Bose-Einstein condensates with negative scattering length

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Summary

- BECs with negative scattering length
- BEC in a harmonic trap: Gaussian variational approach
- Bright solitons and their properties
- Simulating the ENS experiment with bright solitons
- Including an axial optical lattice
- Conclusions

BECs with negative scattering length

Many experiments have been devoted to the study of dilute and ultracold Bose-Einstein condensates (BECs) with positive s-wave scattering length

$$a_s > 0 \;, \tag{1}$$

which implies an effective repulsion between atoms (^{87}Rb, ^{23}Na). There are instead few experiments with negative s-wave scattering length

$$a_s < 0 \;, \tag{2}$$

which implies an effective attraction between atoms.

^{7}Li atoms have a negative scattering length

$$a_s \simeq -14 \cdot 10^{-10} \text{ m} \;. \tag{3}$$

BECs with ^{7}Li atoms have been studied at Rice Univ.* and ENS†.

Recently an attractive BEC with ^{85}Rb atoms has been investigated at JILA‡ by using a Feshbach resonance.

*K.E. Strecker *et al.*, Nature **417**, 150 (2002).

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

‡S.L. Cornish *et al.*, PRL **96**, 170401 (2006).

BEC in a harmonic trap: Gaussian variational approach

The stationary properties of a dilute Bose-Einstein condensates (BEC) are well described by the Gross-Pitaevskii equation (GPE), given by

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

where $\psi(\mathbf{r})$ is the macroscopic wave function of the BEC, here normalized to one, i.e.

$$\int |\psi(\mathbf{r})|^2\ d^3\mathbf{r} = 1\ . \qquad (5)$$

In the GPE μ is the chemical potential, $U(\mathbf{r})$ is the external trapping potential, a_s is the s-wave scattering length and N is the number of condensed atomic bosons.

The GPE can be obtained by minimizing the following energy functional

$$E = \int \left\{\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2 + U(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{2\pi\hbar^2 a_s N}{m}|\psi(\mathbf{r})|^4\right\} d^3\mathbf{r}\ , \qquad (6)$$

with the constraint of Eq. (5).

Let us suppose that the external trap is a spherically-symmetric harmonic potential

$$U(\mathbf{r}) = \frac{1}{2}m\omega_H^2\left(x^2+y^2+z^2\right) = \frac{1}{2}m\omega_H^2 r^2\ . \tag{7}$$

A reasonable variational ansatz for $\psi(\mathbf{r})$ is a Gaussian wave function

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4}a_H^{3/2}\sigma^{3/2}}\exp\left(\frac{-r^2}{2a_H^2\sigma^2}\right)\ , \tag{8}$$

where

$$a_H = \sqrt{\frac{\hbar}{m\omega_H}} \tag{9}$$

is the characteristic harmonic length and σ is the variational parameter, that is the scaled width of the BEC.

By inserting this trial wave function in the GPE energy functional and integrating over spatial coordinates one finds the effective energy

$$\bar{E} = \frac{2E}{\hbar\omega_H} = \frac{3}{2}\frac{1}{\sigma^2} + \frac{3}{2}\sigma^2 + \Gamma\frac{1}{\sigma^3}\ , \tag{10}$$

which is a function of the variational parameter σ, with $\Gamma = \sqrt{\frac{2}{\pi}}\frac{a_s N}{a_H}$ the interaction strength.

The best choice of σ is obtained by minimizing the energy $\bar{E}(\sigma)$, i.e.

$$0 = \frac{\partial \bar{E}}{\partial \sigma} = -3\frac{1}{\sigma^3} + 3\sigma^3 - 3\Gamma\frac{1}{\sigma^4} \, . \tag{11}$$

Obviously σ must also satisfy the condition

$$\frac{\partial^2 \bar{E}}{\partial \sigma^2} > 0. \tag{12}$$

It follows that

$$\sigma > 1 \quad \text{for} \quad \Gamma > 0 \, ,$$

while

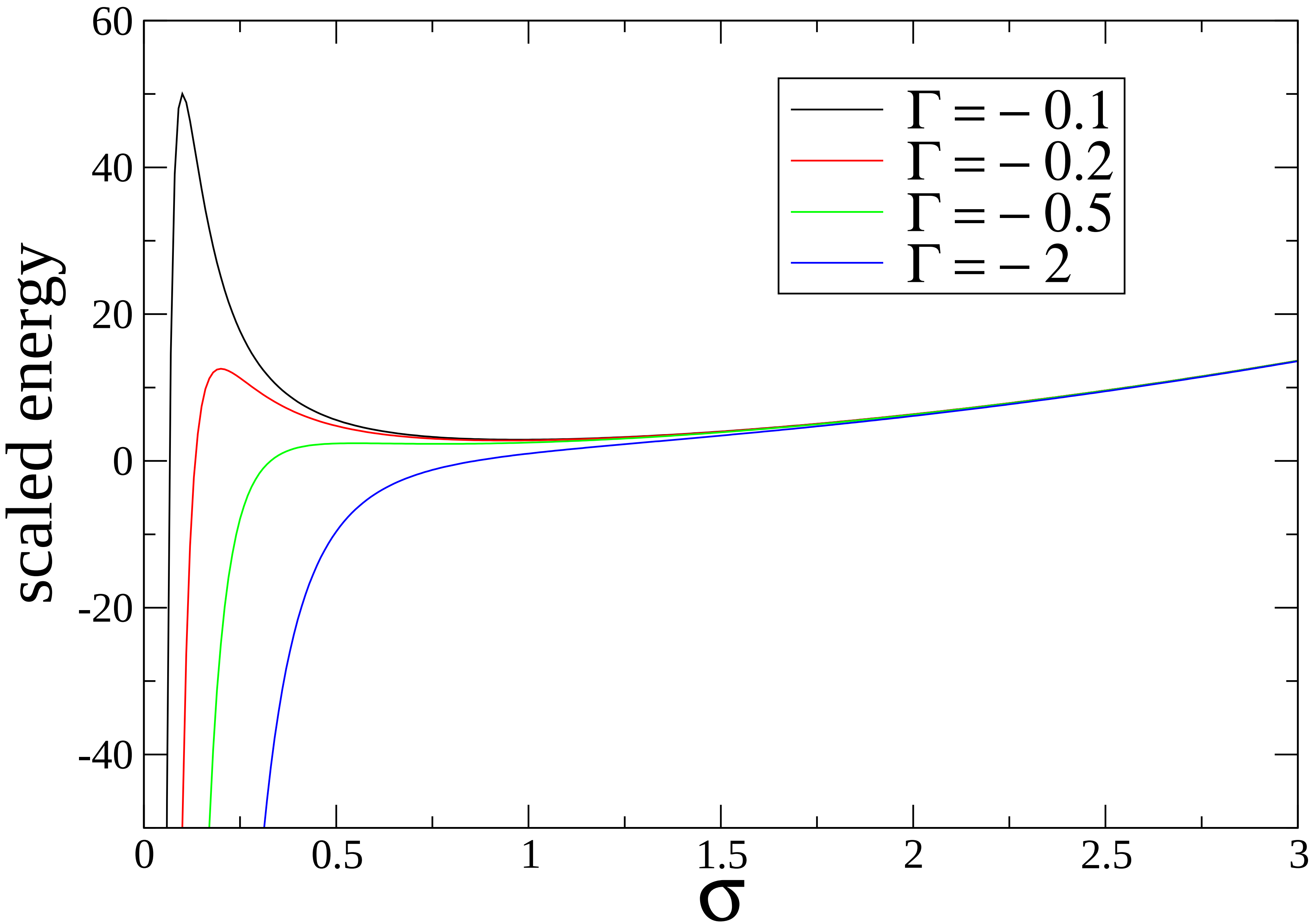
$$\sigma_c < \sigma < 1 \quad \text{for} \quad -\Gamma_c < \Gamma < 0 \, ,$$

with $\sigma_c = 1/5^{1/4} \simeq 0.67$ and $\Gamma_c = 4/5^{5/4} \simeq 0.53$.

