Scattering of matter-wave soliton from a narrow barrier: transmission coefficient and induced collapse

Based on [F. Lorenzi and L. Salasnich, arXiv preprint 2310.02018]

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Outline of the talk

1. Matter-wave solitons in quasi-1D setting
2. Dimensional reduction for the Gross-Pitaevskii equation
3. Numerical methods
4. Results

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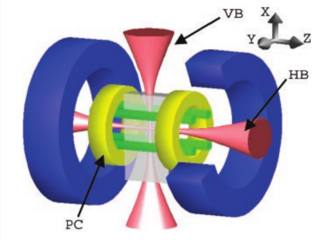
Brief recap of solitons in BEC



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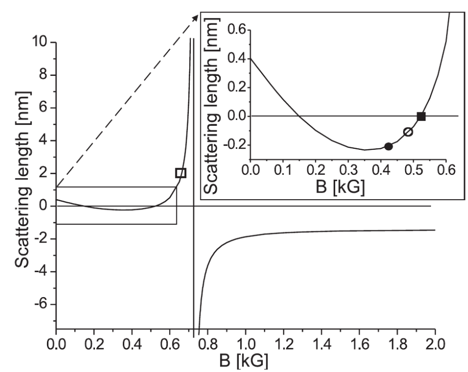
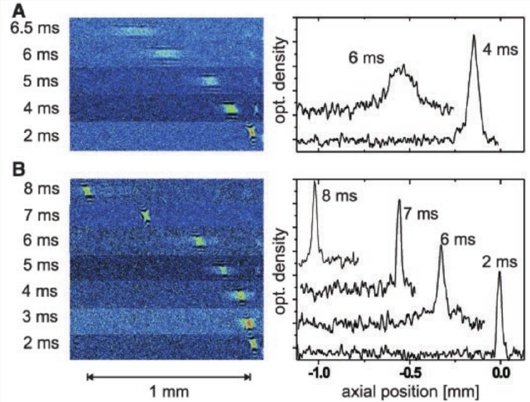


Fig. 2. Predicted magnetic field dependence of the scattering length a for ^{7}Li in state $|F = 1, m_F = 1\rangle$ (*11*). (**Inset**) Expanded view of the 0 to 0.6 kG interval with the various values of a used to study soliton formation. (□) Initial BEC; (■) ideal BEC gas; (○) attractive gas; (●) soliton.

(b)

[L. Khaykovich et al., Science **296** 1290 (2002)]

Brief recap of solitons in BEC



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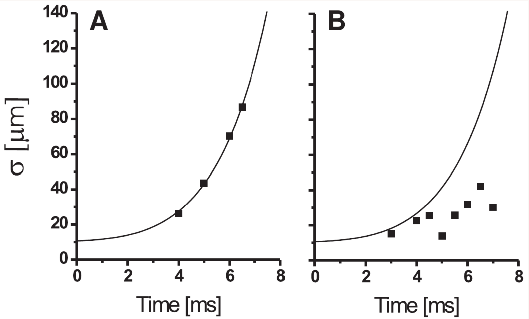


(b)

[L. Khaykovich et al., Science **296** 1290 (2002)]

Basic model: 1D-Gross-Pitaevskii

Gross-Pitaevskii equation in 1D can be used to study the axial wavefunction f:

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

where

$$g_{1D} = \frac{g(N-1)}{2\pi l_\perp}.$$

The 1D interaction parameter can be expressed starting from the 3D one, written in terms of atom number N and s-wave scattering length a_s

$$g = \frac{4\pi\hbar^2 a_s}{m},$$

and with

$$l_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}},$$

the characteristic length of the harmonic confinement.

Soliton solution of the 1D equation

When $a_s < 0$, the equation admits soliton solutions. Assuming a travelling velocity v, we substitute the wave

$$f(x,t) = \phi(x - vt)e^{i\left(mv^2/2-\mu\right)t/\hbar}$$

in the 1D-GPE, and obtain a stationary equation. Solving the equation, if $\zeta = x - vt$, we have

