Effective equations for the quasi-one dimensional collision of a matter-wave soliton with a narrow barrier

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We report the result of systematic numerical simulation of the collision of a matter-wave soliton with a narrow potential barrier in the mean-field approximation. We investigate how the choice of the dimensional reduction for the Gross-Pitaevskii equation impacts the description of some features of the process, namely the transmission coefficient and the onset of mean-field collapse. Our results show that, by using the non-polynomial Schrodinger equation, the regime of high barrier energy and high velocity, described by the three-dimensional Gross-Pitaevskii equation is inaccessible, but by adopting a slight modification of the transverse width equation, corresponding the the true variational solution, the efficacy of the method is restored. We also provide a precise estimation of the critical velocity and barrier width for barrier-induced mean-field collapse in the full 3D case.

I. INTRODUCTION

Dynamics of quantum bright solitons in an attractive Bose-Einstein condensates (BEC) have been intensely studied, since current experimental capabilities offer an unprecedented opportunity to test many-body theories in a ultracold Bose gas. Moreover, several technological applications are based on the possibility to generate and manipulate matter-wave solitons, such as interferometry [**?**], quantum computing [], and quantum-enhanced metrology [].

On the theoretical point of view,

The experimental possibility to generate bright matter-wave solitons has been demonstrated about two decades ago [**?**]. [**?**]

The problem of collision with a narrow potential building block of The recent interest in matter-wave interferometry is stimulating novel theoretical investigation on the usage of the Gross-Pitaevskii equation (GPE) as a predictive tool. In the typical setup of an interferometer, a matter-wave soliton is split by using a barrier (acting analogously as an optical beam splitter) and then recombined in a later stage, after the two split solitons have undergone the two different paths. The process is able to give information about the differential phase accumulated by the split solitons and has applications in metrology. In a typical interferometer, the paths are set by a deep potential geometry that sets the motion along a single dimension, and this is typically achieved using a tight transverse harmonic potential. Along the free dimension, another weak harmonic potential is set, or the path is arranged in a ring geometry.

On the theoretical point of view, by adding a barrier to the NLSE it becomes non integrable.

The collision dynamics with a potential barrier is particularly interesting, as it enables the possibility to create "Schrodinger cat" states, exploring quantum entanglement phenomena [**? ?**]. Furhtermore, atomic interferometers implemented are getting increasing interest [**? ?**], and in these devices, the potential barrier represents the analogous to an optical beam splitter for an optical interferometer. The GPE model predicts a peculiar behavior of the interaction with the barrier: for sufficiently low velocities, the impinging soliton is either fully transmitted or fully reflected. This aspect has been investigated [**?**] and is frequently referred to as the particle behavior of the impinging soliton. It has been argued that the passage signals the quantum change???

On the mean-field size, various dimensional reduction methods have been proposed...

The paper is organized as follows: in **??** we review the GPE model and the various methods that are available for obtaining a dimensional reduction. Also we briefly review the numerical method we are going to use. In section **??** we compare the ground states of the various dimensional reduction schemes, focusing in a strongly nonlinear regime, focusing also on the description of the transverse width. We also In section **??** we investigate the behaviour of the transmission coefficient for the collision process, and compare the effective equations. We conclude the work in **??**. [...]

We believe the present work to be a useful contribution to the field of matter-wave soliton interferometr and quantum computing.

II. EFFECTIVE EQUATIONS

A. Gross-Pitaevskii equations

The model is based on the Hartree approximation for bosons [**?**], using which it is possible to derive the following Lagrangian, called Gross-Pitaevskii Lagrangian, for the field ψ.

$$\mathcal{L} = \int d^3\mathbf{r}\ \psi^* \left[i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - U - \frac{g}{2}(N-1)|\psi|^2 \right] \psi, \tag{1}$$

where U is the potential set inside the trap, N is the number of particles, and g is the contact potential, that can be linked to the s-wave scattering length a_s with the expression $g = \frac{4\pi\hbar^2 a_s}{m}$. The associated Euler-Lagrange (EL) equation is called GPE. Since it is an equation in three spatial dimensions, in our context we will refer to it as the 3D-GPE.