Thus, for $a_s < 0$ it exist a critical strength

$$\frac{|a_s|N}{a_H} = \sqrt{\frac{\pi}{2}}\frac{4}{5^{5/4}} \simeq 0.67 \tag{13}$$

above which the local minumum of the energy does not exist anymore. Above this critical strength there is the so-called collapse of the condensate. For ^{7}Li atoms of Rice Univ. experiment: $N_c \simeq 1300$.



Scaled energy $\bar{E}$ as a function of the variational parameter σ for different values of the scaled interaction strength $\Gamma = \sqrt{\frac{2}{\pi}}\frac{a_s N}{a_H}$.

Let us now consider an attractive BEC ($a_s < 0$) with an anisotropic harmonic trapping potential

$$U(\mathbf{r}) = \frac{1}{2}m\omega_\perp^2(x^2 + y^2) + \frac{1}{2}m\omega_z^2 z^2 \ , \tag{14}$$

By using the transverse harmonic length

$$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \ , \tag{15}$$

as unit of length, and $\hbar\omega_\perp$ as unit of energy, the scaled GPE energy functional reads

$$E = \int \left\{ \frac{1}{2}|\nabla\psi(\mathbf{r})|^2 + \left[\frac{1}{2}(x^2 + y^2) + \frac{\lambda^2}{2}z^2\right] |\psi(\mathbf{r})|^2 + 2\pi\gamma|\psi(\mathbf{r})|^4 \right\} d^3\mathbf{r} \ , \tag{16}$$

with

$$\lambda = \frac{\omega_z}{\omega_\perp} \qquad \text{trap anisotropy}$$

$$\gamma = \frac{|a_s|N}{a_\perp} \qquad \text{interaction strength.}$$

To study this problem we use the Gaussian ansatz[§]

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4}\sigma\eta^{1/2}} \exp\left\{-\frac{(x^2+y^2)}{2\sigma^2} - \frac{z^2}{2\eta^2}\right\}, \tag{17}$$

where σ and η are, respectively, transverse and axial widths. Inserting this ansatz into the energy functional, we obtain the effective energy

$$\bar{E} = \frac{1}{\sigma^2} + \sigma^2 + \frac{1}{2\eta^2} + \frac{\lambda^2}{2}\eta^2 - \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^2\eta}\,. \tag{18}$$

We look for values of σ and η that minimize energy $\bar{E}$ and get

$$-\frac{1}{\sigma^3} + \sigma + \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^3\eta} = 0\,, \tag{19}$$

$$-\frac{1}{\eta^3} + \lambda^2\eta + \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^2\eta^2} = 0\,. \tag{20}$$

These equations give local minima only if the curvature of $E(\eta,\sigma)$ is positive.

Remarkably, there is a **local minumum** also with $\lambda = 0$, i.e. also **without axial confinement**: this is the so-called bright soliton. This bright soliton collapses at a critical strength $\gamma_c \simeq 0.78$.

[§]L.S., A. Parola, and L. Reatto, PRA **66**, 043603 (2002).

We can also study the dynamics of the attractive BEC by using the Lagrangian¶

$$L = \dot{\sigma}^2 + \frac{1}{2}\dot{\eta}^2 - \bar{E}(\sigma,\eta) \ . \tag{21}$$

The equations of motion are

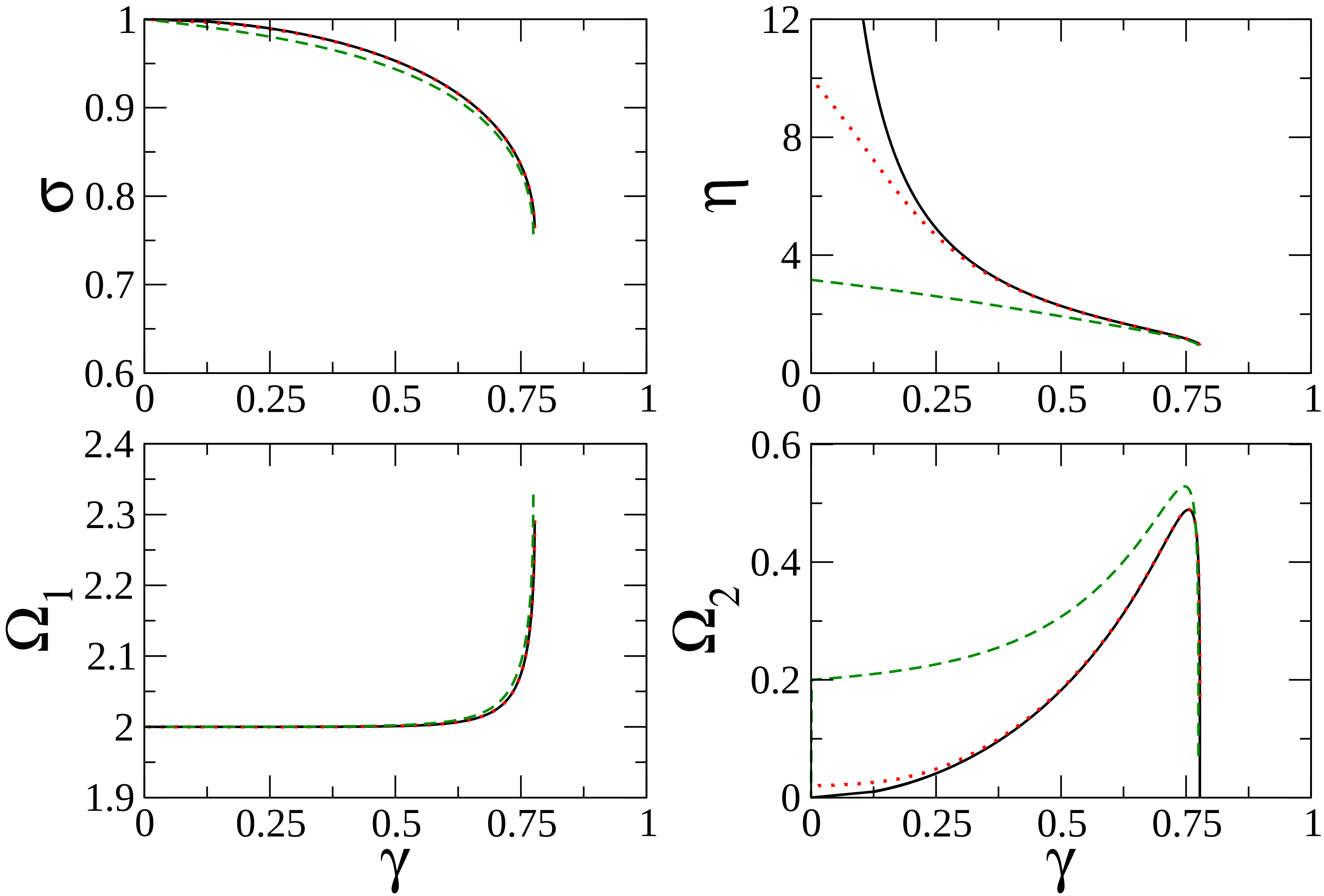
$$\ddot{\sigma} - \frac{1}{\sigma^3} + \sigma + \sqrt{\frac{2}{\pi}}\ \gamma\frac{1}{\sigma^3\eta} = 0 \ , \tag{22}$$

$$\ddot{\eta} - \frac{1}{\eta^3} + \lambda^2\eta + \sqrt{\frac{2}{\pi}}\ \gamma\frac{1}{\sigma^2\eta^2} = 0 \ . \tag{23}$$

From these equations one can quite easily derive the frequencies Ω_1 and Ω_2 of small oscillations around the local minima.