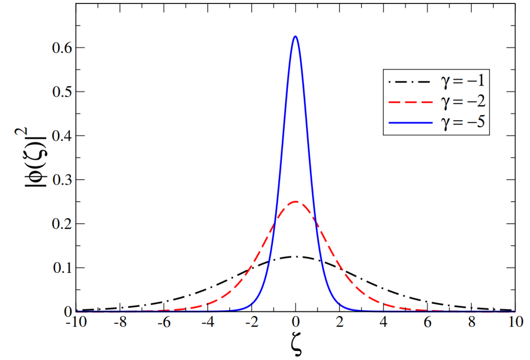
$$\phi(\zeta) = \sqrt{\frac{m|\gamma|}{8\hbar^2}}\,\mathrm{sech}\left(\frac{m|\gamma|}{4\hbar^2}\zeta\right),$$

with $\gamma = (N-1)|a_s|/l_\perp$, and

$$\mu = -\frac{m\gamma^2}{16\hbar^2}.$$

Physically speaking, we can say that the interplay between **attractive interaction** and **kinetic energy** exactly balances, so the matter-wave stay constant in time.

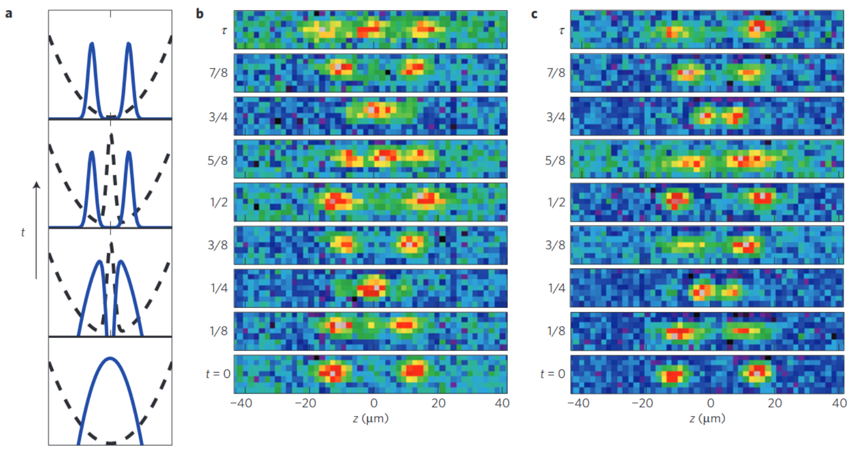
Soliton solution of the 1D equation



Soliton solution of the 1D equation

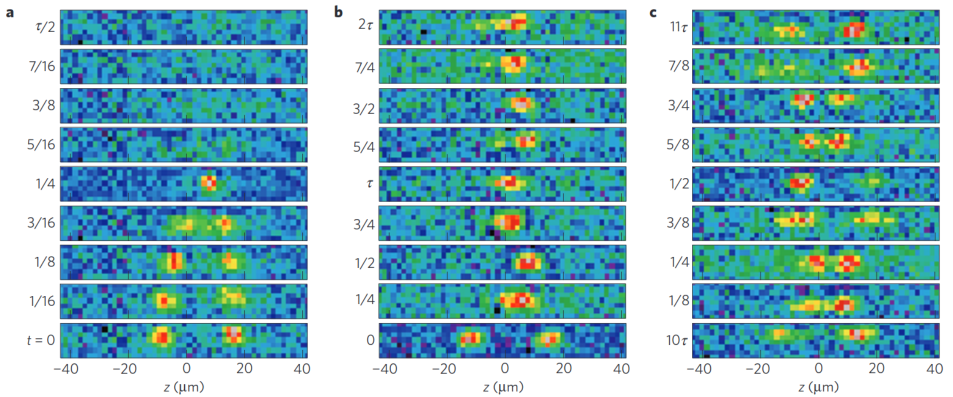
Analogous 1D model can be found also in fiber optics, where the interplay between Kerr-induced **self-phase modulation** and **dispersion** of the group velocity produces the same result. In this context, and in the mathematical literature, the same equation is called Nonlinear Schrödinger equation (NLSE, or NS).

