Physico-mathematical methods for the solution of the Gross-Pitaevskii equation

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Summary

- Bose-Einstein condensation and Gross-Pitaevskii equation
- Gaussian variational approach
- Nonpolynomial Schrödinger equation
- Exact solutions with negative scattering length
- Simulating the ENS experiment with bright solitons
- Conclusions

Bose-Einstein Condensation and Gross-Pitaevskii equation

The N-body stationary Schrödinger equation

$$\hat{H}\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = \epsilon \ \Psi(\mathbf{r}_1, ..., \mathbf{r}_N) \ , \tag{1}$$

where

$$\hat{H} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U(\mathbf{r}_i) \right] + \sum_{i<j} V(\mathbf{r}_i, \mathbf{r}_j) \tag{2}$$

is the N-body Hamiltonian, can be obtained by minimizing the energy functional

$$E[\Psi] = \int \Psi^*(\mathbf{r}_1, ..., \mathbf{r}_N) \hat{H} \Psi(\mathbf{r}_1, ..., \mathbf{r}_N) \ d^3\mathbf{r}_1 ... d^3\mathbf{r}_N \tag{3}$$

with the constraint

$$\int |\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)|^2 \ d^3\mathbf{r}_1 ... d^3\mathbf{r}_N = 1 \ . \tag{4}$$

In the case of a Bose-Einstein condensate (BEC), all identical bosons are in the same single-particle quantum state $\psi(\mathbf{r})$. It is quite natural to write the N-body wave function of a BEC as

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = \psi(\mathbf{r}_1) \ ... \ \psi(\mathbf{r}_N) \ . \tag{5}$$

By inserting this wave function in the energy functional, it becomes

$$E[\psi] \ = \ N \int \psi^*(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) \right] \psi(\mathbf{r}) \ d^3\mathbf{r} \tag{6}$$

$$+ \ \frac{1}{2} N(N-1) \int |\psi(\mathbf{r})|^2 |\psi(\mathbf{r}')|^2 V(\mathbf{r},\mathbf{r}') \ d^3\mathbf{r} \ d^3\mathbf{r}' \tag{7}$$

In the case of a dilute BEC, the inter-atomic interaction can be taken as

$$V(\mathbf{r},\mathbf{r}') = G \ \delta(\mathbf{r}-\mathbf{r}') \ , \tag{8}$$

where

$$G = \frac{4\pi\hbar^2 a_s}{m} \tag{9}$$

is the inter-atomic strength with a_s the s-wave scattering length fixed by experiments. This potential is called Fermi pseudo-potential.

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

$$a_s > 0 \, , \tag{10}$$

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

$$a_s < 0 \, , \tag{11}$$

which implies an effective attraction between atoms.

^{7}Li atoms have a negative scattering length

$$a_s \simeq -14 \cdot 10^{-10} \text{ m} \, . \tag{12}$$

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).

By using the Fermi pseudo-potential, the energy functional of the BEC is further simplified and reads

$$E[\psi] = N \int \psi^*(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{1}{2} G N (N-1) |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) \; d^3\mathbf{r} \; . \qquad (13)$$

By minimizing this single-particle energy functional with the constraint

$$\int |\psi(\mathbf{r})|^2 \; d^3\mathbf{r} = 1 \qquad (14)$$

one obtains the so-called Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + G(N-1)|\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = \mu \; \psi(\mathbf{r}) \; , \qquad (15)$$

where μ is the Lagrange multiplier fixed by the normalization. Usually one sets N instead of $N-1$ for a large number of particles. Note that μ satisfies the equation

$$\mu = \frac{\partial E}{\partial N} \; . \qquad (16)$$

Thus, μ is the chemical potential of the system.

Gaussian variational approach

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

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{4\pi\hbar^2 a_s N}{m}|\psi(\mathbf{r})|^2\right]\psi(\mathbf{r}) = \mu\ \psi(\mathbf{r})\ , \tag{17}$$

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

$$\int |\psi(\mathbf{r})|^2\ d^3\mathbf{r} = 1\ . \tag{18}$$

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

$$E = \int \left\{\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2 + U(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{2\pi\hbar^2 a_s N}{m}|\psi(\mathbf{r})|^4\right\}\ d^3\mathbf{r}\ , \tag{19}$$

with the constraint of Eq. (18).

