Solitons and vortices in Bose-Einstein condensates with finite-range interaction

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Summary

- Bose-Einstein condensates and Hartree equation
- Finite-range potential and modified Gross-Pitaevskii equation
- Solitons with the 1D MGPE
- Vortices with the 3D MGPE
- Conclusions
Let us consider a system of $N$ identical bosonic particles of mass $m$ described by the many-body Hamiltonian

$$
\hat{H} = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + U(r_i) \right] + \frac{1}{2} \sum_{i \neq j}^{N} V(r - r') ,
$$

where $U(r)$ is the external trapping potential and $V(r)$ is the two-body interaction potential.

Let us assume that all the bosonic particles are in a pure Bose-Einstein condensate, characterized by the same single-particle wave function $\psi(r)$. Moreover, let us assume that the symmetric many-body wavefunction of the system is given by

$$
\psi(r_1, r_2, ..., r_{N-1}, r_N) = \psi(r_1) \psi(r_2) ... \psi(r_{N-1}) \psi(r_N) ,
$$

which is clearly invariant exchanging two coordinates.
Bose-Einstein condensates and Hartree equation (II)

The expectation value of $\hat{H}$ with respect to $\Psi$ gives

$$E[\psi(r)] = \langle \Psi | \hat{H} | \Psi \rangle = N \int d^3r \psi^*(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right] \psi(r)$$

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

Extremizing this energy functional with respect to $\psi(r)$, and taking also into account the following constraint of normalization

$$\int d^3r |\psi(r)|^2 = 1 ,$$

one immediately finds

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + (N - 1) \int d^3r' V(r - r') |\psi(r')|^2 \right] \psi(r) = \mu \psi(r) ,$$

which is the so-called Hartree equation for identical bosons and $\mu$ is the chemical potential (Lagrange multiplier) of the system.
The Hartree equation is a nonlinear Schrödinger equation with a nonlocal nonlinearity. However, to describe Bose-Einstein condensates in ultracold and dilute atomic gases, the inter-atomic potential $V(r)$ is usually approximated by the zero-range Fermi pseudo-potential, namely

$$V(r - r') = g_0 \delta(r - r') ,$$

where $\delta(r)$ is the Dirac delta function and $g_0$ is the strength of the zero-range interaction ($g_0 > 0$ repulsion, $g_0 < 0$ attraction). In this way the Hartree equation for bosons becomes

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + (N - 1)g_0 |\psi(r)|^2 \right] \psi(r) = \mu \psi(r) ,$$

which is the familiar Gross-Pitaevskii equation\(^1\) (GPE), i.e. a nonlinear Schrödinger equation with cubic nonlinearity.

In the Hartree equation for bosons there is the mean-field nonlocal potential

\[ U_{mf}(r) = \int d^3r' |\psi(r')|^2 V(r - r') \, . \]  
\( (8) \)

Substituting \( r' = r + s \) in the right side of Eq. (8) and expanding \( \psi(r + s) \) in powers of \( s \) one gets at the second order\(^2\)

\[ U_{mf}(r) = g_0 |\psi(r)|^2 + g_2 \nabla^2 |\psi(r)|^2 , \]  
\( (9) \)

where

\[ g_0 = \int d^3s \, V(s) = \tilde{V}(0) \quad \text{and} \quad g_2 = \frac{1}{2} \int d^3s \, s^2 \, V(s) = -\frac{1}{2} \tilde{V}''(0) \]  
\( (10) \)

with \( \tilde{V}(q) \) the Fourier transform of \( V(r) \).

Thus, by using Eq. (9) the Hartree equation for bosons becomes

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + U(r) + (N-1)g_0|\psi(r)|^2 + g_2(N-1)\nabla^2|\psi(r)|^2\right] \psi(r) = \mu \psi(r),$$

(11)

which is a modified Gross-Pitaevskii equation (MGPE). The MGPE can also be obtained from the Hartree equation of bosons by using the two-body pseudo-potential

$$V(r) = g_0 \delta(r) + \frac{g_2}{2}(\vec{\nabla}^2 \delta(r) + \delta(r) \vec{\nabla}^2),$$

(12)

where the Laplace operators $\vec{\nabla}^2$ and $\vec{\nabla}^2$ act respectively on left and right functions giving the appropriate symmetrization on the effective local potential.

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In 2003 Garcia-Ripoll, Konotop, Malomed, and Perez-Garcia\textsuperscript{4} studied spherically-symmetric solutions of the MGPE with a harmonic trapping potential

\[ U(r) = \frac{1}{2} m \omega^2 r^2. \]  

(13)

In the case \( g_0 < 0 \) they found solitonic solutions of the MGPE which are stabilized against collapse by the finite-range parameter \( g_2 \), as shown also by Parola, Salasnich, Reatto solving the Hartree equation\textsuperscript{5}.

In 2014 Veksler, Fishman, and Ketterle\textsuperscript{6} showed that for a quasi-1D Bose-Einstein condensate made of dilute atoms the MGPE gives rise to small but observable corrections to the GPE.


