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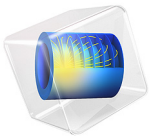


Gross–Pitaevskii Equation for Bose–Einstein Condensation

This tutorial model solves the Gross–Pitaevskii Equation for the ground state of a Bose–Einstein condensate in a harmonic trap, using the Schrödinger Equation physics interface in the Semiconductor Module. The equation is essentially a nonlinear single-particle Schrödinger Equation, with a potential energy contribution proportional to the local particle density. The eigenvalue study is not suitable for solving this kind of nonlinear eigenvalue problems. Instead, a stationary study is used with a global equation enforcing the normalization of the wave function to solve for the ground state solution. The result for a large number of particles compares well with the Thomas–Fermi approximation as expected.

Introduction

The Gross–Pitaevskii equation was first developed to analyze the vortex lines in superfluids in the 60s (Ref. 1 and Ref. 2). It describes the system of a collection of identical bosons, and takes on the form of a nonlinear single-particle Schrödinger equation:

$$-\hbar^2\nabla\cdot\left(\frac{\nabla\psi(\mathbf{r})}{2m}\right)+V(\mathbf{r})\psi(\mathbf{r})+NU_0|\psi(\mathbf{r})|^2\psi(\mathbf{r})=E\psi(\mathbf{r}) \quad (1)$$

where $V(\mathbf{r})$ is an external potential, N is the number of bosons in the system, and U_0 is the interaction strength.

For this model, we assume a Bose–Einstein condensate of ^{87}Rb atoms trapped in an axisymmetric harmonic potential:

$$V(\mathbf{r})=\frac{1}{2}m\omega_0^2(3r^2+z^2)$$

The interaction strength is given by

$$U_0=\frac{4\pi\hbar^2 a_s}{m}$$

where a_s is the s-wave scattering length.

The ground state wave function and eigenenergy are solved for a condensate with one million atoms. The result compares well with the Thomas–Fermi approximation as expected.

Model Definition

The parameters used in the model are atomic mass $m = 1.443 \cdot 10^{-25}$ kg, trap angular frequency $\omega_0 = 2\pi \cdot 10$ rad/s, and scattering length $a_s = 5.2$ nm. The equation is easily set up using the Schrödinger Equation interface.

Because the nonlinear interaction term involves the unknown wave function, this equation cannot be solved using the eigenvalue study. The problem is solved in two studies. In the first eigenvalue study, the ground state solution of noninteracting bosons in the harmonic trap is computed. In the second study, the nonlinear interaction term is added, so is a global equation enforcing the normalization of the wave function. The combined equations are solved in a stationary solver, using the solution from the first study as the initial condition.

Results and Discussion

Figure 1 summarizes the result for the ground state Bose–Einstein condensate with one million atoms: the total potential energy is shown in gray, and the real part of the wave function is shown in color (the imaginary part is zero for a bound state).

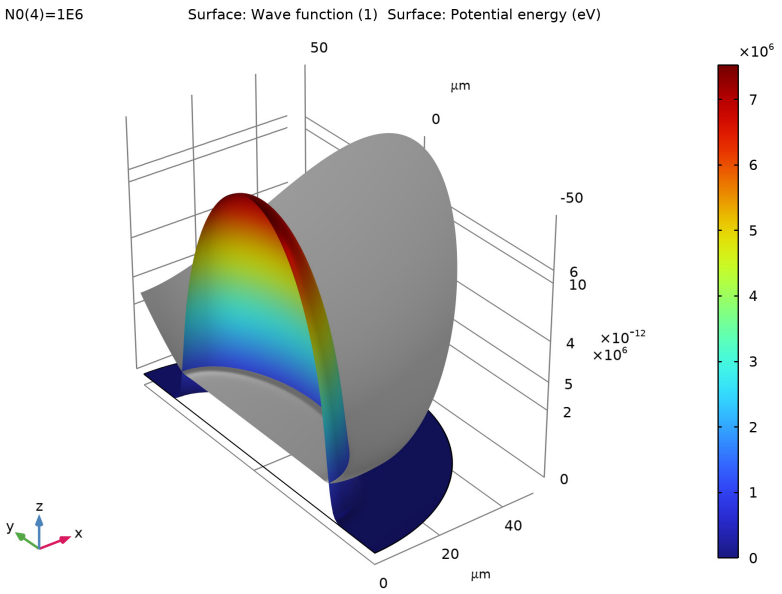


Figure 1: Summary plot for the ground state solution.