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

$$U(\mathbf{r}) = \frac{1}{2} m\omega_H^2 \left(x^2 + y^2 + z^2\right) = \frac{1}{2} m\omega_H^2 r^2 \; . \tag{20}$$

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

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4} a_H^{3/2} \sigma^{3/2}} \exp\left(\frac{-r^2}{2a_H^2\sigma^2}\right) , \tag{21}$$

where

$$a_H = \sqrt{\frac{\hbar}{m\omega_H}} \tag{22}$$

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

$$\bar{E} = \frac{2E}{\hbar\omega_H} = \frac{3}{2}\frac{1}{\sigma^2} + \frac{3}{2}\sigma^2 + \Gamma\frac{1}{\sigma^3} , \tag{23}$$

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.

$$0 = \frac{\partial \bar{E}}{\partial \sigma} = -3\frac{1}{\sigma^3} + 3\sigma^3 - 3\Gamma\frac{1}{\sigma^4} \, . \tag{24}$$

Obviously σ must also satisfy the condition

$$\frac{\partial^2 \bar{E}}{\partial \sigma^2} > 0. \tag{25}$$

It follows that

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

while

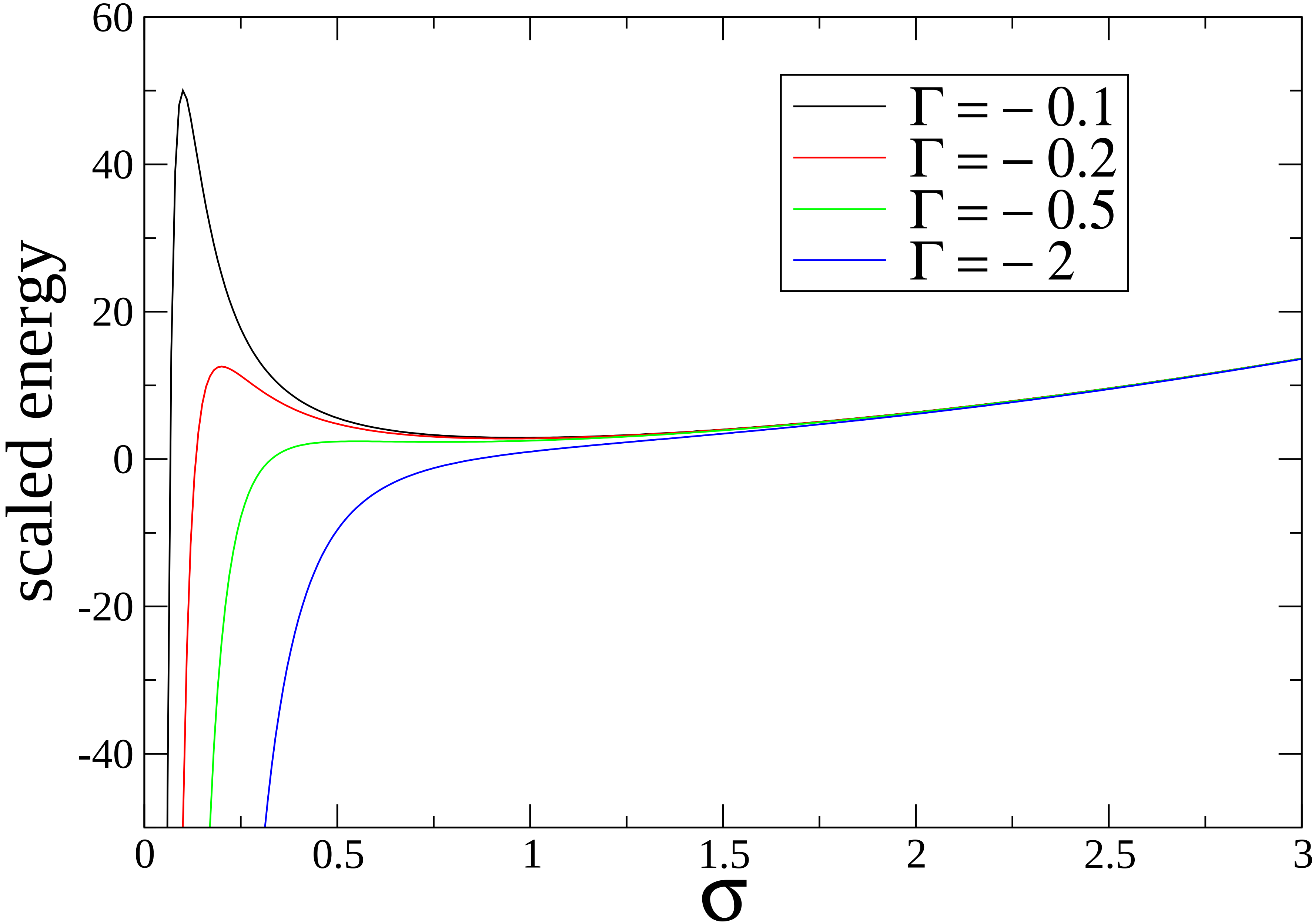
$$\sigma_c < \sigma < 1 \quad \text{for} \quad -\Gamma_c < \Gamma < 0 \, ,$$