Colliding solitons: preparation



[J. H. V. Nguyen et al., Nat. Lett. Phys. **10**, 918 (2014)]

Colliding solitons: collapse, merging



[J. H. V. Nguyen et al., Nat. Lett. Phys. **10**, 918 (2014)]

The phenomenon of collapse and barrier-induced collapse

Solutions of the (elliptic) NLSE with an attracting nonlinearity

$$i\partial_t \psi + \Delta\psi + |\psi|^{2\sigma}\psi = 0$$
$$\psi(\mathbf{x}, 0) = \varphi(\mathbf{x}),$$

can blow up in finite time in so-called **critical** and **supercritical dimensions** of the domain. Finite time blowup represents a violent energy transfer from large to small scales where dissipative processes can act efficiently (e.g. three-body losses), so the physical validity of the NLSE approximation is violated. Mathematical treatments of the blowup solutions are based on the "variance identity" for the variance defined as

$$V(t) = \int d^d\mathbf{x}\ |\mathbf{x}|^2 |\psi(\mathbf{x}, t)|^2,$$

The phenomenon of collapse and barrier-induced collapse

that reads

$$\frac{1}{8}\frac{d^2}{dt^2}V(t) = H - \frac{d\sigma - 2}{2\sigma + 2}\int d^d\mathbf{x}\ |\psi|^{2\sigma+2}.$$

Of course this treatment is valid for static soliton solutions, and the presence of external potentials (for example **harmonic potentials**) is out of the scope of the analysis.

In the quasi-1D scenario for BECs, which corresponds to the $d = 3$ case with strong transverse confinment, one may define the adimensional value

$$\gamma = (N-1)\frac{|a_s|}{l_\perp}$$

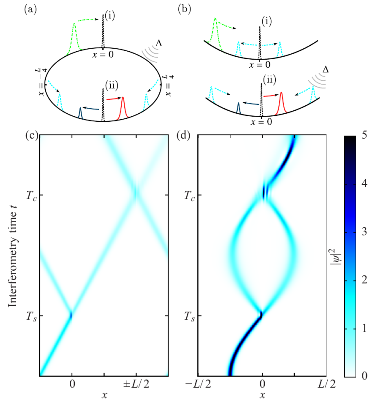
where a_s is the s-wave scattering length, N the number of atoms in the soliton, $l_\perp$ the characteristic length of the harmonic confinment. If no barrier is present, the critical value for stability has been assessed to $\gamma_c \approx 0.67$.

The phenomenon of collapse and barrier-induced collapse

It had been shown that, in presence of the potential in form of a **narrow barrier**, the collapse can be **triggered** by the interaction of the matter-wave with the barrier, resulting in an increase of the axial density.

[C. Sulem, P.L. Sulem, *The Nonlinear Schrödinger equation: self focusing and wave collapse*, Springer (2007)]

Soliton interferometry



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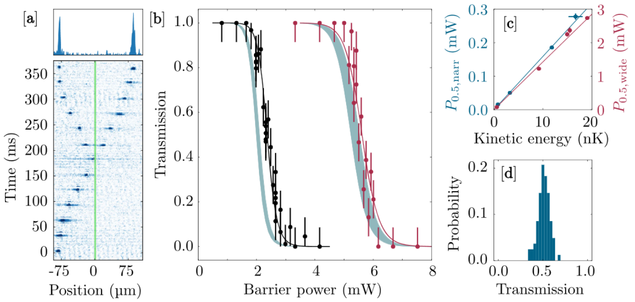
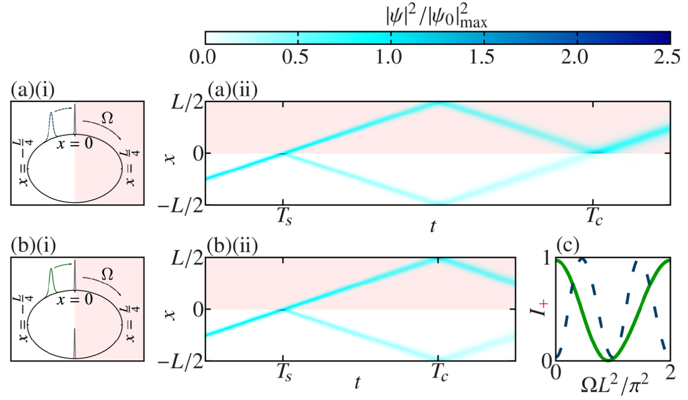


(b)

(a): [J.L. Helm et al., Phys. Rev. Lett. **114**, 134101 (2015)],
(b):[O.J. Wales et al., Comm. Phys. **5** 51 (2020)]

