Derivation of the Gross-Pitaevskii equation and applications

Luca Salasnich

Dipartimento di Fisica e Astronomia "Galileo Galilei", Università di Padova

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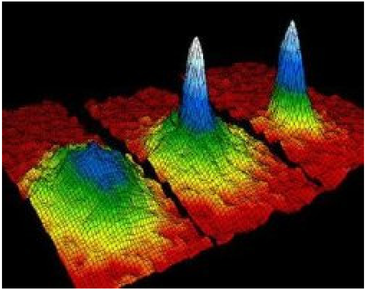
Summary

- Bose-Einstein condensation with ultracold atoms
- Gross-Pitaevskii equation
- Dimensional reduction: from 3D to 1D
- 1D GPE and bright solitons
- Improved dimensional reduction: the 1D NPSE
- Solitons in experiments with ultracold atoms
- Conclusions

Bose-Einstein condensation with ultracold atoms (I)

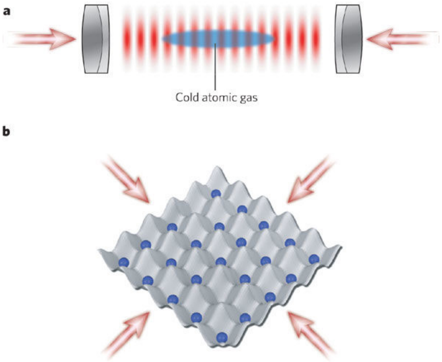
In 1995 Eric Cornell and Carl Wieman, Wolfgang Ketterle, and Randy Hulet achieved Bose-Einstein condensation (BEC) cooling very dilute gases of ^{87}Rb, ^{23}Na atoms, ^{7}Li atoms.



The BEC critical temperature is about $T_c \simeq 100$ nanoKelvin. The gas, made of dilute and ultracold neutral alkali-metal atoms, is in a meta-stable state which can survive for minutes.

Bose-Einstein condensation with ultracold atoms (II)

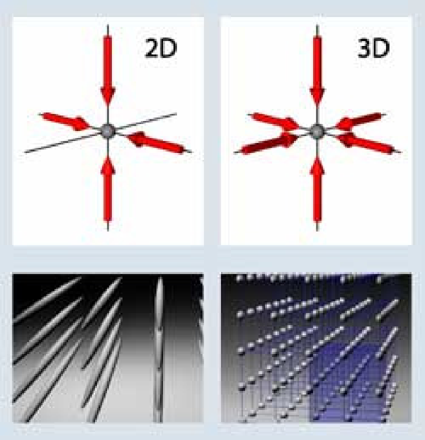
In 2002 the experimental group of Immanuel Bloch obtained with counter-propagating laser beams inside an optical cavity, stationary optical lattice which can trap ultracold atoms.



The resulting optical potential can trap neutral atoms in the minima of the optical lattice due to the electric dipole of atoms.

Bose-Einstein condensation with ultracold atoms (III)

Now the study of neutral atoms trapped with light is a very hot topic of research.



Changing the intensity and shape of the optical lattice, it is now possible to trap atoms in very different configurations. One can have many atoms per site but also one atom per site.

Gross-Pitaevskii equation (I)

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).

Gross-Pitaevskii equation (II)

The Gross-Pitaevskii equation, that is a nonlinear Schrödinger equation with cubic nonlinearity, can be deduced from the many-body quantum Hamiltonian of N identical spinless particles

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + U(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V(\mathbf{r}_i - \mathbf{r}_j) \ , \qquad (3)$$

where $U(\mathbf{r})$ is the external potential and $V(\mathbf{r} - \mathbf{r}')$ is the inter-atomic potential.
The time-dependent Schrödinger equation of this many-body system is given by

$$i\hbar \frac{\partial}{\partial t} \boldsymbol{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \hat{H} \boldsymbol{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t), \qquad (4)$$

where $\boldsymbol{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t)$ is the time-dependent many-body wavefuction.