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

$$\frac{|a_s|N}{a_H} = \sqrt{\frac{\pi}{2}}\frac{4}{5^{5/4}} \simeq 0.67 \tag{26}$$

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

$$U(\mathbf{r}) = \frac{1}{2} m \omega_\perp^2 (x^2 + y^2) + \frac{1}{2} m \omega_z^2 z^2 \ , \tag{27}$$

By using the transverse harmonic length

$$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \ , \tag{28}$$

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

$$E = \int \left\{ \frac{1}{2} |\nabla\psi(\mathbf{r})|^2 + \left[\frac{1}{2}(x^2 + y^2) + \frac{\lambda^2}{2} z^2 \right] |\psi(\mathbf{r})|^2 + 2\pi\gamma |\psi(\mathbf{r})|^4 \right\} d^3\mathbf{r} \ , \tag{29}$$

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[§]

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4}\sigma\eta^{1/2}} \exp\left\{-\frac{(x^2+y^2)}{2\sigma^2} - \frac{z^2}{2\eta^2}\right\}, \tag{30}$$

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

$$\bar{E} = \frac{1}{\sigma^2} + \sigma^2 + \frac{1}{2\eta^2} + \frac{\lambda^2}{2}\eta^2 - \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^2\eta}\,. \tag{31}$$

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

$$-\frac{1}{\sigma^3} + \sigma + \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^3\eta} = 0\,, \tag{32}$$

$$-\frac{1}{\eta^3} + \lambda^2\eta + \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^2\eta^2} = 0\,. \tag{33}$$

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¶

$$L = \dot{\sigma}^2 + \frac{1}{2}\dot{\eta}^2 - \bar{E}(\sigma, \eta) \; . \qquad (34)$$