The ground state solution can be compared with the Thomas–Fermi approximation, where the kinetic energy term in the nonlinear Schrödinger equation is neglected and the particle density profile takes on the shape of the trapping potential (upside down) by a simple algebraic solution of the remaining equation. The figure below compare the computed density with the result from the Thomas–Fermi approximation in the axial and radial directions.

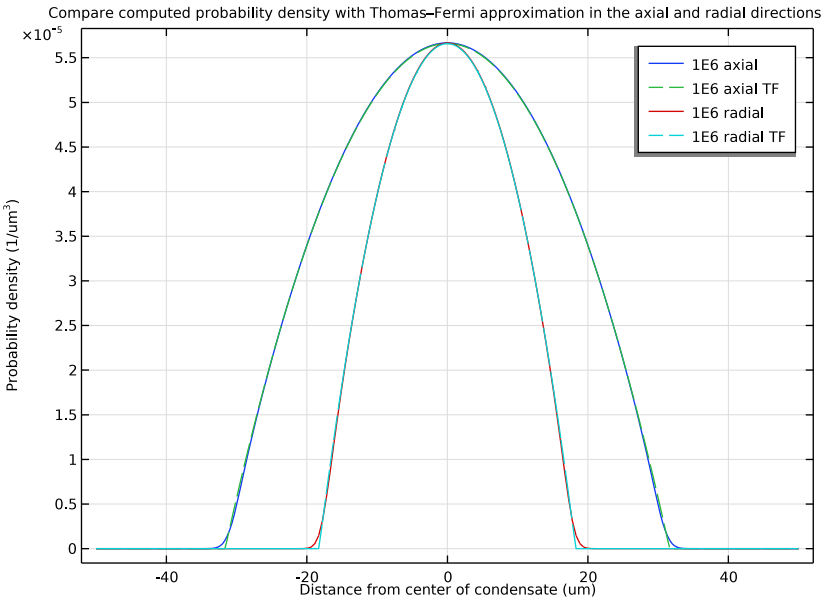


Figure 2: Comparison of computed density with Thomas–Fermi approximation in the axial and radial directions.

References

1. E.P. Gross, "Structure of a quantized vortex in boson systems", *Il Nuovo Cimento*, vol. 20, no. 3, pp 454–457, 1961. doi:10.1007/BF02731494.

2. L.P. Pitaevskii, "Vortex lines in an imperfect Bose gas", *Sov. Phys. JETP*, vol. 13, no. 2, pp 451–454, 1961.

Application Library path: `Semiconductor_Module/Quantum_Systems/gross_pitaevskii_equation_for_bose_einstein_condensation`

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Semiconductor>Schrödinger Equation (schr)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Eigenvalue**.

6 Click **Done**.

GEOMETRY 1

The Model Wizard ended at the **Settings** pane for the **Geometry** node in the Model Builder tree structure. We can use this opportunity to select a convenient length unit.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **µm**.

Enter the parameters for the trap and the Rb-87 condensate.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
w0	2*pi*10[Hz]	62.832 Hz	Trap frequency
ma	86.909[g/mol]/ N_A_const	1.4432E-25 kg	Atomic mass of Rb-87
as	5.2[nm]	5.2E-9 m	Scattering length
U0	4*pi*hbar_const^2* as/ma	5.0356E-51 J·m³	Interaction strength

Name	Expression	Value	Description
N0	1	1	Number of atoms
wr	w0*sqrt(3)	108.83 Hz	Transverse trap frequency
Rr0	(15*U0*w0*N0/(4*pi*ma*wr^3))^0.2	1.1522E-6 m	Transverse T-F size
Rz0	(15*U0*wr^2*N0/(4*pi*ma*w0^4))^0.2	1.9956E-6 m	Longitudinal T-F size
rho0	15*N0/(8*pi*Rr0^2*Rz0)	2.2529E17 1/m³	T-F peak density

Create a half circle for the modeling domain.

