



Vortex Lattice Formation in a Rotating Bose—Einstein Condensate

This tutorial model solves the Gross–Pitaevskii equation for the vortex lattice formation in a rotating Bose–Einstein condensate bound by a harmonic trap. The equation is essentially a nonlinear single-particle Schrödinger equation, with the interparticle interaction represented by a potential-energy contribution proportional to the local particle density. The time evolution in the rotating frame with phenomenological damping is configured with built-in features of the Schrödinger Equation physics interface. Nucleation of vortices is seen starting at the periphery of the condensate. Subsequently the system goes through a period of spectacular dynamical instability before settling down in the low-energy state of a vortex lattice. The Optimization Module is used for parameter estimation from the numerical results. The time scales of the initial oscillation and the eventual collapse of the ellipticity parameter agree well between simulation and the experimental data published by Madison and others.

Introduction

Madison and others published their experimental work in 2001 ([Ref. 1](#)) showing a series of striking images (Fig. 3 in the paper) that vividly demonstrated the nucleation and formation of a vortex lattice in a cloud of Bose–Einstein condensate atoms stirred by a rotating laser field. In the same figure they also plotted the time evolution of the ellipticity, showing an initial oscillation followed by a collapse of the ellipticity to near zero when the system goes through a period of dynamical instability before settling down in the low-energy state of a vortex lattice.

This model follows the theoretical approach of Tsubota and others ([Ref. 2](#)) to simulate this spectacular time evolution process by solving the Gross–Pitaevskii equation in the rotating frame with phenomenological damping ([Ref. 3](#)). Particular attention is paid to match the model parameters to the actual experimental conditions in [Ref. 1](#), thus achieving a better agreement of the time evolution of the ellipticity with the published data (see comments throughout the [Modeling Instructions](#) section for details).

Model Definition

The parameters used in the model are detailed in the [Modeling Instructions](#) section. The equation is easily set up using built-in features of the **Schrödinger Equation** interface. In particular, the **Rotating Frame** feature is used to follow the cloud in the rotating frame, and the **Dissipation** feature is used for the phenomenological damping, which is crucial for the system to relax into the low-energy state of a vortex lattice.

First the stationary state of the condensate is solved for using two studies in the same way as the related model example [Gross–Pitaevskii Equation for Bose–Einstein Condensation](#). This produces the initial condition for the subsequent transient study.

Following the approach of Tsubota and others ([Ref. 2](#)) for the time dependent study, a chemical potential term is added to the Gross–Pitaevskii equation, and a global equation is used to adjust the chemical potential so as to maintain a constant total number of atoms.

When the time-dependent solution has been obtained, an optimization study is used to analyze the result. At each time point, the computed particle density profile is fitted to the Thomas–Fermi approximation density profile in order to extract the ellipticity parameter to be compared with the experimental data.

Results and Discussion

[Figure 1](#) summarizes the result for the time evolution of the rotating Bose–Einstein condensate by showing the particle density as a function of time. After an initial period of oscillation/rotation of the condensate, its periphery starts to see vortices forming around 300 ms. A period of dynamical instability follows with vortices moving randomly. Eventually the system settles into the low-energy state of a vortex lattice.