Sagnac soliton interferometry



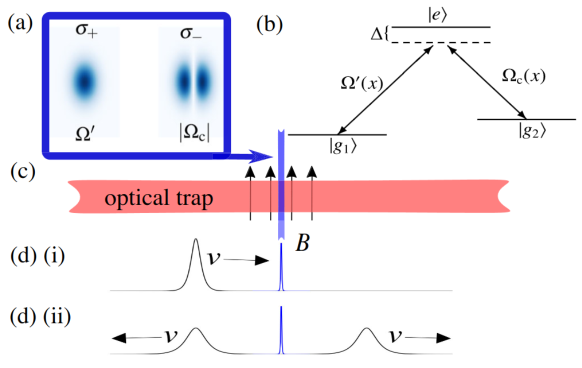
[J.L. Helm et al., Phys. Rev. Lett. **114**, 134101 (2015)]

Very narrow potentials

Using spatially dependent dressed states, it is possible to realize sub-wavelength barrier potentials in the form of

$$V(x) = \frac{\hbar^2}{2m}\left(\frac{\Omega'\partial_x\Omega_c - \Omega_c\partial_x\Omega'}{\Omega'^2 + \Omega_c^2}\right)^2$$

By using different Hermite-Gauss modes, really narrow potentials in the order of ~ 0.1 soliton width or less can be achieved.



[C. L. Grimshaw et al., Phys. Rev. Lett. **129**, 040401 (2022)]

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Research questions

- How can we take into account fully the **dynamical features** of the matter-wave solitons?
- Is it possible to resort to a **1D effective equation** to describe the dynamics, without referring to a time-consuming 3D model?
- In the context of matter-wave interferometry, how can we **efficiently predict barrier-induced collapse** or transverse mode dynamics?
- How is **trap transverse anisotropy** influencing the stability of the trapped solitons?
- To what extent is the **mean-field approach** sufficient to describe matter-wave solitons? What are the alternatives?

3D Gross-Pitaevskii equation

Starting from the GP Lagrangian in 3D:

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

with

$$g = \frac{4\pi\hbar^2 a_s}{m},$$

one can compute the corresponding Euler-Lagrange equation:

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

we call it 3D-GPE. Now assume to have an external potential

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

3D Gross-Pitaevskii equation

with very high $\omega_\perp$. Assuming a factorization

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

we are tempted to assume that, due to the fact that the first excited level of the transverse potential is well above the nonlinear energy of the condensate, the transverse degree of freedom is frozen to the transverse ground state (Gaussian):

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

So, one can substitute inside the 3D-GPE to find the familiar 1D-GPE by separation:

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

where we defined $g_{1D} = g(N-1)/(2\pi l_\perp)$.

Nonpolynomial Schrödinger Equation (NPSE)

A better approach is to assume a **variable transverse width**

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

Writing the 3D GP Lagrangian, we may hope to integrate along the transverse variables

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

Computing the derivatives, we have

$$\mathcal{L} = \int dx \int dy\,dz\, f^*\phi^* \left[i\hbar\phi\frac{\partial}{\partial t}f + i\hbar f\phi\left(\frac{y^2+z^2}{\sigma^3} - \frac{1}{\sigma}\right)\frac{\partial}{\partial t}\sigma + \right.$$
$$\left. \frac{\hbar^2}{2m}\left(f\nabla_\perp^2\phi + f\frac{\partial^2}{\partial x^2}\phi + \phi\frac{\partial^2}{\partial x^2}f\right) - Uf\phi - \frac{1}{2}g(N-1)|f\phi|^2 f\phi\right].$$

Nonpolynomial Schrödinger Equation (NPSE)

Integrating the term proportional to $\frac{\partial}{\partial t}\sigma$ gives 0, as one may realize by looking at the symmetry of its prefactor. However, the term proportional to $\frac{\partial^2}{\partial x^2}\phi$ gives a non-null contribution to the 1D Lagrangian. The integration gives

$$\mathcal{L} = \int dx\, f^* \left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial}{\partial x}^2 - V - \frac{\hbar^2}{2m\sigma^2}\left(1 + \left(\frac{\partial}{\partial x}\sigma\right)^2\right) - \frac{m\omega_\perp^2}{2}\sigma^2 - \frac{1}{2}\frac{N-1}{2\pi\sigma^2} g|f|^2 \right] f.$$

Let us now consider the corresponding Euler-Lagrange equations. These will be computed for f and σ, thus σ is a proper variational parameter, and constitute a set of coupled PDE and ODE.