GEOMETRY 1

Circle 1 (c1)

1 In the **Geometry** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

3 In the **Radius** text field, type 50.

4 In the **Sector angle** text field, type 180.

5 Locate the **Rotation Angle** section. In the **Rotation** text field, type -90.

6 Click **Build All Objects**.

Set a convenient energy unit for the eigenenergy.

SCHRÖDINGER EQUATION (SCHR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Schrödinger Equation (schr)**.

2 In the **Settings** window for **Schrödinger Equation**, locate the **Model Properties** section.

3 Find the **Eigenvalue study** subsection. In the λ_{scale} text field, type 1[nK]*k_B_const.

Enter the atomic mass and the trap potential energy.

Atomic Mass

1 In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation (schr)** click **Effective Mass 1**.

2 In the **Settings** window for **Effective Mass**, type Atomic Mass in the **Label** text field.

3 Locate the **Effective Mass** section. In the $\mathbf{m}_{\mathrm{eff,e,11}}$ text field, type ma.

Trap Potential Energy

1 In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation (schr)** click **Electron Potential Energy 1**.

2 In the **Settings** window for **Electron Potential Energy**, type `Trap Potential Energy` in the **Label** text field.

3 Locate the **Electron Potential Energy** section. From the V_e list, choose **User defined**. In the associated text field, type `0.5*ma*w0^2*(3*r^2+z^2)`.

A tighter trap potential is entered in the radial direction than the axial direction, which will result in an elongated condensate.

Create an appropriate mesh.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extra fine**.

4 Click **Build All**.

We will use the ground state solution of the noninteracting particle as the initial condition for the nonlinear eigenvalue problem posed by the Gross–Pitaevskii equation.

STUDY 1: EIGENVALUE FOR INITIAL CONDITION

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1: Eigenvalue for Initial Condition` in the **Label** text field.

Step 1: Eigenvalue

1 In the **Model Builder** window, under **Study 1: Eigenvalue for Initial Condition** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.

3 In the **Desired number of eigenvalues** text field, type `1`.

4 In the **Home** toolbar, click **Compute**.

Now we can add the nonlinear interaction term.

Trap Potential Energy

In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation (schr)** right-click **Trap Potential Energy** and choose **Duplicate**.

Interaction Energy

1 In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation (schr)** click **Trap Potential Energy 1**.

2 In the **Settings** window for **Electron Potential Energy**, type `Interaction Energy` in the **Label** text field.

3 Locate the **Electron Potential Energy** section. In the V_e text field, type `N0*U0*schr.Pr`.

The **Electron Potential Energy** feature is accumulative, so this term will be added to the **Trap Potential Energy** term above in the final equation to be solved.

Set up a global equation enforcing the normalization of the single-particle wave function to enable the stationary study to solve for the nonlinear eigenvalue problem.

4 Click the **Show More Options** button in the **Model Builder** toolbar.

5 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Equation-Based Contributions**.

6 Click **OK**.

Global Equations 1 (ODE1)

1 In the **Physics** toolbar, click **Global** and choose **Global Equations**.

2 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.

3 In the table, enter the following settings:

Name	f(u,ut,utt, t) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/s)	Description
E0	`(1-schr.int(2*pi*r*schr.Pr))`	1	0	

4 In the **Model Builder** window, click **Schrödinger Equation (schr)**.

5 In the **Settings** window for **Schrödinger Equation**, locate the **Model Properties** section.

6 Find the **Stationary study** subsection. In the *E* text field, type `E0*1[nK]*k_B_const`.

The global solution variable `E0` for the global equation takes on the value of the eigenenergy in units of nK.

Set up an initial condition node to inherit the solution from the noninteracting particle ground state.

Initial Values 1

In the **Model Builder** window, right-click **Initial Values 1** and choose **Duplicate**.

Initial Values 2

1 In the **Model Builder** window, click **Initial Values 2**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *psi* text field, type `schr.Psi`.

Now we can set up the stationary study to solve for the condensate.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Stationary

Click **Add Study** button again to close the window.

1 In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.

2 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

3 From the **Study** list, choose **Study 1: Eigenvalue for Initial Condition, Eigenvalue**.

Sweep the number of atoms from 1 to 1 million.