Ω_1 and Ω_2 are the frequencies of **breathing modes** along radial and axial direction.

¶L.S., Int. J. Mod. Phys. B **14** 405 (2000).



Gaussian variational approach to the **attractive BEC**. Top: Widths σ and η. Bottom: Breathing frequencies ω_1 and ω_2. All *vs* interaction strength γ. Trap anisotropy: black solid line ($\lambda = 0$); red dotted line ($\lambda = 0.01$); green dashed line ($\lambda = 0.1$).

Bright solitons and their properties

To investigate in detail the properties of bright soltions we start from the time-dependent 3D GPE given by

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar}{2m}\nabla^2 + U(\mathbf{r}) - \frac{4\pi\hbar^2 |a_s| N}{m} |\psi(\mathbf{r},t)|^2 \right] \psi(\mathbf{r},t) \; , \tag{24}$$

where $\psi(\mathbf{r},t)$ is the wave function of the attractive BEC. Let us suppose that the trapping potential is

$$U(\mathbf{r}) = \frac{1}{2} m\omega_\perp^2 (x^2+y^2) + V(z) \; . \tag{25}$$

By using the transverse harmonic length

$$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \; , \tag{26}$$

as unit of length, and $\hbar\omega_\perp$ as unit of energy, the scaled 3D GPE reads

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{1}{2}\nabla^2 + \frac{1}{2}(x^2+y^2) + V(z) - 4\pi\gamma |\psi(\mathbf{r},t)|^2 \right] \psi(\mathbf{r},t) \; , \tag{27}$$

where

$$\gamma = \frac{|a_s| N}{a_\perp} \; . \tag{28}$$

The 3D GPE is the Euler-Lagrange equation of the following Lagrangian density

$$\mathcal{L} = \psi^*(\mathbf{r},t)\left(i\frac{\partial}{\partial t} + \frac{1}{2}\nabla^2\right)\psi(\mathbf{r},t) - \frac{1}{2}(x^2+y^2)|\psi(\mathbf{r},t)|^2 - V(z)|\psi(\mathbf{r},t)|^2 + 2\pi\gamma|\psi(\mathbf{r},t)|^4 \tag{29}$$

We consider a semi-Gaussian variational ansatz

$$\psi(\mathbf{r},t) = \frac{1}{\pi^{1/2}\sigma(z,t)} \exp\left\{-\frac{(x^2+y^2)}{2\sigma(z,t)^2}\right\} f(z,t)\ . \tag{30}$$

Inserting this expression into the 3D Lagrangian density, integrating over x and y variables, the two Euler-Lagrange equations are

$$\sigma(z,t) = \left(1 - 2\gamma|f(z,t)|^2\right)^{1/4}. \tag{31}$$

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) + \frac{1}{2}\left(\frac{1}{\sigma(z,t)^2} + \sigma(z,t)^2\right) - 2\gamma\frac{|f(z,t)|^2}{\sigma(z,t)^2}\right] f(z,t) \tag{32}$$

Eq. (34) with Eq. (31) is the so-called nonpolynomial Schrodinger equation (NPSE).‖

‖L.S., A. Parola, and L. Reatto, PRA **65**, 043614 (2002).

Under the weak-coupling condition $g|f(z,t)|^2 \ll 1$ one finds

$$\sigma(z,t) \simeq 1 \ , \tag{33}$$

and the NPSE becomes the 1D GPE

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) - 2\gamma|f(z,t)|^2\right] f(z,t) \ . \tag{34}$$

Remarkably, with

$$V(z) = 0$$

the 1D GPE admits a self-localized stationary solution

$$f(z,t) = \sqrt{\frac{\gamma}{2}} \ sech^2\left(\gamma z\right) \ \exp\left(-i\mu t\right) \ , \tag{35}$$

where $\mu = -2\gamma^2$. This is the ground-state of the attractive 1D GPE with $V(z) = 0$ and there is **no collapse**.

This solution is called **bright soliton** because the 1D GPE with $V(z) = 0$ admits also the shape-invariant time-dependent solution

$$f(z,t) = \sqrt{\frac{\gamma}{2}} \ sech^2\left(\gamma(z-vt)\right) \ \exp\left(iv(z-vt)\right) \ \exp\left(i(v^2-\mu)t\right) \ , \tag{36}$$

where the center-of-mass velocity v is arbitrary (it does not depend on system paramters).

Let us now consider the NPSE with $V(z) = 0$. It can be written as

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{1-3\gamma|f(z,t)|^2}{\sqrt{1-2\gamma|f(z,t)|^2}}\right] f(z,t) \tag{37}$$