Nonpolynomial Schrödinger Equation (NPSE)

$$i\hbar\frac{\partial}{\partial t}f=\left[-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}^{2}+V+\frac{\hbar^2}{2m}\frac{1}{\sigma^2}+\frac{m\omega_\perp^2}{2}\sigma^2+\frac{N-1}{2\pi\sigma^2}g|f|^2\right]f$$

$$-m\omega_\perp^2\sigma+\left[\frac{\hbar^2}{m}+\frac{N-1}{2\pi}g|f|^2\right]\sigma^{-3}+\frac{\hbar^2}{m}\sigma^{-3}\left(\sigma\frac{\partial}{\partial x}^{2}\sigma-\left(\frac{\partial}{\partial x}\sigma\right)^2\right)=0.$$

We obtain a differential equation for σ (we called it NPSE+) that can be turned into an algebraic equation as in the standard derivation of the NPSE by neglecting the derivatives of σ. In fact, the original set of paired equations is

$$i\hbar\frac{\partial}{\partial t}f=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V+\frac{\hbar^2}{2m}\frac{1}{\sigma^2}+\frac{m\omega_\perp}{2}\sigma^2+\frac{N-1}{2\pi\sigma^2}g|f|^2\right]f,$$

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

[L. Salasnich et al., Phys. Rev. A **65**, 043614 (2002)]

Soliton solutions of the NPSE

Scaling length in units of $l_\perp$ and time in units of $\omega_\perp^{-1}$, we search for solutions in which we decouple the soliton motion and the internal state wavefunction

$$f(x,t) = \Phi(x - vt)e^{iv(x-vt)}e^{i\left(v^2/2-\mu\right)t},$$

Substituting in the (scaled) NPSE, the stationary equation is

$$\left[\frac{d^2}{d\zeta^2} - 2\gamma\frac{\Phi^2}{\sqrt{1-2\gamma\Phi^2}} + \frac{1}{2}\left(\frac{1}{\sqrt{1-2\gamma\Phi^2}} + \sqrt{1-2\gamma\Phi^2}\right)\right]\Phi = \mu\Phi,$$

where $\zeta = x - vt$. We have a second order equation with constant of motion

$$E = \frac{1}{2}\left(\frac{d\Phi}{d\zeta}\right)^2 + \mu\Phi^2 - \Phi^2\sqrt{1-2\gamma\Phi^2}.$$

Soliton solutions of the NPSE

One obtains an implicit equation describing the soliton

$$\zeta = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{1-\mu}}\arctan\left[\sqrt{\frac{\sqrt{1-2\gamma\Phi^2}-\mu}{1-\mu}}\right] - \frac{1}{\sqrt{2}}\frac{1}{\sqrt{1+\mu}}\operatorname{arctanh}\left[\sqrt{\frac{\sqrt{1-2\gamma\Phi^2}-\mu}{1+\mu}}\right].$$

The chemical potential, after imposing the normalization condition, is written as

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

The equation for the chemical potential show how we are not getting stable solutions above $\gamma_{\mathrm{c,\ NPSE}} = \frac{2}{3}$.

Cubic-Quintic Schrödinger Equation

Another approach is available: assume now the decomposition

$$\psi(r,x,t) = \phi(x,t)\chi(r,x,t),$$

one can separate the 3D-GPE problem in the coupled equations

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + \tilde{\mu}\phi,$$
$$\widetilde{\mu}\chi = -\frac{\hbar^2}{2m}\nabla_\perp^2\chi + \frac{1}{2}m\omega^2 r^2\chi + \frac{4\pi\hbar^2 a_s}{m}n|\chi|^2\chi,$$

considering n small, we can compute the perturbation in order to obtain a better estimate of the eigenvalue $\widetilde{\mu} = \hbar\omega + g_{1\mathrm{D}}n - g_2 n^2$ to the second order. One obtains

$$g_{1\mathrm{D}} = 2\hbar\omega a_s, \quad g_2 = 24\left(\ln\frac{4}{3}\right)\hbar\omega a_s^2,$$

Cubic-Quintic Schrödinger Equation

and so, an equation of motion,

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + g_{1\mathrm{D}}|\phi|^2\phi - g_2|\phi|^4\phi.$$

This equation is purely 1D, but remarkably can show collapse.