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U + g(N-1)|\psi|^2 \right] \psi \tag{2}$$

Assuming a tight harmonic radial confinment

$$U(x,y,z) = \frac{1}{2}m\omega_\perp^2(y^2+z^2) + V(x) \tag{3}$$

one obtains a characteristic length scale $l_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}}$. The dimensional reduction of the 3D-GPE, for obtaining an effective 1D wave equation, is done in many works by assuming that the wavefunction separates in a constant Gaussian transverse part ϕ, which is the ground state of the transverse harmonic potential, and a time-varying axial component f as

$$\psi(\mathbf{r},t) = f(x,t)\phi(y,z) \tag{4}$$

where

$$\phi(y,z) = \frac{1}{\sqrt{\pi}l_\perp}\exp\left[-\frac{y^2+z^2}{2l_\perp^2} \right] \tag{5}$$

Inserting this ansatz into Eq. (**??**), and integrating along the transverse coordinates, one obtains the corresponding wave equation, called the 1D-GPE:

$$i\hbar\frac{\partial}{\partial t}\phi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(z) + g_{1D}|\phi|^2 \right] \phi \tag{6}$$

where we defined $g_{1D} = \frac{g(N-1)}{2\pi}$. When $g_{1D} < 0$, stable solitons are ground states of the system.

B. Improved equations

However, a better approximation is to consider the separation of the total wavefunction in a transverse Gaussian component with variable width, and to find the equation of motion using a variational principle. This is indeed the approach followed in [**?**]. The function ϕ in the ansatz (**??**) is substituted by

$$\phi(y,z,\sigma(x,t)) = \frac{1}{\sqrt{\pi}\sigma(x,t)}\exp\left[-\frac{y^2+z^2}{2\sigma(x,t)^2} \right] \tag{7}$$

where σ is a function to be determined as a variational parameter. In the work [**?**], the calculations have been done assuming that derivatives of σ are negligible. If one include the terms in the calculations, it is possible to write the following effective 1D Lagrangian (detailed calculations are given in the Appendix)

$$\begin{aligned} \mathcal{L} = \int dx\ f^* \Big[& i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V + \\ & -\frac{\hbar^2}{2m}\frac{1}{\sigma^2}\left(1 + \left(\frac{\partial}{\partial x}\sigma\right)^2\right) - \frac{m\omega_\perp}{2}\sigma^2 - \frac{1}{2}g_{1D}|f|^2 \Big] f. \end{aligned} \tag{8}$$

The corresponding EL equations for f and σ are readily obtained.

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}f = \Big[& -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V + \\ & +\frac{\hbar^2}{2m}\frac{1}{\sigma^2}\left(1 + \left(\frac{\partial}{\partial x}\sigma\right)^2\right) + \frac{m\omega_\perp}{2}\sigma^2 + g_{1D}|f|^2 \Big], \end{aligned} \tag{9}$$

$$\begin{aligned} & \sigma^4 - l_\perp^4\left[1 + 2a_s|f|^2\right] + \\ & + l_\perp^4\left[\sigma\frac{\partial^2}{\partial x^2}\sigma - \left(\frac{\partial}{\partial x}\sigma\right)^2\right] = 0 \end{aligned} \tag{10}$$

By neglecting the derivative of σ, one can obtain the same effective 1D Lagrangian as in Ref. ([**?**]), whose EL equations correspond to

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}f = \Big[& -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V + \\ & +\frac{\hbar^2}{2m}\frac{1}{\sigma^2} + \frac{m\omega_\perp}{2}\sigma^2 + g_{1D}|f|^2 \Big] f, \end{aligned} \tag{11}$$

$$\sigma^2 = l_\perp^2\sqrt{1 + 2a_s(N-1)|f|^2}. \tag{12}$$

Eq. (**??**) is called Non-Polynomial Schrodinger equation (NPSE). We will use the 3D-GPE as a reference equation, and compare the predictions of the 1D-GPE, the NPSE, and the NPSE with the derivatives.