4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
N0 (Number of atoms)	`1 100 1e4 1e6`	

7 In the **Model Builder** window, click **Study 2**.

8 In the **Settings** window for **Study**, type `Study 2: Stationary for Condensate` in the **Label** text field.

9 In the **Home** toolbar, click **Compute**.

The default plot shows the ground state wave function of the condensate with 1 million atoms.

We can compare this result with the Thomas–Fermi approximation.

RESULTS

Compare with Thomas–Fermi Approximation

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Compare with Thomas-Fermi Approximation` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Stationary for Condensate/ Solution 2 (sol2)**.

4 From the **Parameter selection (N0)** list, choose **Last**.

5 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Compare computed probability density with Thomas-Fermi approximation in the axial and radial directions`.

7 Locate the **Plot Settings** section.

8 Select the **x-axis label** check box. In the associated text field, type `Distance from center of condensate (um)`.

9 Select the **y-axis label** check box. In the associated text field, type `Probability density (1/um<sup>3</sup>)`.

Line Graph 1

1 Right-click **Compare with Thomas–Fermi Approximation** and choose **Line Graph**.

2 Select Boundaries 1 and 2 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `schr.Pr`.

5 In the **Unit** field, type `1/um^3`.

6 Select the **Description** check box. In the associated text field, type `axial`.

7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

8 In the **Expression** text field, type `z`.

9 Click to expand the **Legends** section. Select the **Show legends** check box.

10 Find the **Include** subsection. Select the **Description** check box.

11 Right-click **Line Graph 1** and choose **Duplicate**.

Line Graph 2

1 In the **Model Builder** window, click **Line Graph 2**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `max(0,1-z^2/Rz0^2)*rho0/N0`.

4 In the **Description** text field, type `axial TF`.

5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

The particle density profile along the z-axis matches well with the one from the Thomas–Fermi approximation.

To plot the profile along the r-axis, first create a dataset to extend to the negative direction.

Mirror 2D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 2D**.

2 In the **Settings** window for **Mirror 2D**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2: Stationary for Condensate/Solution 2 (sol2)**.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Data** section.

3 From the **Dataset** list, choose **Mirror 2D 1**.

4 Locate the **Line Data** section. Clear the **Bounded by points** check box.

Line Graph 1

In the **Model Builder** window, under **Results>Compare with Thomas–Fermi Approximation** right-click **Line Graph 1** and choose **Duplicate**.

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Parameter selection (N0)** list, choose **Last**.

5 Locate the **y-Axis Data** section. In the **Description** text field, type `radial`.

6 Locate the **x-Axis Data** section. In the **Expression** text field, type `cln1x`.

Line Graph 2

In the **Model Builder** window, right-click **Line Graph 2** and choose **Duplicate**.

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

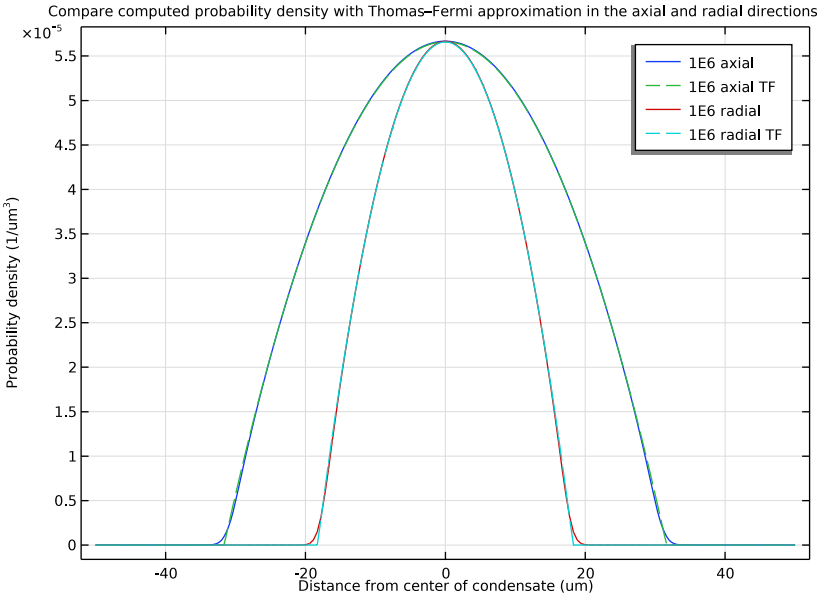
4 From the **Parameter selection (N0)** list, choose **Last**.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `max(0,1-r^2/RrO^2)*rhoO/NO`.

