Atomic soliton transmission and induced collapse in the scattering from a Gaussian barrier

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Summary

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- Dimensional reduction: from 3D to 1D
- 1D GPE and bright solitons
- Improved dimensional reduction: the 1D NPSE
- Further improvement: the 1D NPSE+
- Soliton scattering with a Gaussian barrier
- Conclusions

3D Gross-Pitaevskii equation

Static and dynamical properties of a pure Bose-Einstein condensate made of dilute and ultracold atoms are very well described by the Gross-Pitaevskii equation[1]

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)\frac{4\pi\hbar^2 a_s}{m}|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t)\ , \tag{1}$$

where $U(\mathbf{r})$ is the external trapping potential and a_s is the s-wave scattering length of the inter-atomic potential.
Here $\psi(\mathbf{r},t)$ is the wavefunction of the Bose-Einstein condensate normalized to one, i.e.

$$\int |\psi(\mathbf{r},t)|^2\ d^3\mathbf{r} = 1\ , \tag{2}$$

and such that $n(\mathbf{r}) = N|\psi(\mathbf{r},t)|^2$ is the local number density of the N condensed atoms.

[1] E.P. Gross, Nuovo Cimento **20**, 454 (1961); L.P. Pitaevskii, Sov. Phys. JETP. **13**, 451 (1961).

Dimensional reduction: from 3D to 1D (I)

We have just seen the Gross-Pitaevskii (GP) equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)g|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t) \ , \quad (3)$$

with

$$g = \frac{4\pi\hbar^2}{m}a_s \ . \quad (4)$$

Clearly, this is the Euler-Lagrange equation of the GP action functional

$$S = N\int dt\, d^3\mathbf{r}\, \psi^*(\mathbf{r},t)\Big(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\nabla^2-U(\mathbf{r})-\frac{N-1}{2}g|\psi(\mathbf{r},t)|^2\Big)\psi(\mathbf{r},t) \ . \quad (5)$$

Let us now consider a very strong harmonic confinement of frequency $\omega_\perp$ along y and z and a generic confinement $V(x)$ along x, namely

$$U(\mathbf{r}) = V(x) + \frac{1}{2}m{\omega_\perp}^2(y^2+z^2). \quad (6)$$

Dimensional reduction: from 3D to 1D (II)

On the basis of the chosen external confinement, we adopt the ansatz

$$\psi(\mathbf{r}, t) = f(x, t) \frac{1}{\pi^{1/2} \ell_{\perp}} \exp\left(-\frac{y^2 + z^2}{2 {\ell_{\perp}}^2} \right) , \tag{7}$$

where $f(x, t)$ is the axial wave function and $\ell_{\perp} = \sqrt{\hbar/(m\omega_{\perp})}$ is the characteristic length of the transverse harmonic confinement.

By inserting Eq. (7) into the GP action (5) and integrating along x and y, the resulting effective action functional depends only on the field $f(z, t)$.

One easily finds that the Euler-Lagrange equation of the axial wavefunction $f(x, t)$ reads

$$i\hbar \frac{\partial}{\partial t} f(x, t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + g_{1D} |f(x, t)|^2 \right] f(x, t) , \tag{8}$$

where

$$g_{1D} = \frac{(N-1)g}{2\pi {\ell_{\perp}}^2} = 2(N-1)\hbar\omega_{\perp} a_s \tag{9}$$

is the effective one-dimensional interaction strength and the additive constant $\hbar\omega_{\perp}$ has been omitted because it does not affect the dynamics.

1D GPE and bright solitons (I)

In the absence of axial confinement, i.e. $V(x) = 0$, the 1D GPE becomes

$$i\hbar \frac{\partial}{\partial t} f(x,t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + g_{1D} |f(x,t)|^2 \right] f(x,t) \; . \qquad (10)$$

This is a 1D nonlinear Schrödinger equation with cubic nonlinearity.
In 1972 Vladimir Zakharov and Aleksei Shabat[2] found that this equation admits solitonic solutions, such that

$$f(x,t) = \phi(x - vt) e^{i\theta(x,t)}, \qquad (11)$$

where $\theta(x,t)$ is a phase and v is the arbitrary velocity of propagation of the solution, which has a shape-invariant axial density profile:

$$n(x,t) = N|f(x,t)|^2 = N|\phi(x - vt)|^2 \; . \qquad (12)$$

[2] V.E. Zakharov and A.B. Shabat, Sov. Phys. JETP **34**, 62 (1972).