[L. Khaykovich et al., Phys. Rev. A **74**, 023607 (2006)]

Signatures of collapse

Looking at the equations, we notice that the NPSE gives us an algebraic equation for the transverse width.

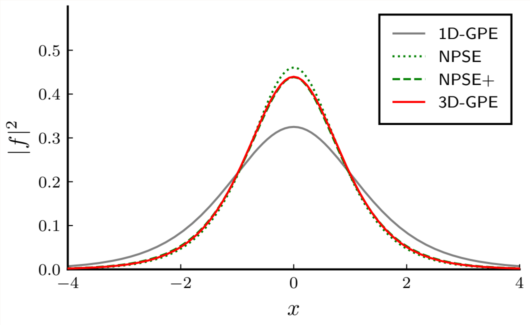
$$\sigma^2 = l_\perp^2 \sqrt{1 + 2a_s(N-1)|f|^2}.$$

We expect, for highly localized field f, to have **null** or **complex** transverse width, if

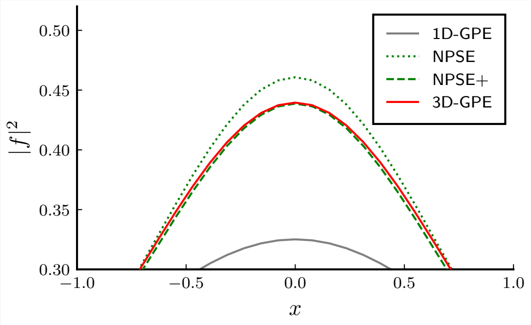
$$1 + 2a_s(N-1)|f|^2 < 0.$$

In the 3D-GPE and NPSE+ case, numerical simulations in imaginary time show that, when running above the critical 3D nonlinearity, the localization of the solution make it occupy only few mesh sites. So we assume, as a collapse numerical signature, a probability per point of 0.3 .

Localized soliton-like solutions

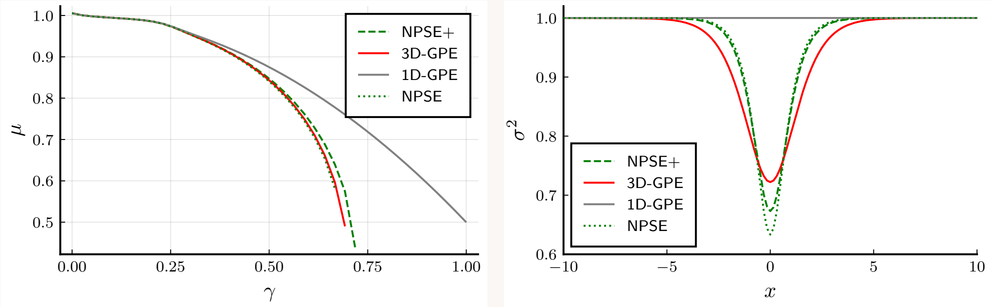


(a) Soliton solutions compared. $\gamma = 0.65$



(b) Zoom applied to the top part of the soliton solutions.

Chemical potential and transverse width



Trap anisotropy

Using an anisotropic transverse potential

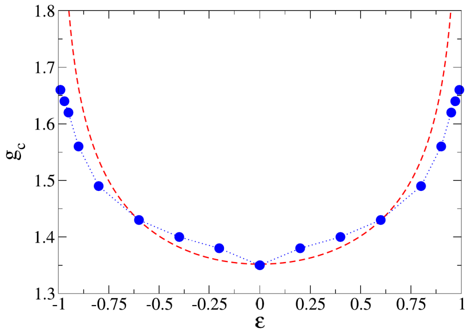
$$U(y,z) = \frac{m}{2}\left(\omega_1^2 y^2 + \omega_2^2 z^2\right),$$

one defines

$$\omega_1 = \lambda_1 \omega_\perp, \quad \omega_2 = \lambda_2 \omega_\perp,$$

and normalized parameters λ_1 and λ_2 can be expressed using the ellipticity

$$\lambda_1 = \sqrt{1-\epsilon}, \quad \lambda_2 = \sqrt{1+\epsilon}.$$



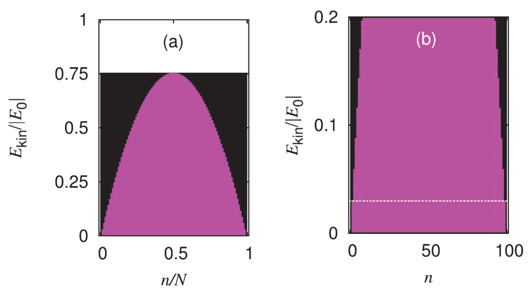
In the plot $g_c = 2\gamma$.