The equations of motion are

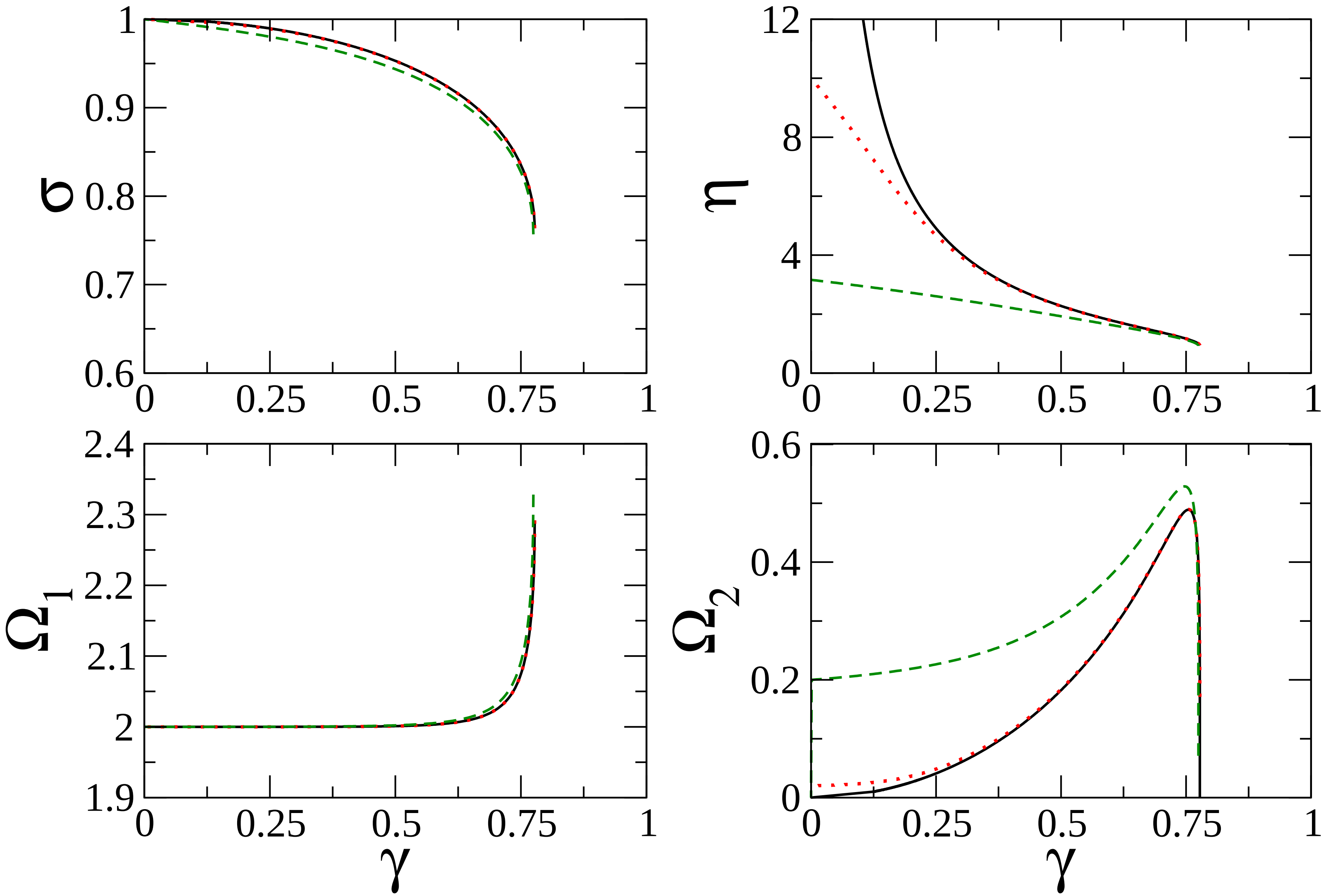
$$\ddot{\sigma} - \frac{1}{\sigma^3} + \sigma + \sqrt{\frac{2}{\pi}} \; \gamma \frac{1}{\sigma^3 \eta} = 0 \; , \qquad (35)$$

$$\ddot{\eta} - \frac{1}{\eta^3} + \lambda^2 \eta + \sqrt{\frac{2}{\pi}} \; \gamma \frac{1}{\sigma^2 \eta^2} = 0 \; . \qquad (36)$$

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 ($\lambda = 0.1$).

Nonpolynomial Schrödinger equation

To investigate the dynamics of a BEC we start from the time-dependent 3D GPE given by

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left[-\frac{\hbar}{2m}\nabla^2+U(\mathbf{r})+\frac{4\pi\hbar^2 a_s N}{m}|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t)\ , \qquad (37)$$