and admits the stationary self-localized solution

$$f(z,t) = \phi(z) \exp\left(-i\mu t\right) , \tag{38}$$

where $\phi(z)$ is given by the implicity formula

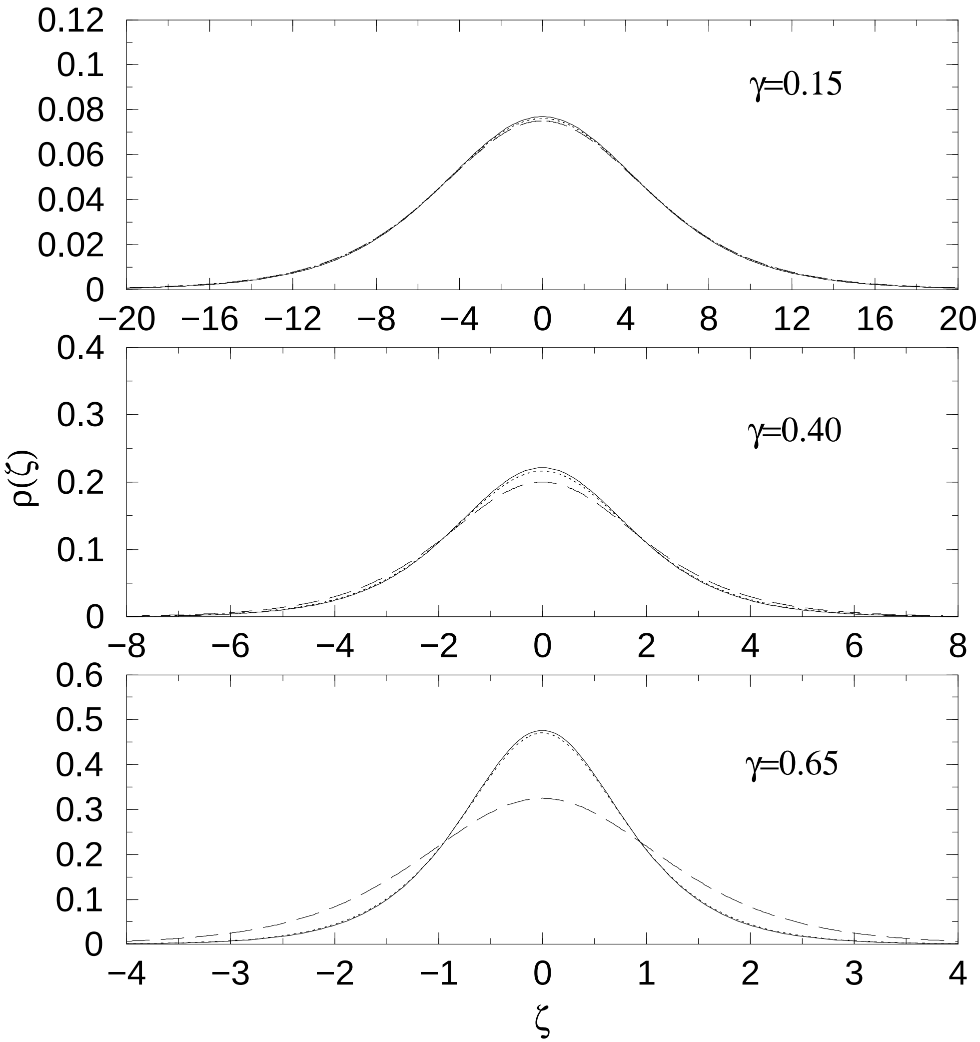
$$\sqrt{2}\, z = \sqrt{\frac{1}{1-\mu}}\text{Arctanh}\left(\sqrt{\frac{\sqrt{1-2\gamma\phi^2}-\mu}{1-\mu}}\right) - \sqrt{\frac{1}{1+\mu}}\tan^{-1}\left(\sqrt{\frac{\sqrt{1-2\gamma\phi^2}-\mu}{1+\mu}}\right) , \tag{39}$$

with μ given by the implicity formula $2\gamma = \frac{2\sqrt{2}}{3}(2\mu+1)\sqrt{1-\mu}$.
This 3D bright soliton exists up to the critical strength

$$\gamma_c = \left(\frac{|a_s|N}{a_\perp}\right)_c = \frac{2}{3} . \tag{40}$$

Above this value there is the **collapse of the bright soliton**.

Stationary 3D bright soliton: NPSE gives practically the same results of the 3D GPE.**



Axial density profile $\rho(z)$ of the BEC bright soliton: 3D GPE (full line), NPSE (dotted line), 1D GPE (dashed line). $\gamma = |a_s|N/a_\perp$.

L.S., A. Parola, and L. Reatto, PRA **66, 043603 (2002).

Simulating the ENS experiment with bright solitons

In the ENS experiment[††] with bright solitons made of ^{7}Li atoms the longitudinal potential

$$V(z) = \frac{m}{2}\omega_z^2 z^2 \, , \tag{41}$$

is <u>expulsive</u> (inverted parabola) because

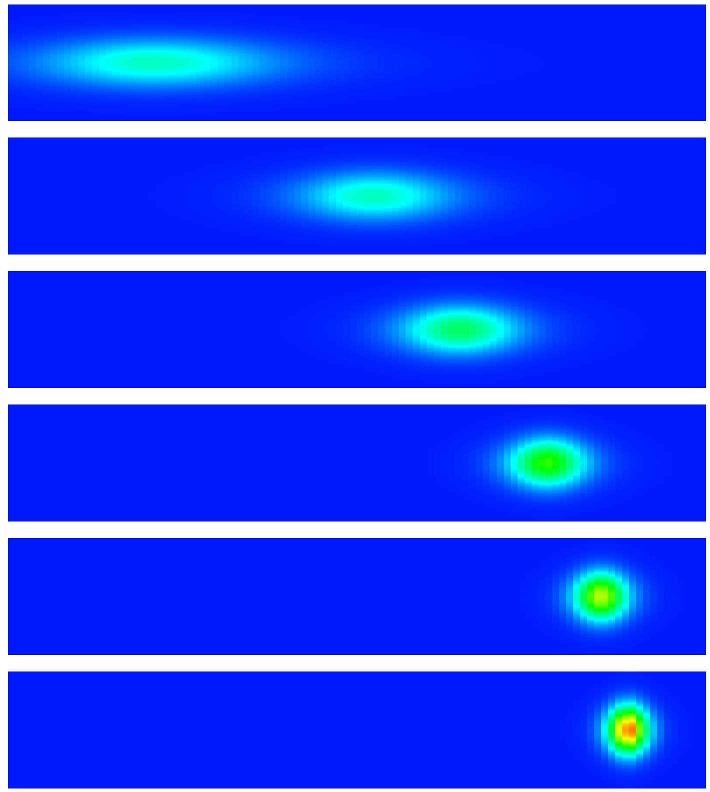
$$\omega_z = 2\pi i \times 78 \text{ Hz} \tag{42}$$

is an *imaginary* longitudinal frequency. In the experiment the s-wave scattering length a_s of ^{7}Li atoms is modified by the Feshbach-resonance technique.

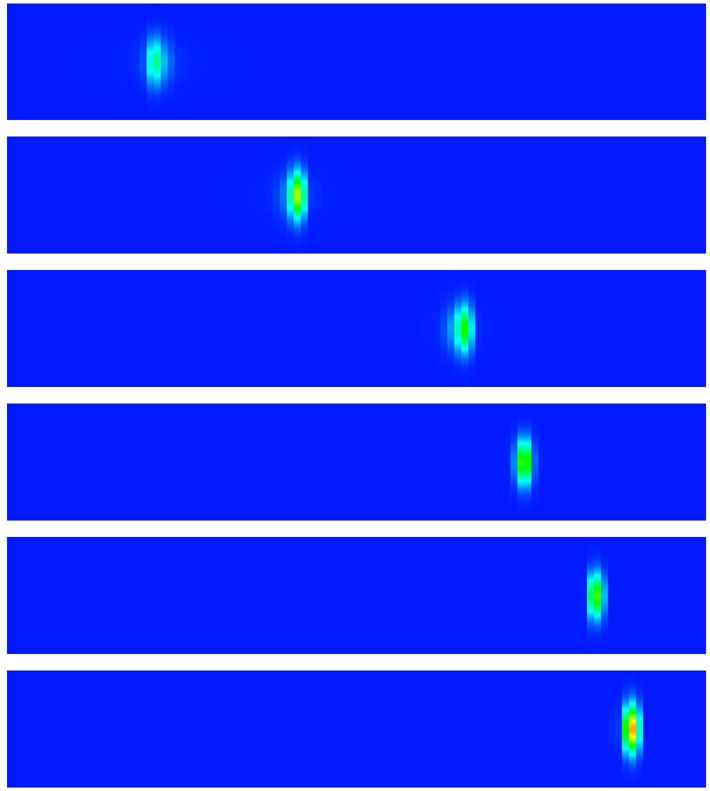
We have quite succesfully simulated this experiment by using the NPSE.[‡‡]