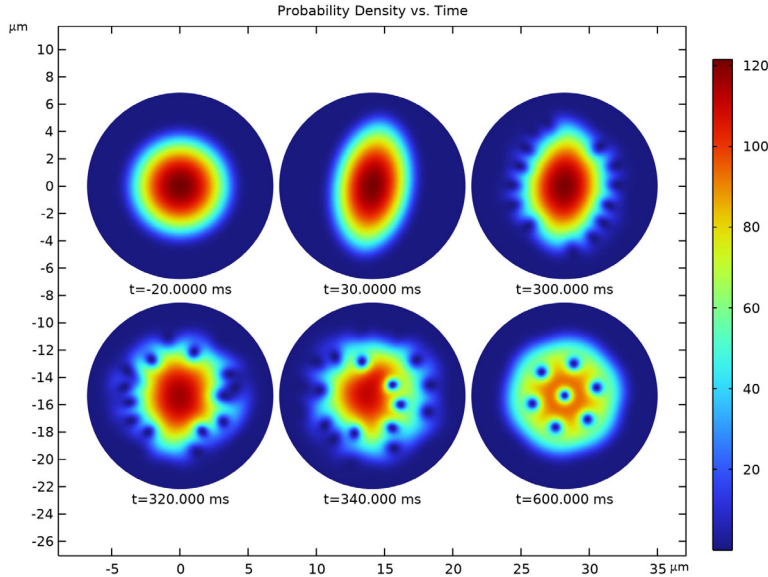


Figure 1: Time evolution of the particle density profile.

In addition to the figure, the model generates a mesmerizing movie of the time evolution of the particle density profile. Make sure to check it out!

Due to practical limitations on the optical imaging system in the experimental setup, it is not possible to obtain the images of the density profile as shown in [Figure 1](#) while the atoms are still being trapped. Instead, in the experiment, the atoms are released from the trap and the cloud is allowed to freely expand for a duration of 25 ms to a size of about 300 μm . The aspect ratio of the cloud also changes dramatically before and after the free expansion — an initial cigar shape becomes a final pancake shape, with the long and short dimensions swapped before and after the expansion. Keep this in mind when comparing the simulated in-trap density profile with the published images of the after-expansion atom cloud.

The stationary 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. [Figure 2](#) below compares the computed density with the result from the Thomas–Fermi approximation in the X direction.

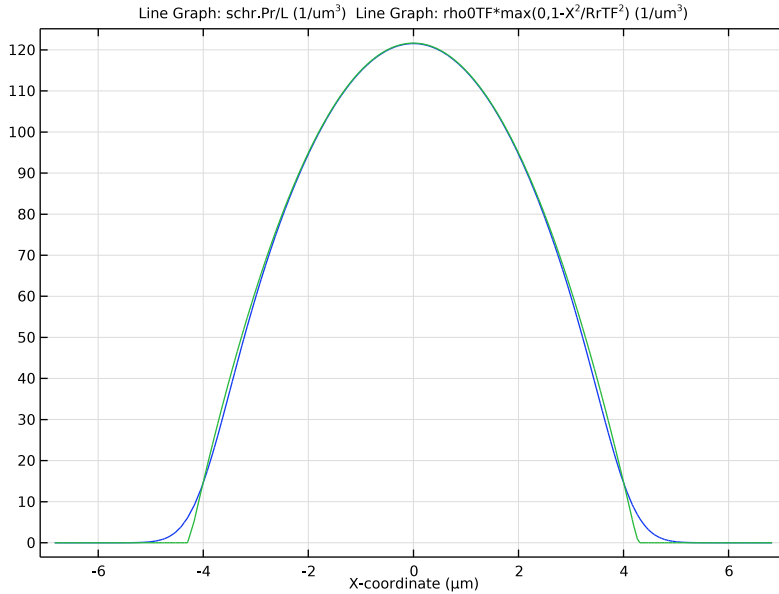


Figure 2: Comparison of computed density with Thomas–Fermi approximation in the X direction.

The time evolution process shown in Figure 1 can be distilled to a single ellipticity parameter, which is obtained by fitting the particle density profile to a simple function to extract the major and minor axes of the ellipse. For the simulated in-trap density profiles shown in Figure 1, the Thomas–Fermi approximation provides a good fit function. By fitting it to the simulated density profile at each time point, the ellipticity parameter can be computed as a function of time. Figure 3 shows the result. The time scales of the initial oscillation and the eventual collapse agree very well with the data shown in Fig. 3 of the experimental paper (Ref. 1). The magnitude is slightly different but this is understandable, given the possible shape change before and after the free expansion as discussed above.