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

$$U(\mathbf{r})=\frac{1}{2}m\omega_\perp^2(x^2+y^2)+V(z)\ . \qquad (38)$$

By using the transverse harmonic length

$$a_\perp=\sqrt{\frac{\hbar}{m\omega_\perp}}\ , \qquad (39)$$

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

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left[-\frac{1}{2}\nabla^2+\frac{1}{2}(x^2+y^2)+V(z)+2\pi g|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t)\ , \qquad (40)$$

where

$$g=\frac{2a_s N}{a_\perp}\ . \qquad (41)$$

The 3D GPE is the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \psi} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\psi}} - \nabla \frac{\partial \mathcal{L}}{\partial \nabla \psi} = 0 \ , \tag{42}$$

of the following Lagrangian density

$$\mathcal{L} = \psi^*(\mathbf{r},t)\left(i\frac{\partial}{\partial t} + \frac{1}{2}\nabla^2\right)\psi(\mathbf{r},t) - \frac{1}{2}(x^2+y^2)|\psi(\mathbf{r},t)|^2 - V(z)|\psi(\mathbf{r},t)|^2 - \pi g|\psi(\mathbf{r},t)|^4 \ . \tag{43}$$

We remind that the Euler-Lagrange equation (42) is obtained by extermizing the action functional

$$A[\psi] = \int dt \ L = \int dt \ d^3\mathbf{r} \ \mathcal{L}(\psi, \nabla\psi, \dot{\psi}) \ , \tag{44}$$

where

$$L = \int d^3\mathbf{r} \ \mathcal{L}(\psi, \nabla\psi, \dot{\psi}) \tag{45}$$

is the full Lagrangian obtained from the Lagrangian density.

We consider a semi-Gaussian variational ansatz

$$\psi(\mathbf{r},t) = \frac{1}{\pi^{1/2}\sigma(z,t)} \exp\left\{-\frac{(x^2+y^2)}{2\sigma(z,t)^2}\right\} f(z,t) \ . \tag{46}$$

Inserting this expression into the 3D Lagrangian density and integrating over x and y variables, we obtain an effective 1D Lagrangian density

$$\bar{\mathcal{L}} = f^*(z,t)\left[i\frac{\partial}{\partial t}f(z,t) + \frac{1}{2}\frac{\partial^2}{\partial z^2} - V(z) - \frac{1}{2}\left(\frac{1}{\sigma(z,t)^2} + \sigma(z,t)^2\right) - \frac{1}{2}g\frac{|f(z,t)|^2}{\sigma(z,t)^2}\right] f(z \tag{47}$$

The two Euler-Lagrange equations of this effective Lagrangian density with respect to $\sigma(z,t)$ and $f(z,t)$ are

$$\sigma(z,t) = \left(1 + g|f(z,t)|^2\right)^{1/4} \ , \tag{48}$$

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) + \frac{1}{2}\left(\frac{1}{\sigma(z,t)^2} + \sigma(z,t)^2\right) + g\frac{|f(z,t)|^2}{\sigma(z,t)^2}\right] f(z,t) \tag{49}$$

Eq. (49) with Eq. (48) is the so-called nonpolynomial Schrodinger equation (NPSE).‖

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

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

$$\sigma(z,t) \simeq 1 \; , \tag{50}$$

and the NPSE becomes the familiar 1D GPE (cubic nonlinearity)

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) + g|f(z,t)|^2 \right] f(z,t) \; . \tag{51}$$

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

$$\sigma(z,t) \simeq g^{1/4}|f(z,t)|^{1/2}. \tag{52}$$

and the NPSE becomes a 1D nonlinear Schrodinger equation with quadratic nonlinearity

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) + \frac{3}{2}g^{1/2}|f(z,t)| \right] f(z,t) \tag{53}$$

Exact solutions with negative scattering length

Let us consider the self-focusing ($a_s < 0$) 1D GPE without external potential, i.e. $V(z) = 0$. It is given by

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) - 2\gamma|f(z,t)|^2\right] f(z,t) \ , \tag{54}$$

where $\gamma = -|g|/2$.