Gross-Pitaevskii equation (III)

The time-dependent many-body Schrödinger equation is the Euler-Lagrange equation of the following many-body action functional

$$S = \int dt \; d^3\mathbf{r}_1 \; ... \; d^3\mathbf{r}_N \; \mathbf{\Psi}^*(\mathbf{r}_1, ..., \mathbf{r}_N, t) \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \mathbf{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t) \; . \tag{5}$$

In the case of a pure Bose-Einstein condensate one assumes all bosons in the same time-dependent single-particle orbital (Hartree approximation)

$$\mathbf{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \prod_{i=1}^{N} \psi(\mathbf{r}_i, t) \; . \tag{6}$$

Inserting this ansatz into the many-body action functional one gets

$$\begin{aligned} S &= N \int dt \; d^3\mathbf{r} \; \psi^*(\mathbf{r}, t) \Big(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - U(\mathbf{r}) \\ &- \frac{N-1}{2} \int d^3\mathbf{r}' \; |\psi(\mathbf{r}', t)|^2 V(\mathbf{r} - \mathbf{r}') \Big) \psi(\mathbf{r}, t) \; . \end{aligned} \tag{7}$$

Gross-Pitaevskii equation (IV)

The Euler-Lagrange equation of the previous action functional reads

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)\int d^3\mathbf{r}' \; |\psi(\mathbf{r}',t)|^2 V(\mathbf{r}-\mathbf{r}')\right]\psi(\mathbf{r},t) \; . \tag{8}$$

This is the time-dependent Hartree equation for N identical bosons in the same single-particle state $\psi(\mathbf{r},t)$.
In the case of dilute gases we assume (Fermi pseudo-potential) that

$$V(\mathbf{r}) \simeq g \; \delta^{(3)}(\mathbf{r}) \tag{9}$$

with $\delta^{(3)}(\mathbf{r})$ the Dirac delta function and, by construction,

$$g = \int V(\mathbf{r}) \; d^3\mathbf{r} \; . \tag{10}$$

From 3D scattering theory, the s-wave scatering length a_s of the inter-atomic potential can be written (Born approximation) as

$$a_s = \frac{m}{4\pi\hbar^2}\int V(\mathbf{r}) \; d^3\mathbf{r} \; . \tag{11}$$

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

From the Hartree equation we have obtained the Gross-Pitaevskii (GP) equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)g|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t) \; , \qquad (12)$$

with

$$g = \frac{4\pi\hbar^2}{m}a_s \; . \qquad (13)$$

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

$$S = N\int dt\, d^3\mathbf{r}\; \psi^*(\mathbf{r},t)\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\nabla^2-U(\mathbf{r})-\frac{N-1}{2}g|\psi(\mathbf{r},t)|^2\right)\psi(\mathbf{r},t) \; . \qquad (14)$$

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

$$U(\mathbf{r}) = \frac{1}{2}m{\omega_\perp}^2(x^2+y^2)+\mathcal{U}(z) \; . \qquad (15)$$

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

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

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

where $f(z, t)$ is the axial wave function and $a_{\perp} = \sqrt{\hbar/(m\omega_{\perp})}$ is the characteristic length of the transverse harmonic confinement.
By inserting Eq. (16) into the GP action (14) 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 $f(z, t)$ reads

$$i\hbar \frac{\partial}{\partial t} f(z, t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \mathcal{U}(z) + \gamma |f(z, t)|^2 \right] f(z, t) , \tag{17}$$

where

$$\gamma = \frac{(N-1)g}{2\pi {a_{\perp}}^2} \tag{18}$$

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. $\mathcal{U}(z) = 0$, the 1D GPE becomes

$$i\hbar \frac{\partial}{\partial t} f(z,t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \gamma |f(z,t)|^2 \right] f(z,t) \; . \qquad (19)$$

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

$$f(z,t) = \phi(z - vt) e^{i(mv^2/2 - \mu)t/\hbar}, \qquad (20)$$

where v is the arbitrary velocity of propagation of the solution, which has a shape-invariant axial density profile:

$$n(z,t) = N|f(z,t)|^2 = N|\phi(z - vt)|^2 \; . \qquad (21)$$

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

1D GPE and bright solitons (II)

Setting $\zeta = z - vt$, the 1D stationary GP equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{d\zeta^2} + \gamma |\phi(\zeta)|^2 \right] \phi(\zeta) = \mu \; \phi(\zeta) \; , \tag{22}$$