C. Generalization of splitting energy bound

The soliton solution has been obtained for the chemical potential of the stationary solution [**?**]:

$$(1-\mu)^{3/2} - \frac{3}{2}(1-\mu)^{1/2}\frac{3}{2\sqrt{2}}\gamma = 0 \tag{13}$$

where $\gamma = |a_s|N/a_\perp$. Using this equation we are able to find the ground state energy of the nonlinear wave equation corresponding to an N-particle soliton. The minimum splitting kinetic energy follows from the theoretical considerations in [**? ? ?**],

$$E_k > E_G(N-n) + E_G(n) - E_G(N), \tag{14}$$

which follows from energy conservation, supposing zero final kinetic energy, after the interaction. From the 1D-GPE, the ground state energy function is

$$E_G(N) = -\frac{N}{6} m a_s^2 \omega_\perp^2 N^2, \tag{15}$$

instead, if we use a NPSE model, the energy can be written as $E_G(n) = \int_0^n dn' \mu(n')$. The consequent forbidden region in the T, v plane is described by the following inequality for the 1D-GPE where T is the transmission coefficient.

D. Numerical method

All the equations are solved using the Split Step Fourier Method (SSFM), with Strang time splitting [**?**].

III. NUMERICAL RESULTS

1. Shape of the solitons for highly nonlinear regime Fig. **??** Fig. **??**
2. sigma 2 for the cases Fig. **??**
3. chemical potential for the various equations (NPSE is not satisfying the variational principle, VK criterion) Fig. **??**.
4. Numerical verification of the VK criterion.
5. Fake collapse of NPSE during barrier interaction (fixed by NPSE+) Fig. **??**
6. transmission heatmap for G3, NPSE, NPSE+, Fig. **??**
7. transmission vs velocity for NPSE and NPSE+ Fig. **??**
8. transmission vs velocity for the collapsing case Fig. **??**

IV. CONCLUSIONS

V. APPENDIX

Let us start again from the 3D Lagrangian

$$\mathcal{L} = \int dx \int dy\, dz\ f^* \phi^* \left[i\hbar\partial_t + \right. \\ \left. + \frac{\hbar^2}{2m}\nabla^2 - U - \frac{1}{2} g_0 (N-1)|f\phi|^2 \right] f\phi, \tag{16}$$

we are interested in integrating along the transverse coordinates without neglecting the terms proportional to

figures/fig1_0.65_ground_states.pdf

FIG. 1. Comparison of the ground state of the 3D-GPE, the 1D-GPE, the NPSE, and the NPSE with derivatives. $\gamma = 0.65$.

$\partial_z \sigma$ and $\partial_z^2 \sigma$. The novel terms arise from $i\hbar\partial_t(f\phi)$ and $\frac{\hbar}{2m}\nabla^2(f\phi)$. By separating the derivatives, we have

$$\mathcal{L} = \int dz \int dx dy f^* \phi^* \left[i\hbar\phi\partial_t f + i\hbar f\phi \left(\frac{y^2+z^2}{\sigma^3} - \frac{1}{\sigma} \right) \partial_t\sigma + \right. \\ \left. + \frac{\hbar^2}{2m}(f\nabla_\perp^2\phi + f\partial_x^2\phi + \phi\partial_x^2 f) - Uf\phi - \frac{1}{2} g_0 (N-1)|f\phi|^2 f\phi \right]. \tag{17}$$

[...]

[1] Khaykovich, L., Schreck, F., Ferrari, G., Bourdel, T., Cubizolles, J., Carr, L. D., Castin, Y., and Salomon, C. (2002). Formation of a matter-wave bright soliton.

figures/fig2_0.65_ground_states_zoom.pdf

FIG. 2. Comparison of the ground state of the 3D-GPE, the 1D-GPE, the NPSE, and the NPSE with derivatives. $\gamma = 0.65$. Zoomed in.

figures/fig3_compare_sigma2_065.pdf

FIG. 3. Comparison of the σ^2 [...] . $\gamma = 0.65$

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[2] J. Helm splitting
[3] Mazzarella

FIG. 4.

figures/0.65_ground_states.pdf

FIG. 5.

figures/0.65_ground_states.pdf

FIG. 6.

figures/compare_lines.pdf

FIG. 7.

figures/compare_lines.pdf

FIG. 8.