This equation admits a self-localized stationary solution

$$f(z,t) = \sqrt{\frac{\gamma}{2}}\ sech^2(\gamma z)\ \ \exp\left(-i\mu t\right) \ , \tag{55}$$

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

$$f(z,t) = \sqrt{\frac{\gamma}{2}}\ sech^2(\gamma(z-vt))\ \ \exp\left(iv(z-vt)\right)\ \ \exp\left(i(v^2-\mu)t\right) \ , \tag{56}$$

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

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

$$i\frac{\partial}{\partial t}f(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{1-3\gamma|f(z,t)|^2}{\sqrt{1-2\gamma|f(z,t)|^2}}\right] f(z,t) \tag{57}$$

and admits the stationary self-localized solution

$$f(z,t) = \phi(z)\exp\left(-i\mu t\right) , \tag{58}$$

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

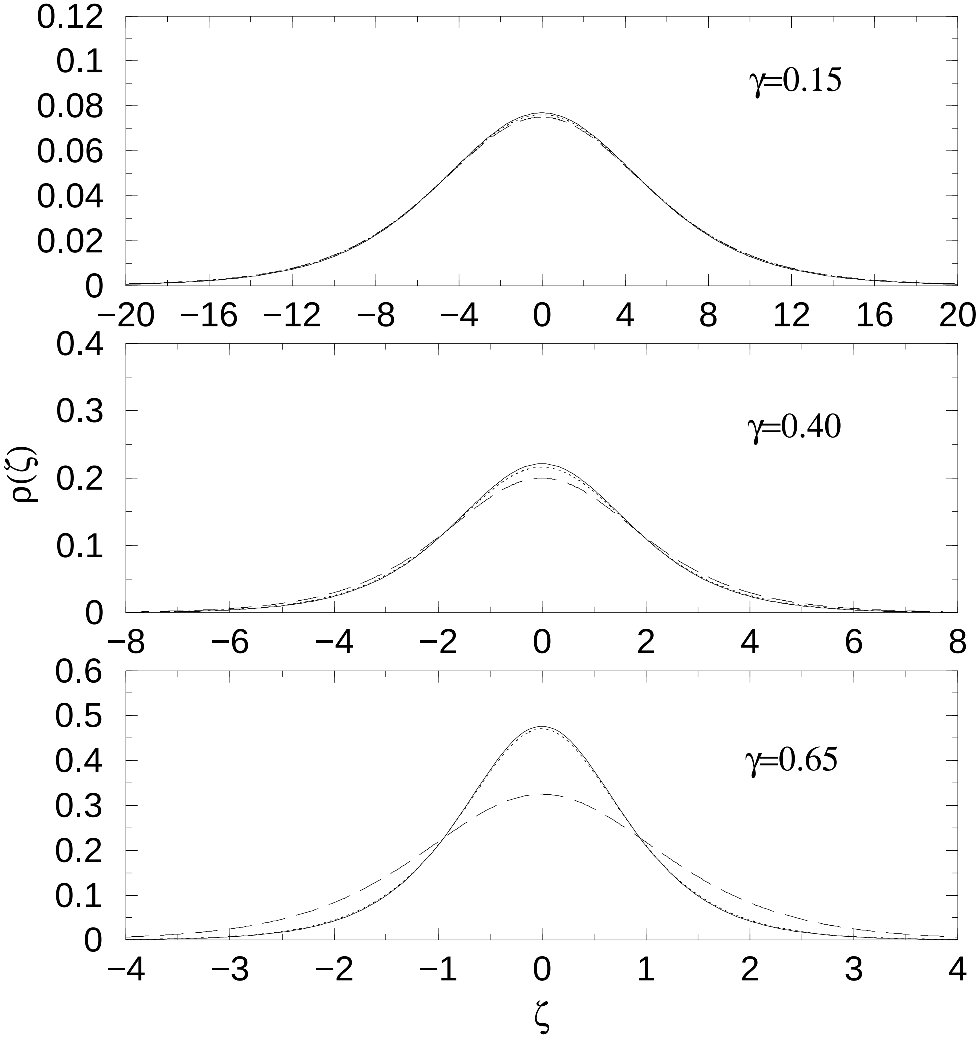
$$\sqrt{2}\, z = \sqrt{\frac{1}{1-\mu}}\text{Arctanh}\left(\sqrt{\frac{\sqrt{1-2\gamma\phi^2}-\mu}{1-\mu}}\right) - \sqrt{\frac{1}{1+\mu}}\tan^{-1}\left(\sqrt{\frac{\sqrt{1-2\gamma\phi^2}-\mu}{1+\mu}}\right) , \tag{59}$$