[††] L. Khaykovich, F. Schreck, G. Ferrari, T. Bourdel, J. Cubizolles, L. D. Carr, Y. Castin, C. Salomon, Science **296**, 1290 (2002)

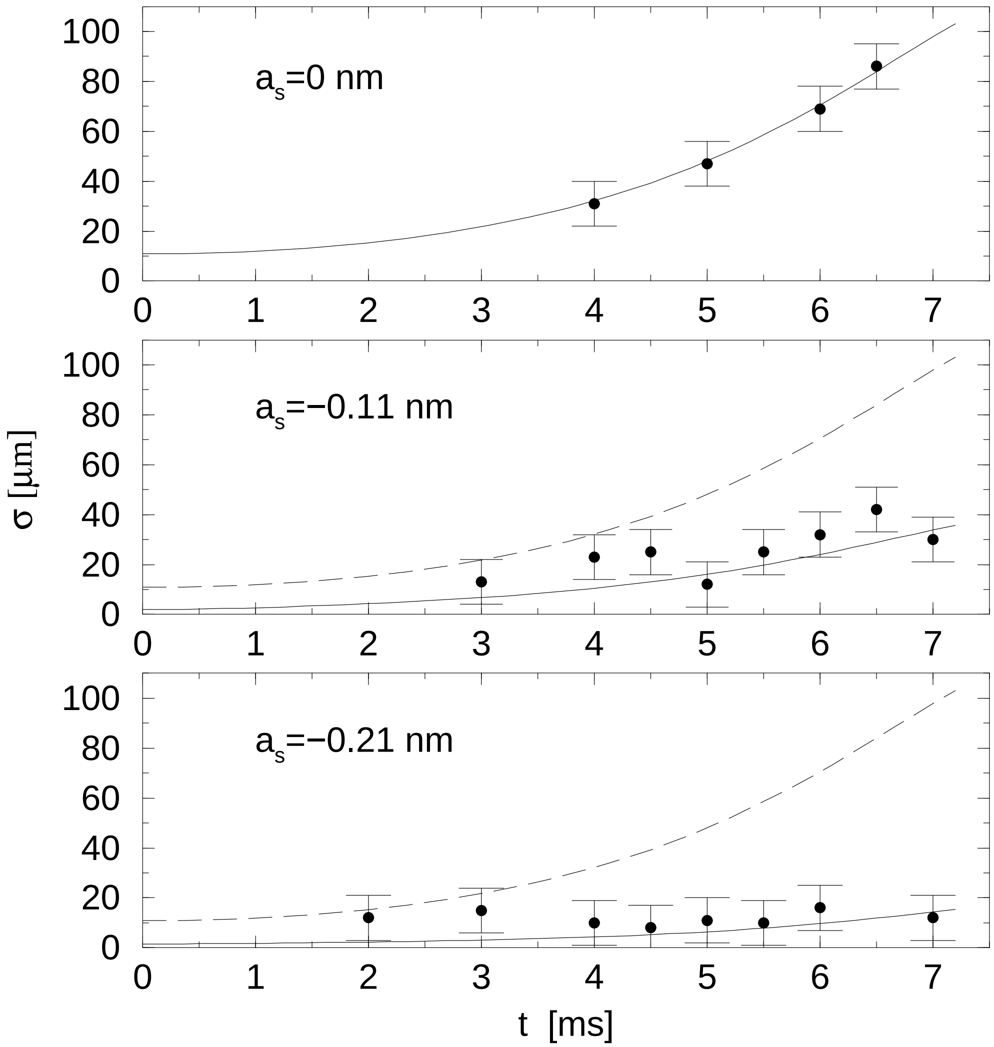
[‡‡] L.S., PRA **70**, 053617 (2004).



Density of the ^{7}Li BEC in the expulsive potential obtained by solving the NPSE. The BEC cloud propagates over 1 mm. Case with $a_s = 0$ (ideal gas). There are $N = 4 \times 10^3$ atoms. Six frames from bottom to top: $t = 2$ ms, $t = 3$ ms, $t = 4$ ms, $t = 5$ ms, $t = 6$ ms, $t = 7$ ms. Red color corresponds to highest density.



Density of the ^{7}Li BEC in the expulsive potential obtained by solving the NPSE. The BEC cloud propagates over 1 mm. Case with $a_s = -0.21$ nm ("bright soliton"). There are $N = 4 \times 10^3$ atoms. Six frames from bottom to top: $t = 2$ ms, $t = 3$ ms, $t = 4$ ms, $t = 5$ ms, $t = 6$ ms, $t = 7$ ms. Red color corresponds to highest density.



Root mean square size of the longitudinal width of the BEC as a function of the propagation time t. The filled circles are the experimental data of ENS experiment. The dashed line is the ideal gas ($a_s = 0$) curve. The solid line is obtained from the numerical solution of the NPSE.

Including an axial optical lattice

Let us now consider the inclusion of a periodic potential (optical lattice) acting along axis z on the properties of an attractive BEC. The external potential is

$$U(\mathbf{r}) = \frac{1}{2}(x^2 + y^2) + V(z) \,, \tag{43}$$

where

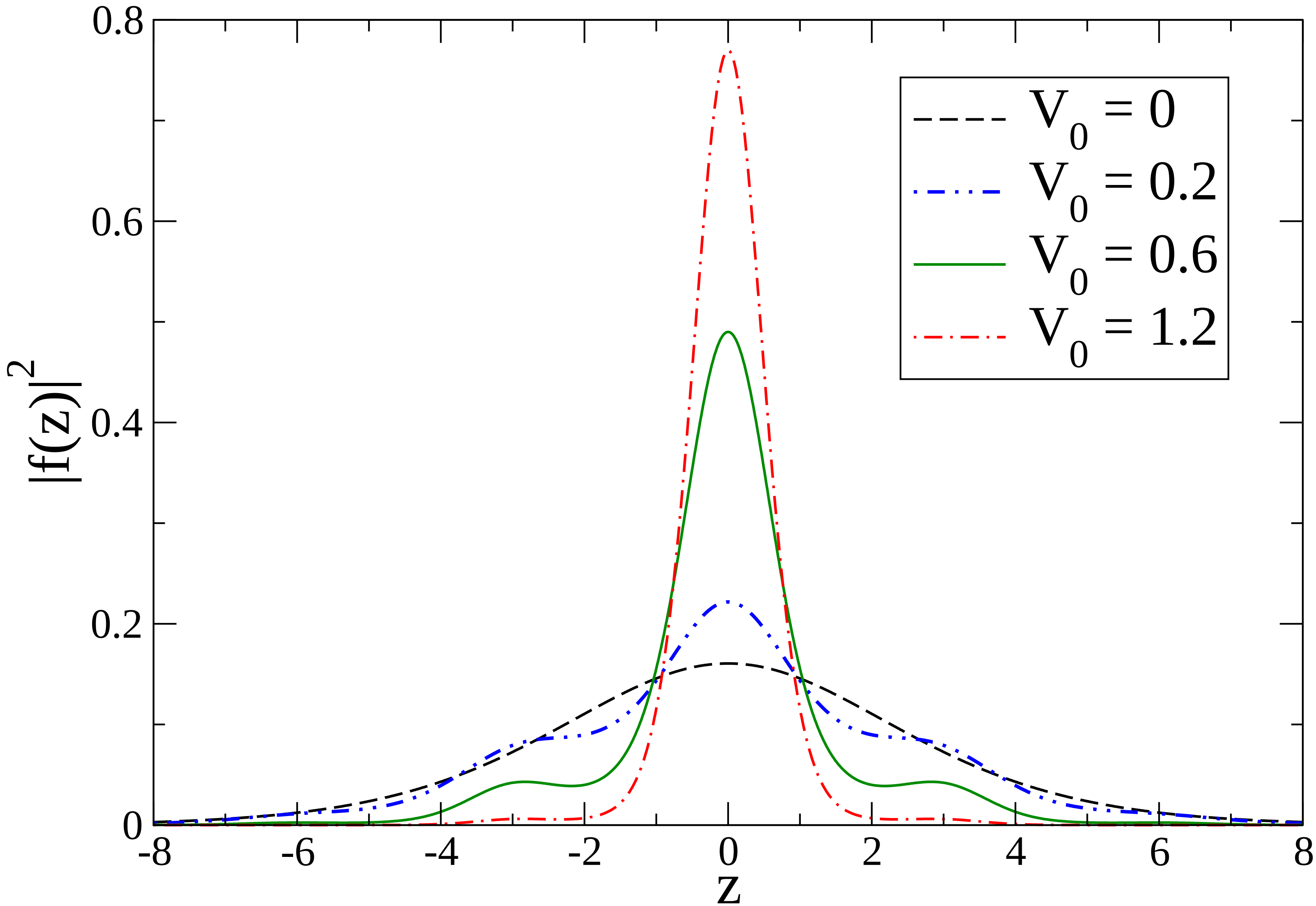
$$V(z) = -V_0 \cos(2k_L z) \,. \tag{44}$$