[G. Mazzarella and L. Salasnich, Phys. Lett. A **373** 4434 (2009)]

Splitting dynamics: mean-field and beyond mean-field

Physical interpretation of GPE wavefunction can be thought of Hartree product states. But one can also interpret $|\psi|^2$, in a more general wat, to be the **single-particle density**. Stepwise behavior of the GPE solutions signals that, at the mean-field some states are not accessible.

$$E_{\text{kin}} > E_G\,(N-n)+E_G\,(n)-E_G(N).$$



[B. Gertjerenken et al., Phys. Rev. A **86**, 033608 (2012)]

Outline of the talk

Split-Step Fourier time marching scheme

- Strang splitting, better performance over Lie-Trotter splitting.
- Accuracy to the second order in time and to every order in space.
- High efficiency in the spatial discretization.

The drawback of the method - or the feature, depending on the point of view - is to implement **periodic boundary conditions** natively. The implementation of absorption boundaries is still possible but not straightforward. We assume the field to be localized away from the boundaries to neglect this problem.

How to integrate the NPSE+ numerically

Recall the NPSE+:

$$i\hbar\frac{\partial}{\partial t}f = \left[-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}^2 + V + \frac{\hbar^2}{2m}\frac{1}{\sigma^2} + \frac{m\omega_\perp^2}{2}\sigma^2 + \frac{N-1}{2\pi\sigma^2}g|f|^2\right]f$$

$$-m\omega_\perp^2\sigma + \left[\frac{\hbar^2}{m} + \frac{N-1}{2\pi}g|f|^2\right]\sigma^{-3} + \frac{\hbar^2}{m}\sigma^{-3}\left(\sigma\frac{\partial}{\partial x}^2\sigma - \left(\frac{\partial}{\partial x}\sigma\right)^2\right) = 0.$$

We use a simple iterative scheme to solve the coupled ODE-PDE system

1. Solve the ODE for σ with Dirichlet boundary conditions with initial f.
2. Use the solution σ to take a SSF step of the PDE for f .

Simulation parameters

We have an isotropic confinement, in which we have units:

- energy $\longrightarrow \hbar\omega_\perp$,
- time $\longrightarrow \omega_\perp^{-1}$,
- length $\longrightarrow l_\perp$.

- 1D simulations a total length of $L = 40$, with a grid of $N = 512$ points.
- 3D simulations, we use a grid of $(N_x, N_y, N_z) = (512, 40, 40)$ points, with total lengths of $(L_x, L_y, L_z) = (40, 10, 10)$.

Collapse threshold is set to a probability per point of 0.3. The time step in both setups is chosen to be $h_t = 0.01$. These parameters have been proven to give a total truncation error in the L_∞ norm of the order of 10^{-4}, and allow for a reasonable computation time of all the calculations.

The code has been written in the Julia programming language.