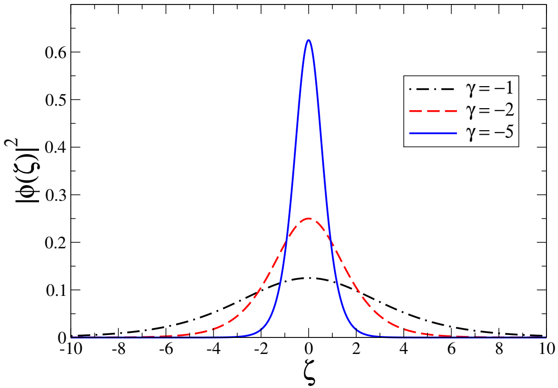
with $\gamma < 0$ (self-focusing), admits the bright-soliton solution

$$\phi(\zeta) = \sqrt{\frac{m|\gamma|}{8\hbar^2}} \; Sech\left[\frac{m|\gamma|}{4\hbar^2} \zeta \right] \tag{23}$$

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

$$\mu = -\frac{m \; \gamma^2}{16 \; \hbar^2} \; . \tag{24}$$

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 bright soliton analytical solution has been obtained from the 1D GPE, which is derived from the 3D GPE assuming a transverse Gaussian with a constant transverse width $a_\perp$.
A more general assumption,[3] is based on a space-time dependent transverse width

$$\psi(\mathbf{r},t) = f(z,t)\frac{1}{\pi^{1/2} a_\perp \sigma(z,t)} \exp\left(\frac{x^2+y^2}{2{a_\perp}^2 \sigma(z,t)^2}\right) , \tag{25}$$

where $f(z,t)$ is the axial wave function and $\sigma(z,t)$ is the adimensional transverse width in units of $a_\perp$.
From this ansatz one gets the **1D nonpolynomial Schrödinger equation** (1D NPSE)

$$i\hbar \frac{\partial}{\partial t} f = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \mathcal{U}(z) + \frac{\gamma |f|^2}{\sigma^2} + \frac{\hbar\omega_\perp}{2}\left(\frac{1}{\sigma^2} + \sigma^2\right)\right] f \, , \tag{26}$$

$$\sigma = \left(1 + \gamma |f|^2\right)^{1/4} . \tag{27}$$

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

Improved dimensional reduction: the 1D NPSE (II)

In the weak-coupling regime $\gamma|f|^2 \ll 1$ one finds $\sigma \simeq 1$ and the 1D NPSE becomes the familiar 1D GPE.
With $\mathcal{U}(z) = 0$ and assuming $\gamma < 0$ the NPSE admits analytical bright soliton solutions. Setting

$$f(z,t) = \phi(z - vt) e^{i(mv^2/2-\mu)t/\hbar}, \tag{28}$$

one finds the bright-soliton solution written in implicit form

$$\zeta = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1-\mu}} \, arctg \left[\sqrt{\frac{\sqrt{1-|\gamma|\phi^2} - \mu}{1-\mu}} \right] \tag{29}$$

$$- \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1+\mu}} \, arcth \left[\sqrt{\frac{\sqrt{1-|\gamma|\phi^2} - \mu}{1+\mu}} \right] , \tag{30}$$

where $\zeta = z - vt$ and $|\gamma| = 2|a_s|(N-1)/a_\perp$.

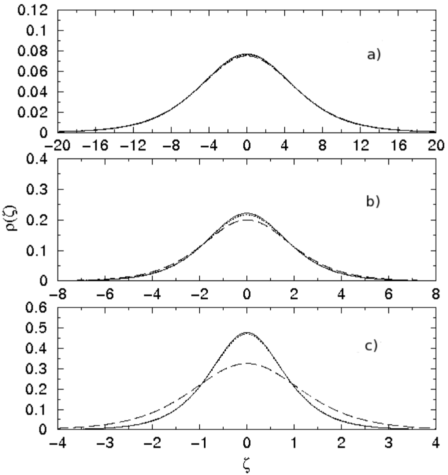
Improved dimensional reduction: the 1D NPSE (III)

In the weak-coupling limit ($\gamma\phi^2 \ll 1$) one finds that the NPSE bright-soliton solution reduces the the 1D GPE one.
However, contrary to the 1D GPE bright soliton, the 1D NPSE bright soliton does not exist anymore, **collapsing** to a Dirac delta function, at

$$\gamma_c = \left(\frac{2a_s(N-1)}{a_\perp} \right)_c = -\frac{4}{3} \, .$$

This analytical result is in extremely good agreement with the numerical solution of the 3D GPE but also with experimental results.