1D GPE and bright solitons (II)

Setting $\zeta = x - vt$ and $\hbar = m = 1$, the 1D stationary GP equation

$$\left[-\frac{1}{2} \frac{d^2}{d\zeta^2} + \gamma |\phi(\zeta)|^2 \right] \phi(\zeta) = \mu \, \phi(\zeta) \; , \tag{13}$$

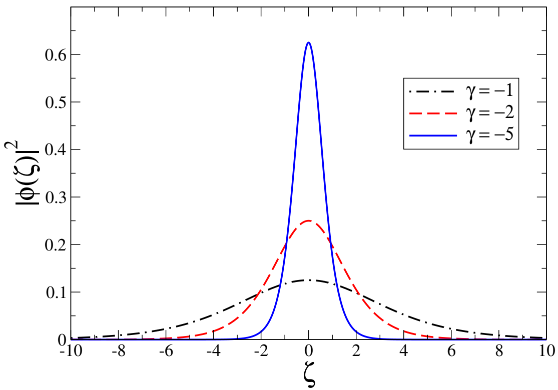
with $\gamma < 0$ (self-focusing), admits the bright-soliton solution

$$\phi(\zeta) = \sqrt{\frac{|\gamma|}{8}} \; Sech \left[\frac{|\gamma|}{4} \zeta \right] \tag{14}$$

with $Sech[x] = \frac{2}{e^x + e^{-x}}$ and

$$\mu = -\frac{\gamma^2}{16} \; . \tag{15}$$

1D GPE and bright solitons (III)



Probability density $|\phi(\zeta)|^2$ of the bright soliton for three values of the nonlinear strength γ. We set $\hbar = m = 1$.

Improved dimensional reduction: the 1D NPSE (I)

The 1D GPE has been derived from the 3D GPE assuming a transverse Gaussian with a constant transverse width $\ell_\perp$.
A more general assumption[3], is based on a space-time dependent transverse width

$$\psi(\mathbf{r},t) = f(x,t)\frac{1}{\pi^{1/2}\sigma(x,t)} \exp\left(-\frac{y^2+z^2}{2\sigma(x,t)^2}\right) , \qquad (16)$$

where $f(x,t)$ is the axial wave function and $\sigma(x,t)$ is the space-time dependent transverse width.
Inserting this ansatz in the 3D GP action functional, after neglecting the spatial derivatives of $\sigma(x,t)$, the Euler-Lagrange equations of $f(x,t)$ and $\sigma(x,t)$ give the **1D nonpolynomial Schrödinger equation** (1D NPSE)

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}f &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + \frac{\hbar^2}{2m\sigma^2} + \frac{m\omega_\perp^2\sigma^2}{2} + \frac{2\hbar^2 a_s(N-1)|f|^2}{m\sigma^2}\right] f , \\ \sigma &= \ell_\perp\left(1+2a_s(N-1)|f|^2\right)^{1/4} . \end{aligned} \qquad (17)$$

[3] LS, A. Parola, L. Reatto, Phys. Rev. A **65**, 043614 (2002)

Improved dimensional reduction: the 1D NPSE (II)

In the weak-coupling regime $|a_s||f|^2 \ll 1$ one finds $\sigma \simeq \ell_\perp$ and the 1D NPSE becomes the familiar 1D GPE.

However, contrary to the 1D GPE bright soliton, the 1D NPSE bright soliton does not exist anymore, **collapsing** at[4]

$$\gamma_c = \left(\frac{a_s(N-1)}{\ell_\perp} \right)_c = -\frac{2}{3} \; . \tag{18}$$

This analytical result is in extremely good agreement with the numerical solution of the 3D GPE: $\gamma_c = -0.67$.

[4]LS, A. Parola, L. Reatto, Phys. Rev. A **66**, 043603 (2002); Phys. Rev. Lett. **91**, 080405 (2003).