Here we use again the transverse harmonic length

$$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \,, \tag{45}$$

as unit of length, and $\hbar\omega_\perp$ as unit of energy.

We use the 3D GPE and the NPSE to investigate the attractive BEC (bright soliton) under these trapping conditions.



The axial density profile, $|f(z)|^2$, of the soliton in periodic potential, with $k_L = 1$ and four different values of V_0. The self-attraction strength is fixed at $g = 2|a_s|N/a_\perp = 0.5$. From: L.S., A. Cetoli, B.A. Malomed, and F. Toigo, PRA **75**, 033622 (2007).

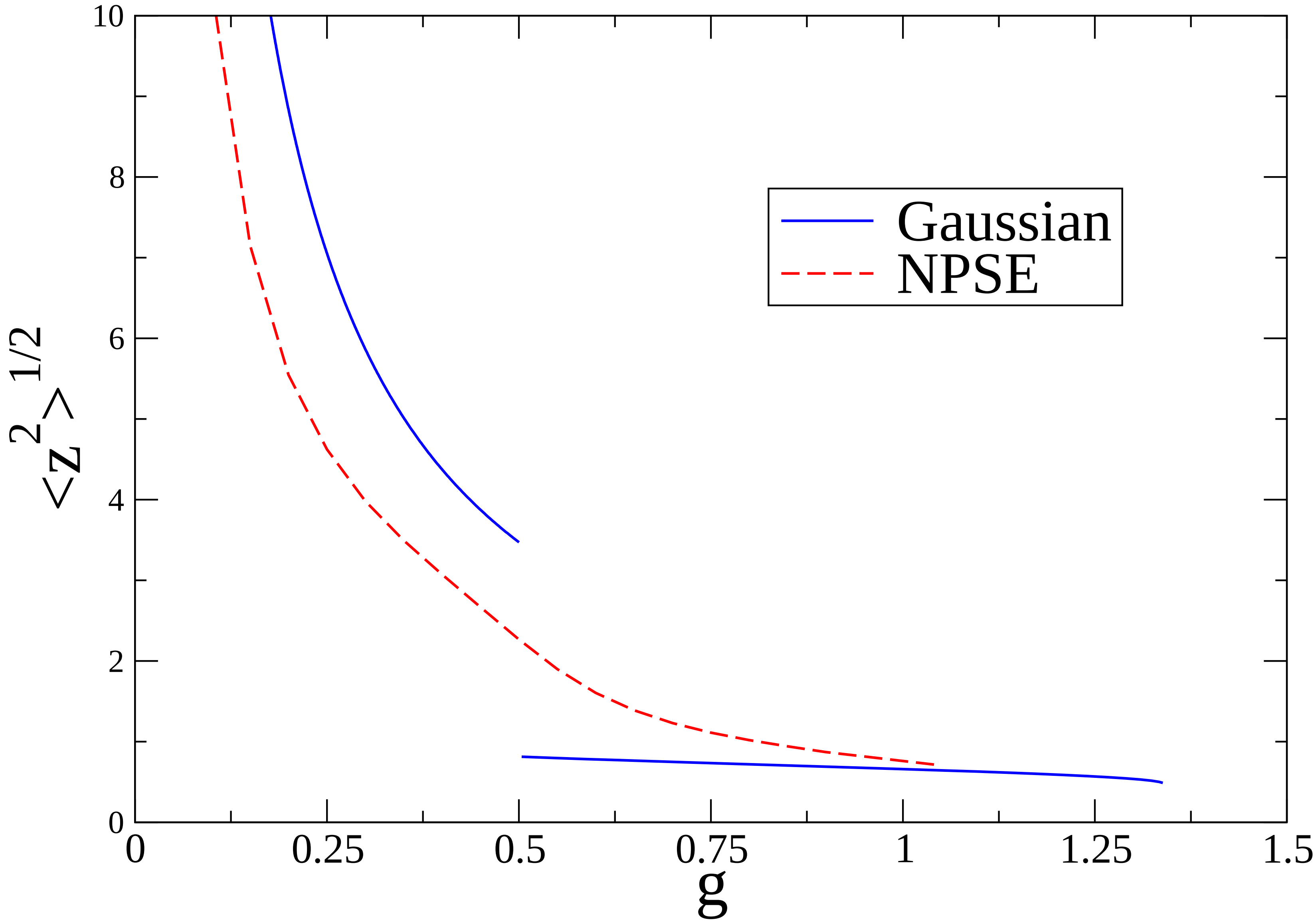


FIG. 2: Axial length of the ground-state bright soliton, $\langle z^2 \rangle^{1/2}$, as a function of self-attraction strength $g = 2|a_s|N/a_\perp$, for $V_0 = 0.4$ and $k_L = 1$. Displayed are results provided by the Gaussian variational and by the NPSE.

From: L.S., A. Cetoli, B.A. Malomed, and F. Toigo, PRA **75**, 033622 (2007).

V_0	g_c	$\sqrt{\langle z^2 \rangle}$	$\sigma(0)$
0	1.33	0.91	0.75
0.1	1.26	0.77	0.68
0.5	1.07	0.64	0.61
1	0.96	0.50	0.60
2	0.85	0.41	0.57

TABLE 1: The critical value of the self-attraction strength, g_c, and the corresponding values of the axial length, $\sqrt{\langle z^2 \rangle}$, and minimal transverse width, $\sigma(0)$, of the soliton in the periodic potential, $V(z) = -V_0 \cos(2k_L z)$, with $k_L = 1$, for different values of V_0, as found from numerical solution of the NPSE.