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

$$\gamma_c = \left(\frac{|a_s|N}{a_\perp}\right)_c = \frac{2}{3} . \tag{60}$$

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

$$V(z) = \frac{m}{2}\omega_z^2 z^2 \, , \tag{61}$$

is expulsive (inverted parabola) because

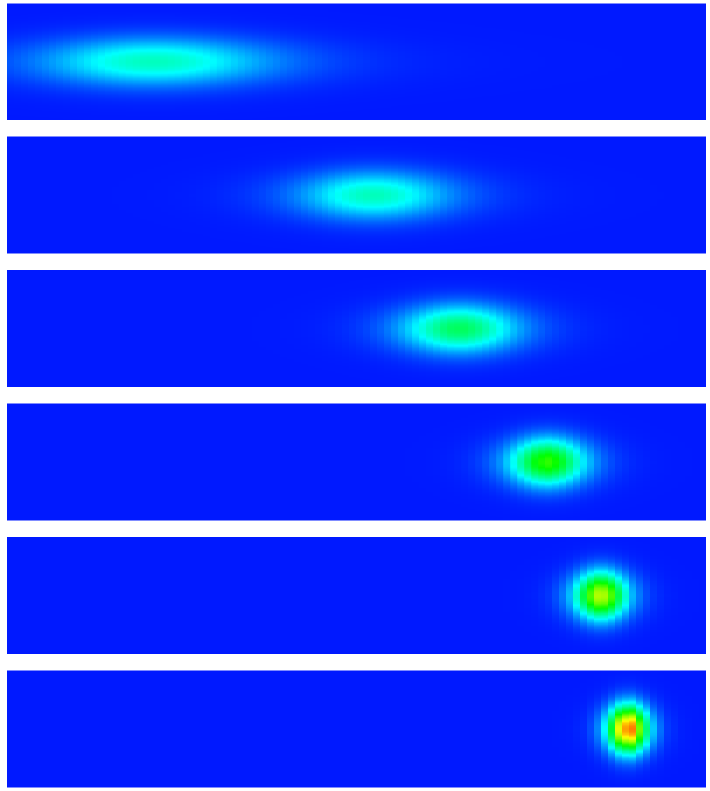
$$\omega_z = 2\pi i \times 78 \text{ Hz} \tag{62}$$

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.

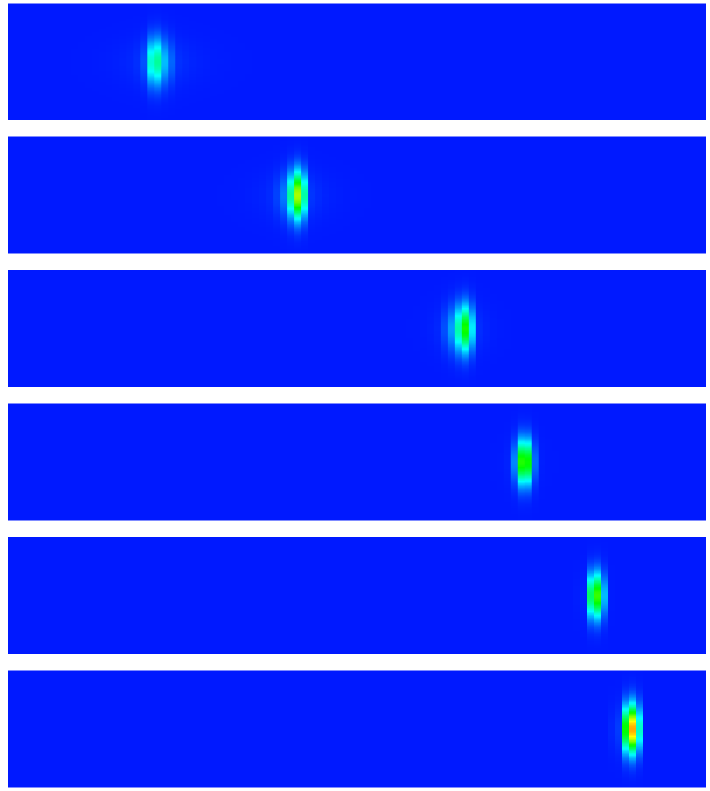
We have quite succesfully simulated this experiment by using the NPSE.‡‡