Further improvement: the 1D NPSE+ (I)

The 1D NPSE is found by neglecting the spatial derivatives of the transverse width $\sigma(x,t)$. An improvement is obtained taking into account these spatial derivatives. In this way we get[5]

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}f &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)+\frac{\hbar^2}{2m}\frac{1}{\sigma^2}\left(1+\left(\frac{\partial}{\partial x}\sigma\right)^2\right)\right. \\ &+ \left.\frac{m\omega_\perp^2}{2}\sigma^2+\frac{2\hbar^2 a_s(N-1)}{m\sigma^2}|f|^2\right]f \end{aligned} \tag{19}$$

that is called **1D NPSE+**, coupled to

$$\begin{aligned} \sigma^4 &- {\ell_\perp}^4\left[1+2a_s(N-1)|f|^2\right] \\ &+ {\ell_\perp}^4\left[\sigma\frac{\partial^2}{\partial x^2}\sigma-\left(\frac{\partial}{\partial x}\sigma\right)^2+\sigma\frac{\partial}{\partial x}\sigma\frac{1}{|f|^2}\frac{\partial}{\partial x}|f|^2\right]=0\,. \end{aligned} \tag{20}$$

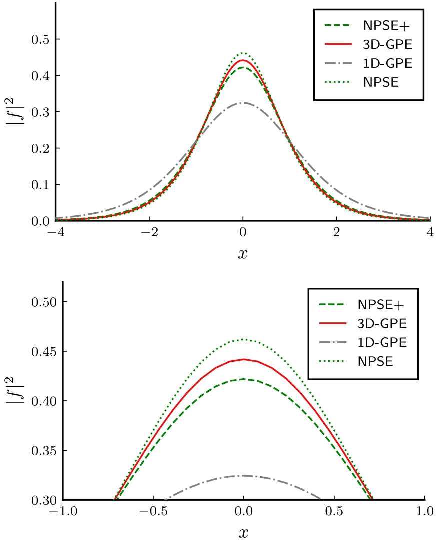
[5] F. Lorenzi and LS, Sci. Rep. **14**, 4665 (2024).

Further improvement: the 1D NPSE+ (II)

We remark that the **1D NPSE+**, as opposed to the 1D NPSE, respects the variational principle, so the corresponding ground state energy is bound to be greater or equal to the true ground state energy of the 3D-GPE.
The **1D NPSE+** gives exactly the 1D NPSE by neglecting the spatial derivatives of $\sigma(x, t)$.

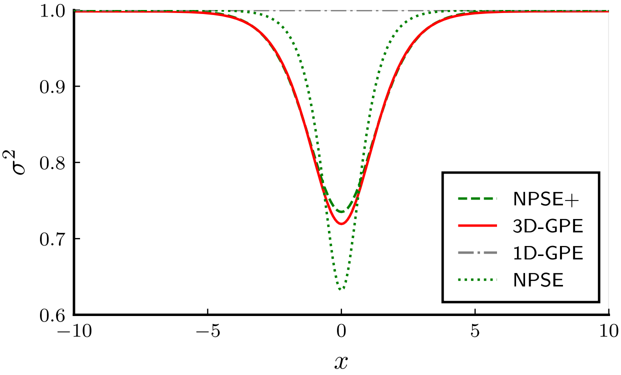
We now use the 3D GPE as a reference equation, and compare the predictions of the 1D GPE, the 1D NPSE, and the **1D NPSE+** for the bright soliton.

Further improvement: the 1D NPSE+ (III)



We set $\gamma = -0.65$ with $\gamma = (N-1)a_s/\ell_\perp$.

Further improvement: the 1D NPSE+ (IV)

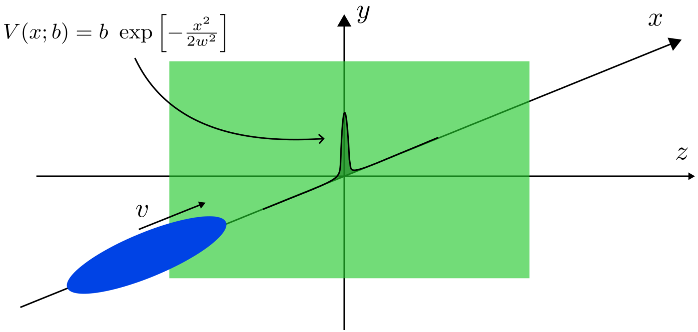


Transverse width $\sigma(x)$ of the bright soliton with $\gamma = 0.65$.
For the 3D GPE we set

$$\sigma^2(x) = \frac{\int dy\, dz\, (y^2 + z^2)|\psi(x, y, z)|^2}{\int dy\; dz\; |\psi(x, y, z)|^2} \ . \tag{21}$$

Soliton scattering with a Gaussian barrier (I)

We now consider the collision of a bright soliton with a barrier.