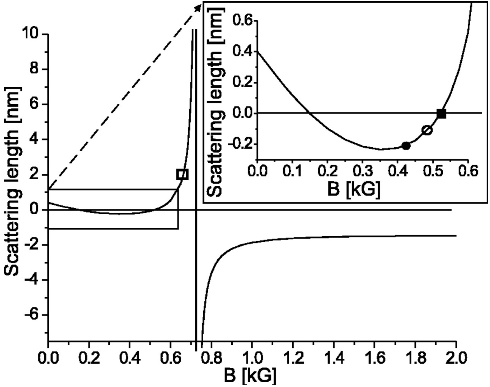
Improved dimensional reduction: the 1D NPSE (IV)



Axial density profile $\rho(\zeta)$ of the Bose-condensed bright soliton: 3D GPE (**full line**), 1D NPSE (dotted line), 1D GPE (dashed line). Length in units $a_\perp = (\hbar/m\omega_\perp)^{1/2}$ and density in units $1/a_\perp$. Three values of the interaction strength: a) $\gamma = 0.3$, b) $\gamma = 0.8$, c) $\gamma = 1.3$.

Solitons in experiments with ultracold atoms (I)

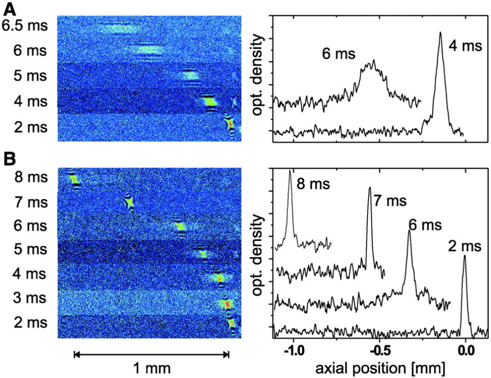
In 2002 there were two relevant experiments about bright solitons with BECs made of ^{7}Li atoms.



Both experiments used the technique of Fano-Feschbach resonance to tune the s-wave scattering length a_s of the inter-atomic potential by means of an **external constant magnetic field**. In the figure: scattering length a_s for ^{7}Li in state $|F = 1, m_F = 1\rangle$.

Solitons in experiments with ultracold atoms (II)

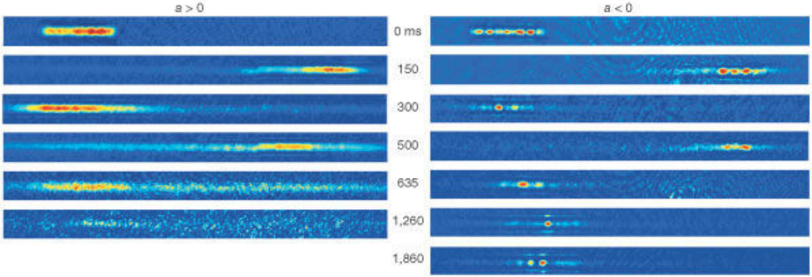
At ENS of Paris, Khaykovich et al. [Science **296**, 1290 (2002)] reported the production of bright solitons in an ultracold ^{7}Li gas. The interaction was tuned with a Feshbach resonance from repulsive to attractive before release in a one-dimensional optical waveguide.



Propagation of the soliton without dispersion over a macroscopic distance of 1.1 millimeter was observed.

Solitons in experiments with ultracold atoms (III)

At Rice University, Strecker et al. [Nature **417**, 150 (2002)] reported the formation of a train of bright solitons of ^{7}Li atoms in a quasi-one-dimensional optical trap.



The solitons were set in motion by offsetting the optical potential, and they were observed to propagate along the axial harmonic potential for many oscillatory cycles without spreading.

Conclusions

- We have derived the **3D GPE** from the many-body action of identical interacting bosons by assuming that all the particles are in the same time-dependent single-particle wavefunction.
- We have shown how to derive the 1D GPE assuming a transverse Gaussian with a constant transverse width $a_{\perp}$.
- 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.
- The study of bright and dark solitons in ultracold atoms is still a hot topic. See, for instance, the recent experiment
  J.H.V. Nguyen, D. Luo, R.G. Hulet, Science **356**, 422 (2017)
  which investigates the collective modes of bright-soliton trains.

Acknowledgements

Thank you for your attention!

Slides online: http://materia.dfa.unipd.it/salasnich/talk-patna19b.pdf