6 In the **Description** text field, type `radial TF`.

7 Locate the **x-Axis Data** section. In the **Expression** text field, type `cln1x`.

8 In the **Compare with Thomas–Fermi Approximation** toolbar, click **Plot**.



Create a composite plot to summarize the ground state wave function and the total potential.

Wave Function (schr)

In the **Model Builder** window, under **Results** right-click **Wave Function (schr)** and choose **Duplicate**.

Summary Plot

1 In the **Model Builder** window, under **Results** click **Wave Function (schr) 1**.

2 In the **Settings** window for **2D Plot Group**, type `Summary Plot` in the **Label** text field.

Imaginary Part

1 In the **Model Builder** window, expand the **Summary Plot** node.

2 Right-click **Imaginary Part** and choose **Delete**.

Surface 1

1 In the **Model Builder** window, expand the **Results>Potential Energy (schr) 1** node.

2 Right-click **Surface 1** and choose **Copy**.

Summary Plot

In the **Model Builder** window, under **Results** right-click **Summary Plot** and choose **Paste Surface**.

Surface 1

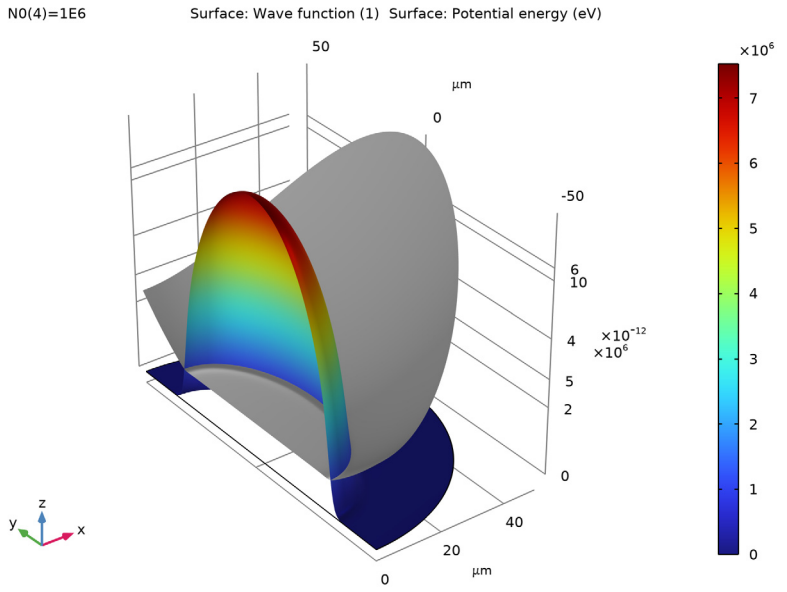
1 In the **Model Builder** window, click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Coloring** list, choose **Uniform**.

4 From the **Color** list, choose **Gray**.

5 In the **Summary Plot** toolbar, click **Plot**.



The flat bottom of the total potential is another indication of the agreement with the Thomas–Fermi approximation.

Finally, for Study 1 disable the additional nodes added for Study 2, so that in the future you can recompute Study 1 with its intended setup.

STUDY 1: EIGENVALUE FOR INITIAL CONDITION

Step 1: Eigenvalue

1 In the **Model Builder** window, under **Study 1: Eigenvalue for Initial Condition** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the tree, select **Component 1 (comp1)>Schrödinger Equation (schr)>Interaction Energy**.

5 Click **Disable**.

6 In the tree, select **Component 1 (comp1)>Schrödinger Equation (schr)> Global Equations 1 (ODE1)**.

7 Click **Disable**.

8 In the tree, select **Component 1 (comp1)>Schrödinger Equation (schr)>Initial Values 2**.

9 Click **Disable**.