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

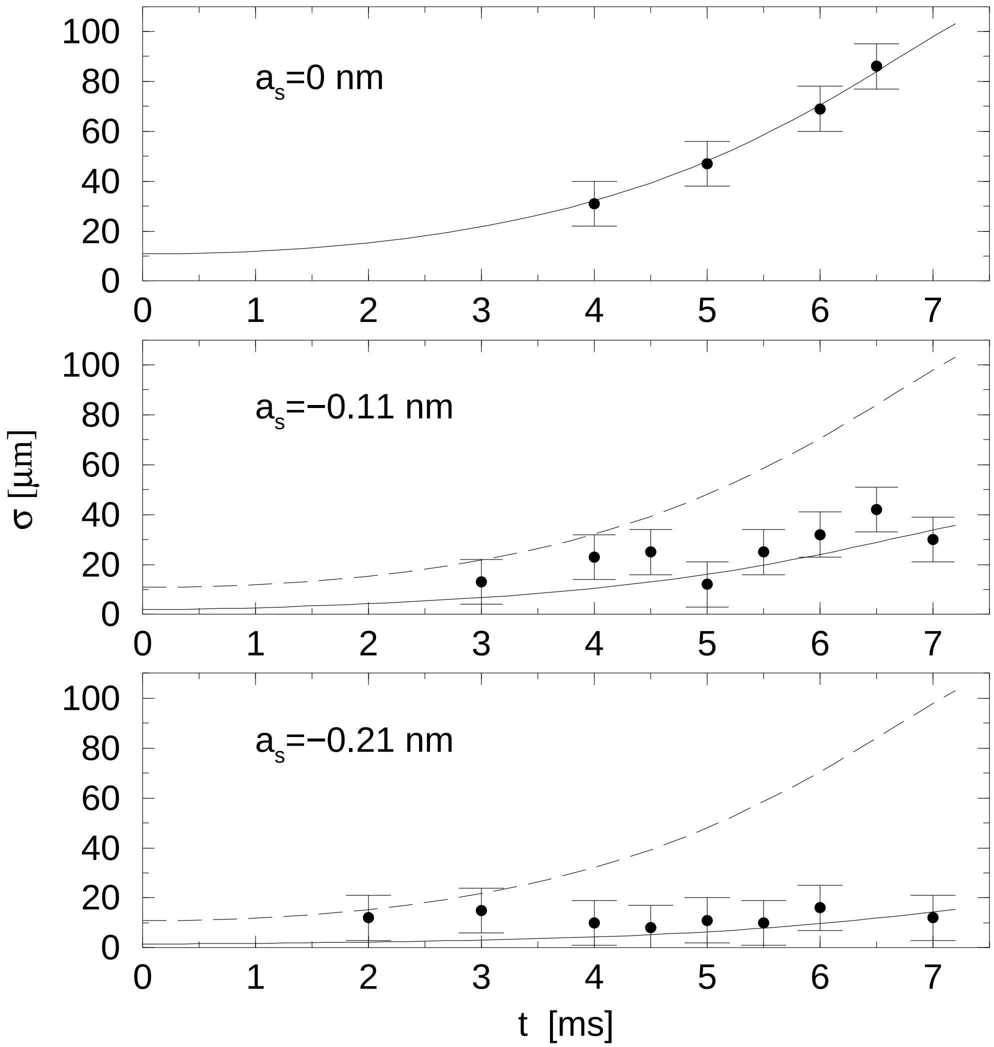
‡‡L.S., PRA **70**, 053617 (2004).



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.

Conclusions

- The Gaussian variational approach can be useful to study the GPE.

- The NPSE, based on a semi-Gaussian approach, is also better.

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

- 1D GPE and NPSE with attractive interaction admit exact analitical solutions: bright solitons.

- 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).

THANKS!!