( 1/a_\perp \), where \( a_\perp = (\hbar/m\omega_\perp)^{1/2} \) is the harmonic length of transverse confinement.

![Figure 1](image-url)
IV. BRIGHT SOLITON IN THE EXPULSIVE POTENTIAL

We now consider the case $\omega_z \neq 0$ in Eq. (3) and try to simulate the experiment of the Ecole Normale Supérieure [4] with $^7$Li alkali-metal vapors. In that experiment a BEC with positive scattering length ($a_s > 0$) has been condensed into a cigar-shaped harmonic trap. The scattering length has been then tuned to a small and negative value ($a_s < 0$) via a Feshbach resonance. The resulting condensate, projected onto the expulsive harmonic potential of Eq. (1), has been observed to propagate over a distance of 1 mm.

Following the paper of Khaykovich et al. [4], we choose as initial condition for a fixed $a_s$ the ground-state of the stationary Eq. (3) with a fully confining harmonic potential: $\omega_\perp = 2\pi \times 710$ Hz and $\omega_z = 2\pi \times 50$ Hz. Then the time-dependent wave function is obtained by the numerical integration of the Eq. (3) with the expulsive potential: $\omega_\perp = 2\pi \times 710$ Hz but $\omega_z = 2\pi i \times 78$ Hz. Note that, as in the experiment, the initial position of the BEC cloud is shifted of 50 $\mu$m on the left with respect to the maximum of the expulsive potential. A critical point is the choice of the number $N$ of atoms. To avoid the collapse we choose $N = 4 \times 10^3$, a value compatible with the experimental data and suggested by the variational theory [13]. The NPSE is solved by using the finite-difference numerical algorithm described in [14].

In Fig. 2 we plot six frames of the density of the BEC with $a_s = 0$. This is the case of an ideal gas and the figure shows that the center of mass $z_{cm}$ follows the law $z_{cm}(t) = z_0 \exp (|\omega_z| t)$. In addition, the longitudinal width of the cloud grows due to the dispersive kinetic term. In Fig. 3 we plot instead the time-dependent density of the BEC with $a_s = -0.21$ nm. Also here the center of mass $z_{cm}$ follows the exponential grow in time but the longitudinal width does not show an appreciable enlargement: the matter wave travels without spreading. It is important to stress that Fig. 2 and Fig. 3 are in remarkable good agreement with the absorption images shown in Fig. 3 of the experimental paper [4] with the same values of the parameters.

In their experiment, Khaykovich et al. [4] have measured the root mean square size $\sigma$ of the longitudinal width versus the propagation time for three values of $a_s$: $a_s = 0$, $a_s = -0.11$ nm, and $a_s = -0.21$ nm. Figure 4 shows their experimental data and our numerical re-
results obtained with the NPSE. For $a_s = 0$ the attractive interaction between atoms is zero and the expansion of the cloud is governed by the kinetic energy and the negative curvature of the longitudinal axial potential. For $a_s = -0.11$ nm the size $\sigma$ of the axial width is consistently below that of a non-interacting gas but the attractive interaction is not strong enough to avoid an appreciable enlargement of the cloud.

For $a_s = -0.21$ nm the enlargement is further reduced but our numerical results suggest that $\sigma$ is not truly constant. This is not surprising because a truly shape-invariant solitary wave is expected only in the absence of a longitudinal potential and with an appropriate initial condition. Nevertheless Fig. 4 shows that our results are fully compatible with the experimental data, which have the resolution limit $\Delta \sigma = 9 \mu$m of the imaging system.

As previously discussed, in the calculations we have chosen $N = 4 \times 10^3$ to avoid the collapse of the BEC with $a_s = -0.21$ nm. In the experiments the collapse actually implies that a fraction of atoms is expelled from the Bose condensate via three-body recombination. This effect can be phenomenologically modelled by including a dissipative term in the GPE or in the NPSE, but a more rigorous treatment requires the solution of coupled time-dependent equations for the Bose condensate and the thermal cloud.

Finally, we note that a sudden shift of the inter-atomic strength $|a_s|N/a_\perp$ to a very large value (for instance via a Feshbach resonance) produces a set of bright solitons (soliton train), which can travel in the expulsive potential. A detailed analysis of the formation of these multi-soliton configurations can be found in our recent papers [8,15].

V. CONCLUSIONS

We have shown that the 1D non-polynomial Schrödinger equation (NPSE) is able to accurately describe the time evolution of an attractive Bose-condensed cloud of $^7$Li atoms in an expulsive harmonic potential. Contrary to the 1D Gross-Pitaevskii equations, the NPSE takes also into account the space-time variations of the transverse width of the Bose-Einstein condensate and its numerical integration is much faster than the numerical solution of the 3D Gross-Pitaevskii equation. The theoretical results of the NPSE have been compared with the experimental data of a recent experiment performed at the Ecole Normale Supérieure de Paris. Both experiment and theory show that, when the inter-atomic strength is sufficiently strong, a localized matter wave is obtained, which travels for a large distance without an appreciable spreading. Our numerical calculations suggest that this solitary wave is not fully shape-invariant but the experimental resolution does not allow one to clarify this point. It is important to stress that the limitations in the current resolution of the experimental imaging system can be overcome by creating a bright soliton with a larger longitudinal width. This can be achieved by using a smaller attractive inter-atomic strength in addition with a weaker expulsive potential.

In conclusion, we observe that to make clear the particle-like nature of a soliton it is essential to investigate its interaction with another soliton. The interference of BEC bright solitons is an important subject which has to be analyzed in detail, having also implications for atom interferometry [16].

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