From: L.S., A. Cetoli, B.A. Malomed, and F. Toigo, PRA **75**, 033622 (2007).

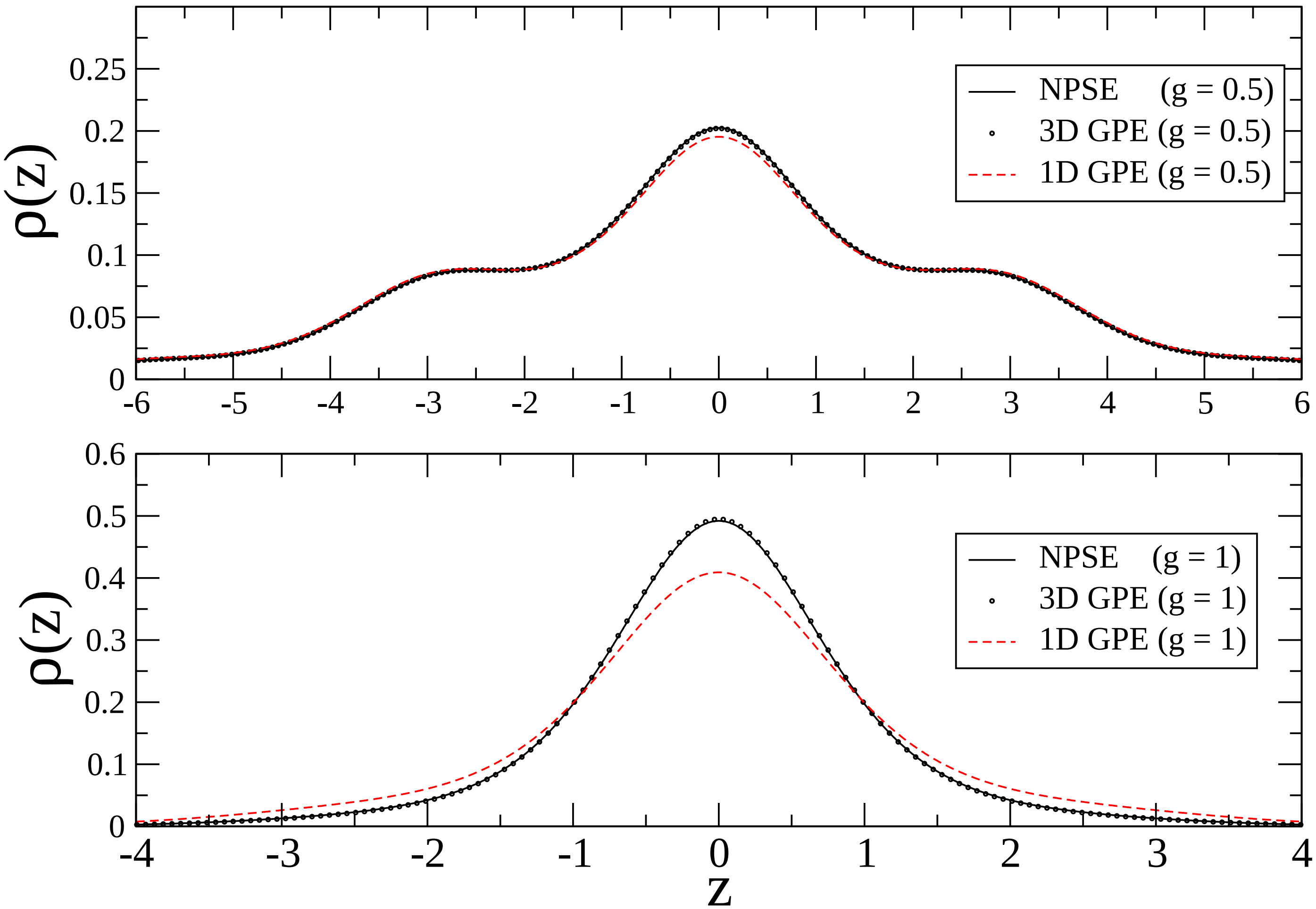


FIG. 3: The axial density profile, $\rho(z)$, of the soliton in potential, with $k_L = 1$ and $V_0 = 0.2$. Comparison between results provided by the different equations: NPSE, 3D GPE, and 1D GPE. In the case of the 3D equation, the axial density is defined as $\rho(z) = \int\int |\psi(\mathbf{r})|^2 dxdy$, while in the other cases it is simply $|f(z)|^2$.

From: L.S., A. Cetoli, B.A. Malomed, and F. Toigo, PRA **75**, 033622 (2007).

To study the dynamics of the bright soltion in the axial optical lattice, we multiply the stationary solution $f_0(z)$ by $\exp(ipz)$, i.e., use initial conditions

$$f(z) = f_0(z) \ \exp(ipz) \ , \tag{46}$$

where p is the momentum of the imposed kick.

We solved the full time-dependent NPSE,

$$i\,\frac{\partial f(z,t)}{\partial t} = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} - V_0 \cos\left(2k_L z\right) + \frac{1-\frac{3}{2}g|f(z,t)|^2}{\sqrt{1-g|f(z,t)|^2}} \right] f(z,t), \tag{47}$$

with the initial condition of Eq. (46), by using a Crank-Nicholson predictor-corrector algorithm in real time. Here the interaction strength g is given by

$$g = \frac{2|a_s|N}{a_\perp} \ .$$

Note that configuration (46) can be created experimentally by means of the so-called phase-imprinting technique.

Our numerical simulations ($136 \times 2 = 272$ runs!) reveal the existence of three different dynamical regimes:

(i) **stable breathers**, i.e., solitons steadily moving at an almost constant velocity, with small-amplitude shape oscillations.

(ii) **dispersive dynamics**, in which case the soliton strongly spreads out in the course of the evolution; here solitons move at a variable speed.

(iii) **localization**, in which a narrow soliton remains trapped in one lattice cell.