The 1D MGPE is obtained from the 3D MGPE assuming the following trapping potential

\[ U(r) = \frac{1}{2} m \omega_\perp^2 (x^2 + y^2) + W(z) \]  \hspace{1cm} (14)

and the following wavefunction

\[ \psi(r) = \frac{e^{-(x^2+y^2)/(2a_\perp^2)}}{\pi^{1/2} a_\perp} \phi(z) , \] \hspace{1cm} (15)

where \( a_\perp = \sqrt{\hbar/(m \omega_\perp)} \) is the characteristic length of the transverse harmonic confinement and \( W(z) \) is a generic axial potential. The corresponding 1D MGPE for the axial wavefunction \( \phi(z) \) reads

\[ \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + W(z) + \gamma_0 |\phi(z)|^2 + \frac{1}{2} \gamma_2 \frac{\partial^2}{\partial z^2} |\phi(z)|^2 \right] \phi(z) = \tilde{\mu} \phi(z) , \] \hspace{1cm} (16)

where \( \gamma_0 = (g_0 - g_2/a_\perp^2)/(2\pi a_\perp^2) \), \( \gamma_2 = g_2/(2\pi a_\perp^2) \) and \( \tilde{\mu} = \mu - \hbar \omega_\perp \).
Solitons with the 1D MGPE (III)

Setting for simplicity $\hbar = m = 1$, $W(z) = 0$, and assuming a real wavefunction $\psi(z)$, the 1D MGPE reads

$$-rac{1}{2} \psi'' + \gamma_0 \psi^2 + \frac{1}{2} \gamma_2 (\psi^2)'' \phi = \mu \phi . \quad (17)$$

If $\gamma_0 > 0$ and $\gamma_2 < 1/2$ this equation admits exact dark soliton solutions $\phi(z)$, with boundary conditions

$$\phi(0) = 0 \quad \text{and} \quad \phi(\pm \infty) = \pm \phi_\infty , \quad (18)$$

given implicitly by\(^7\)

$$\int_0^{\phi(z)^2} \frac{\sqrt{1 - 2 \gamma_2 \xi}}{\sqrt{\xi |\phi_\infty^2 - \xi|}} \, d\xi = 2 \sqrt{\gamma_0} z \quad (19)$$

Setting $\gamma_2 = 0$ one recovers the familiar result

$$\phi(z) = \phi_\infty \tanh (\sqrt{\gamma} \phi_\infty z) . \quad (20)$$

Dark solitons of the 1D MGPE with $\gamma_0 = 1$ and three values of the finite-range strength $\gamma_2$. In the plots we set $\phi_\infty = 1$. 
If $\gamma_0 < 0$ and $\gamma_2 < 1/2$ the 1D MGPE admits exact bright soliton solutions $\phi(z)$, with boundary conditions

$$\phi(0) = \phi_0 \quad \text{and} \quad \phi(\pm \infty) = 0,$$

(21)
given implicitly by

$$\int_{\phi(z)^2}^{\phi_0^2} \frac{\sqrt{1 - 2\gamma_2 \xi}}{\xi \sqrt{\phi_0^2 - \xi}} \, d\xi = 2 \sqrt{|\gamma_0|} \, z$$

(22)

Setting $\gamma_2 = 0$ one recovers the familiar result

$$\phi(z) = \phi_0 \text{sech} \left( \sqrt{|\gamma_0|} \phi_0 \, z \right).$$

(23)

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Bright solitons of the 1D MGPE with $\gamma_0 = -1$ and three values of the finite-range strength $\gamma_2$. In the plots we set $\psi_0 = 1$. 

$$\gamma_0 = -1$$
Vortices with the 3D MGPE (I)

Vortex solutions of the MGPE can be found in 3D by considering $U(r) = 0$ and cylindric symmetry, i.e.

$$
\left[ -\frac{\hbar^2}{2m} \nabla^2 + (N - 1)g_0|\psi(\rho, \theta)|^2 + g_2(N - 1)\nabla^2|\psi(\rho, \theta)|^2 \right] \psi(\rho, \theta) = \mu \psi(\rho, \theta),
$$

(24)

setting

$$
\psi(\rho, \theta) = \phi(\rho) e^{ik\theta},
$$

(25)

with $\rho$ cylindric radial coordinate, $\theta$ cylindric angular coordinate, and $k$ quantum number of circulation. Then one finds

$$
\left[ -\frac{\hbar^2}{2m} \nabla^2_{\rho} + \frac{\hbar^2 k^2}{2m\rho^2} + (N - 1)g_0\phi(\rho)^2 + (N - 1)g_2 \nabla^2_{\rho}\phi(\rho)^2 \right] \phi(\rho) = \mu \phi(\rho),
$$

(26)

where

$$
\nabla^2_{\rho} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right).
$$

(27)
Imposing the boundary condition

\[ \phi(+\infty) = \phi_\infty \]

which gives

\[ \mu = \gamma_0 (N - 1) \phi_\infty^2 \quad (28) \]

and introducing the adimensional variable

\[ x = \frac{\rho}{\xi} \quad \text{with} \quad \xi = \sqrt{\frac{\hbar^2}{2 m \mu}} \quad (29) \]

and wavefunction

\[ f(x) = \frac{\phi(\rho = \xi x)}{\phi_\infty}, \quad (30) \]

the 1D MGPE becomes

\[ \left[ -\nabla_x^2 + \frac{k^2}{x^2} + f(x)^2 + r \nabla_x^2 f(x)^2 \right] f(x) = f(x) \quad (31) \]

with \( s = g_2/(\xi^2 g_0) \).
Quantized vortices of the 1D MGPE with $\gamma_0 > 0$ and three values of the finite-range parameter $s = g_2/(\xi^2 g_0)$. In the plots we set the quantum number $k = 1$. 
Conclusions

- We have derived a modified Gross-Pitaevskii equation (MGPE) from the Hartree equation.
- Our MGPE takes into account finite-range effects.
- MGPE admits dark solitons, bright solitons and quantized vortices which generalize the familiar ones of GPE.
- Finite-range effects can be measured with Bose-Einstein condensates by increasing the density, i.e. by reducing the average distance between bosons.
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