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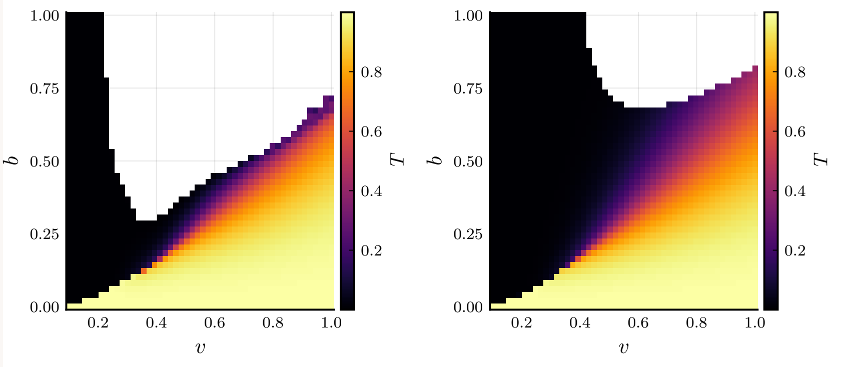
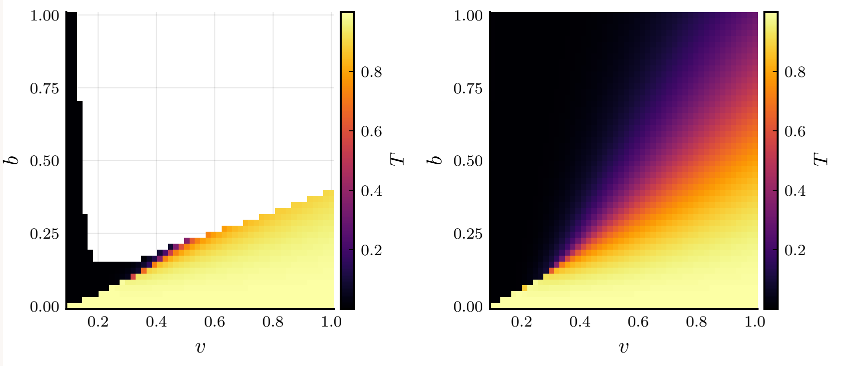


(a) 3D-GPE **(b)** NPSE+

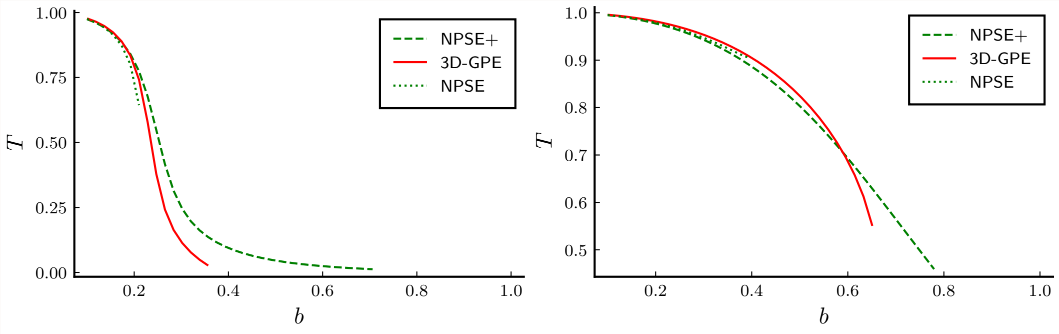
Diagrams of dynamical regimes



(a) NPSE

(b) 1D-GPE

Transmission coefficients



(a) $v = 0.5$ **(b)** $v = 1$

Conclusions and open problems

Conclusions

- Matter-wave soliton represent an exciting field of study, that has interesting applications in interferometry for metrology and sensing.
- The familiar 1D-GPE is a valuable tool, but it is unable to describe the full dynamical features of the solitons, especially when they interact with each other, or with a barrier. Most importantly, it cannot predict collapse of the matter-wave.
- The transverse dynamics of a trapped matter-wave soliton can strongly affect the dynamics, and it is possible to tackle it with effective 1D models.
- Different effective equations predict collapse with different signatures, and the NPSE+ show a remarkable agreement with the full 3D-GPE simulations.

Conclusions and open problems

Open problems:

- How can we effectively describe the dynamics of quantum solitons and their interaction with a barrier?
- To what extent is it possible to generate entangled states using soliton splitting?
- Is the effective range correction important in this case?

Thanks for the attention!

F. Lorenzi and L. Salasnich, *Scattering of matter-wave soliton from a narrow barrier: transmission coefficient and induced collapse*, arxiv.org/abs/2310.02018 .

Relevant references

[1] X. Antoine, W. Bao, and C. Besse. **"Computational Methods for the Dynamics of the Nonlinear Schrödinger/Gross–Pitaevskii Equations".** In: *Comput. Phys. Comm.* 184 (2013), pp. 2621–2633.

[2] X. Antoine, C. Geuzaine, and Q. Tang. **"Perfectly Matched Layer for Computing the Dynamics of Nonlinear Schrödinger Equations by Pseudospectral Methods. Application to Rotating Bose-Einstein Condensates".** In: *Commun. Nonlinear. Sci. Numer. Simulat.* 90 (2020), p. 105406.

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