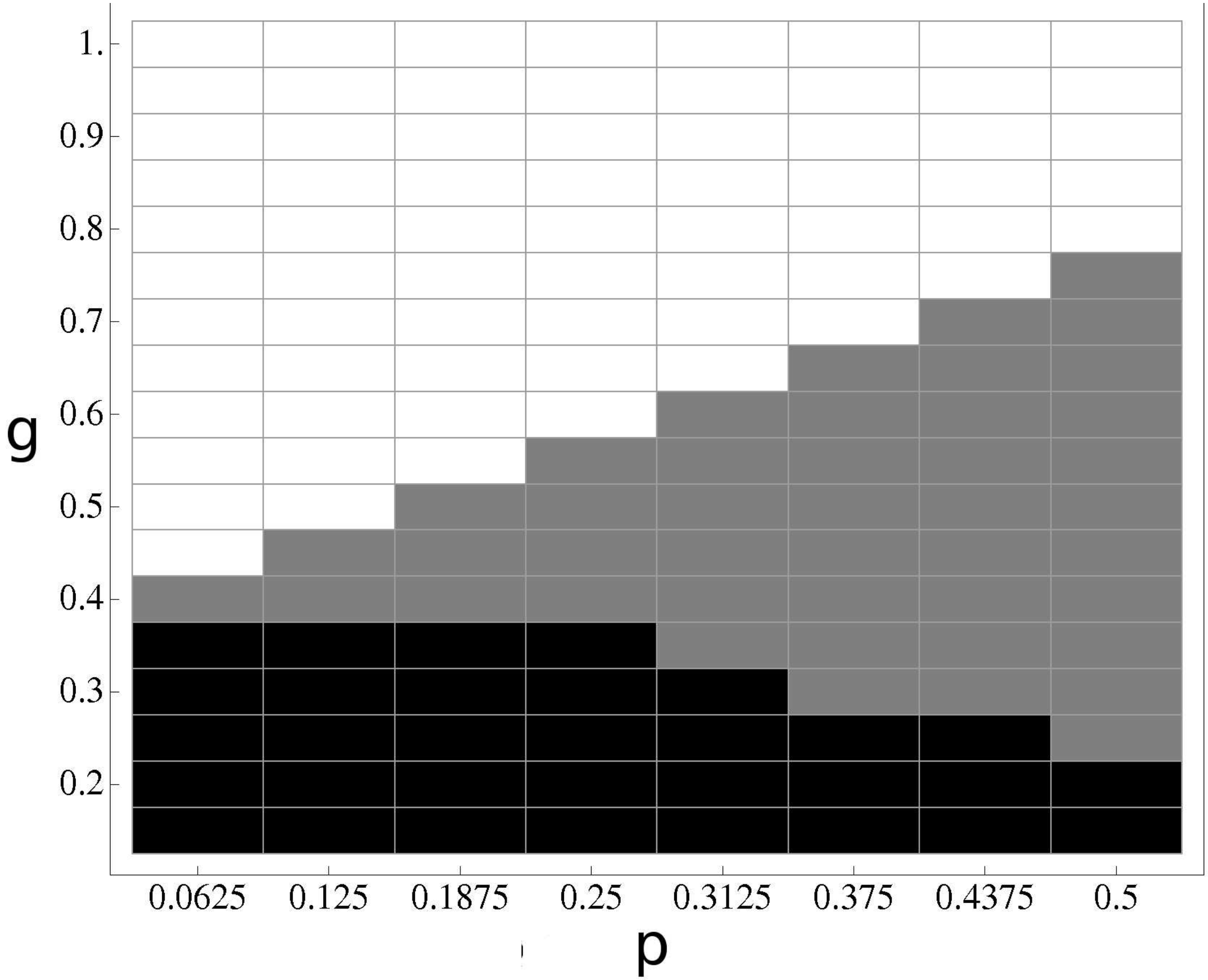


FIG. 6: Dynamical regimes in the plane of (p, g). Black region: steadily moving breather-like solitons; gray region: spreading out of the irregularly moving soliton; white region: localization (the center of mass does not move). Parameters of the optical lattice are $k_L = 1$ and $V_0 = 0.5$.

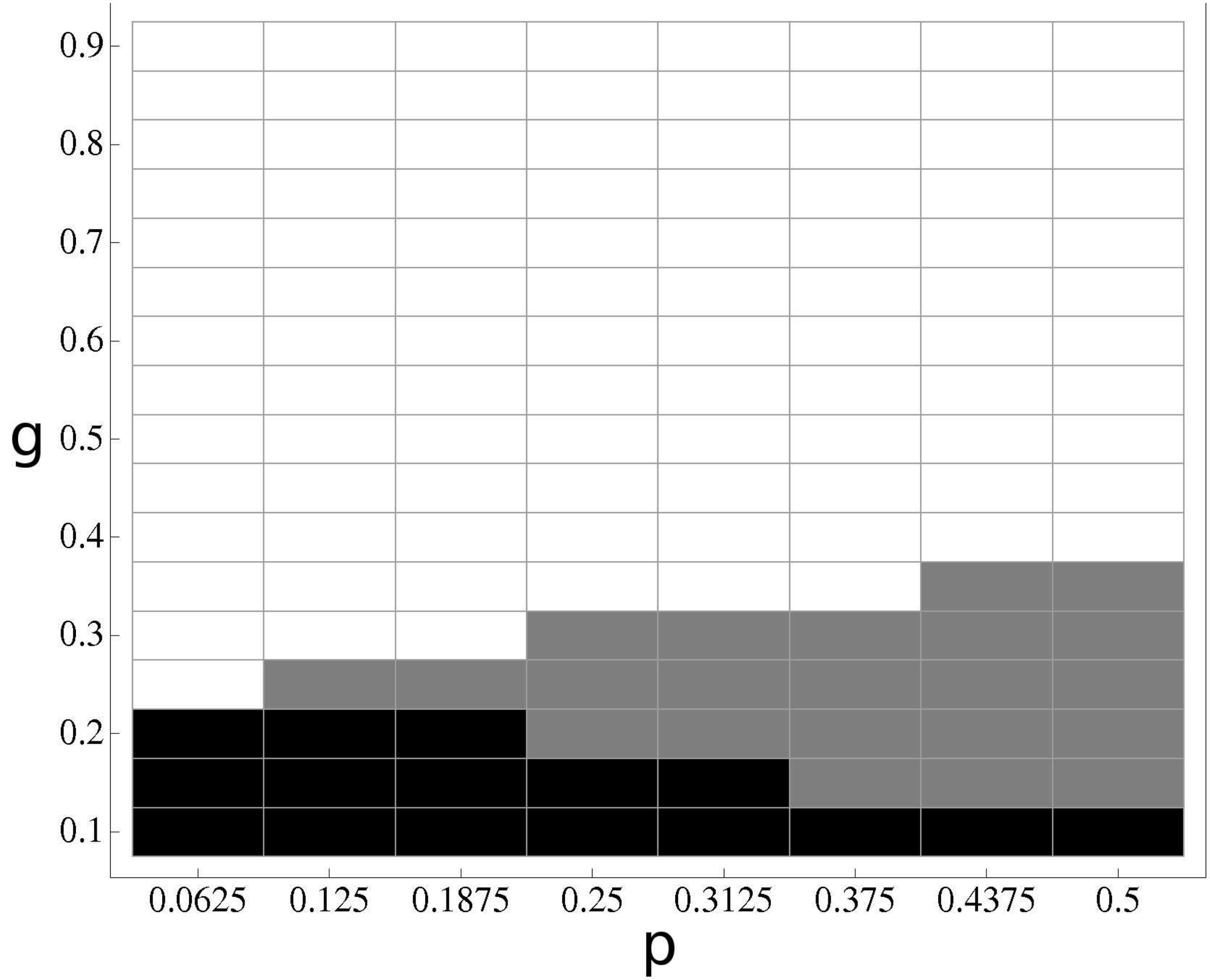


FIG. 7: Dynamical regimes in the plane of (p, g). Black region: steadily moving breather-like solitons; gray region: spreading out of the irregularly moving soliton; white region: localization (the center of mass does not move). Parameters of the optical lattice are $k_L = 1$ and $V_0 = 1$.

Conclusions

- BECs with negative scattering length show interesting properties:
  – collapse above a critical strength;
  – bright soliton solutions.

- By using 3D GPE and NPSE we have succcesfully simulated the only two experiments (Rice Univ. and ENS) on BEC bright solitons (more details on request).

- In an axial optical lattice (AOL) the bright soliton occupies one or many-sites depending on inter-atomic stregth and lattice parameters.

- The behavior of a kicked bright soliton in a AOL shows 3 regimes:
  – breather-like;
  – irregular dynamics;
  – localization.

THANKS!!