We are interested in computing the transmission coefficient for various velocities and barriers. We assume energy in units of $\hbar\omega_\perp$, time in units of $\omega_\perp^{-1}$, and length in units of $\ell_\perp$.

Soliton scattering with a Gaussian barrier (II)

As shown in the previous figure, the barrier is modelled by a Gaussian potential

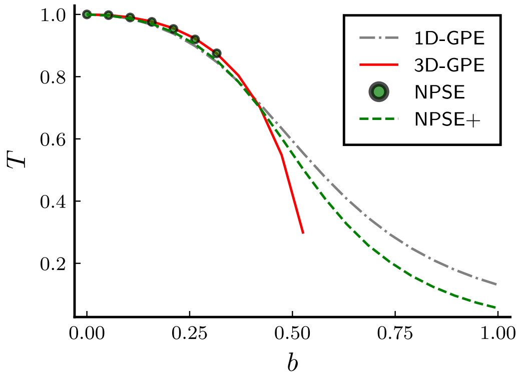
$$V(x) = b\ \exp\left(-\frac{x^2}{2w^2}\right) \tag{22}$$

parametrized by the peak value b and the width w, that we fix at $w = 0.5$.

In our numerical simulations (split-step Fourier method and finite-difference Newton-Raphson), the velocity ranges in $v \in [0.1, 1.0]$, and the barrier in $b \in [0.0, 1.0]$.

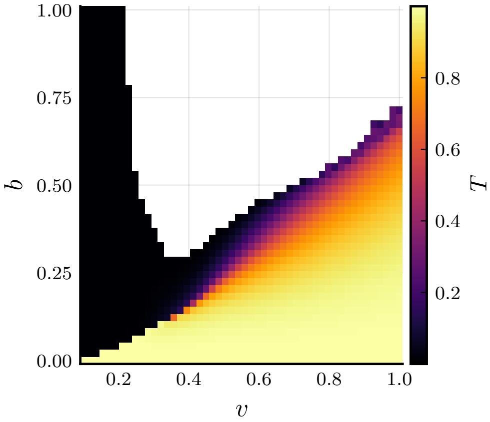
We work with $\gamma = -0.65$, close to $\gamma_c = -0.67$, analyzing also the onset of barrier-induced collapse, happening for high soliton velocity v and high barrier height b.

Soliton scattering with a Gaussian barrier (III)



Transmission coefficient T versus barrier height b with fixed velocity $v = 0.8$ of the bright soliton. v is in units of $\sqrt{\hbar\omega_\perp/m}$, and b is in units of $\hbar\omega_\perp$.

Soliton scattering with a Gaussian barrier (IV)



Transmission coefficient T versus barrier height b and soliton velocity v, showing the collapse region (white area) for the 3D GPE. v is in units of $\sqrt{\hbar\omega_\perp/m}$, b is in units of $\hbar\omega_\perp$.

Conclusions

- From the 3D GPE we have derived the 1D GPE assuming a transverse Gaussian with a constant transverse width $\ell_\perp$.
- The bright soliton solutions of the 1D GPE have been considered.
- A more general assumption with a space-time dependent transverse width (1D NPSE) shows that the quasi-1D bright soliton collapses at a critical interaction strength, in good agreement with 3D GPE static calculations.
- We have found that a fully variational approach leads to the **1D NPSE+**, whose accuracy for stationary problems is however comparable with the 1D NPSE one.
- We have shown that the collapse of the bright solitons can be induced by the scattering with a Gaussian barrier. For this dynamical problem the use of 3D GPE is needed to get fully reliable results.

Acknowledgements

Thank you for your attention!

Slides online:
http://materia.dfa.unipd.it/salasnich/talk-benasque24.pdf

Numerical package:
https://github.com/lorenzifrancesco/SolitonDynamics.jl