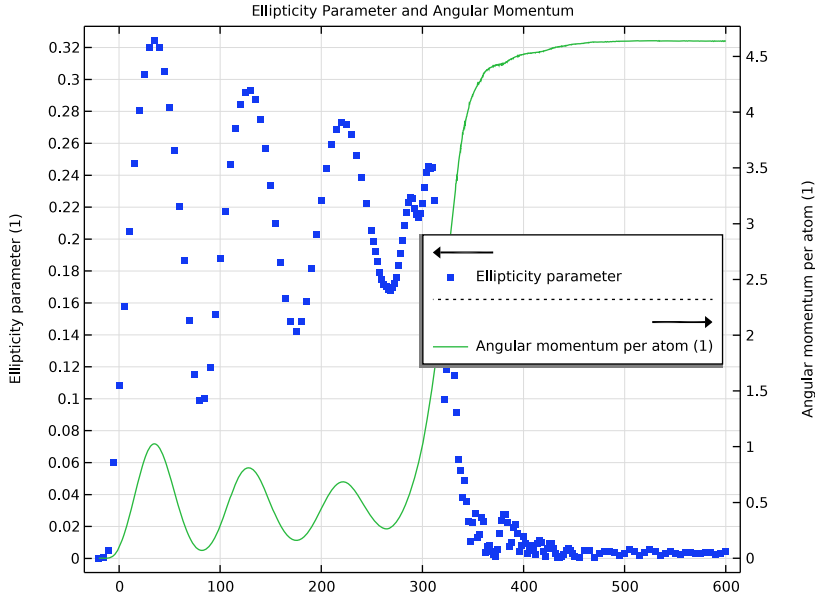


Figure 3: Ellipticity parameter and angular momentum per atom as functions of time.

Another important parameter that characterizes the transition from an oscillating/rotating full cloud to a vortex lattice is the angular momentum, which is also plotted in Figure 3. The general behavior of initial oscillation and eventual gaining of a certain angular momentum in proportional to the number of vortices is consistent with the simulation result by Tsubota and others (Fig. 3 in Ref. 2). However here the time scale of our result is much closer to the experimental data.

As mentioned before, the Optimization Module is used for the fitting. The quality of the fit can be checked by plotting the contours of the fit data (simulated density profile) and

the contours of the fit function (Thomas–Fermi density profile) together and comparing them, as shown in Figure 4.

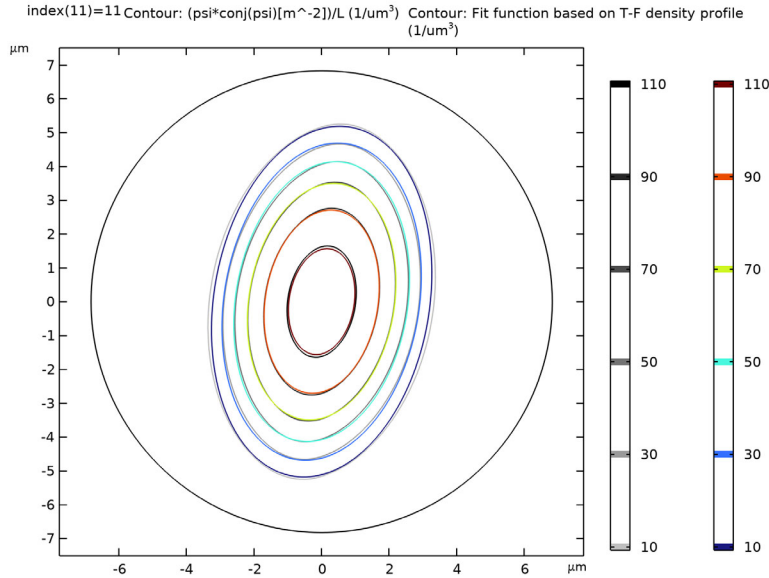


Figure 4: Fit data (simulated density profile; grayscale) and fit function (Thomas–Fermi density profile; color).

References


1. K.W. Madison, F. Chevy, V. Bretin, and J. Dalibard, “Stationary States of a Rotating Bose-Einstein Condensate: Routes to Vortex Nucleation,” *Phys. Rev. Lett.*, vol. 86, p. 4443, 2001.
2. M. Tsubota, K. Kasamatsu, and M. Ueda, “Vortex lattice formation in a rotating Bose-Einstein condensate,” *Phys. Rev. A*, vol. 65, p. 023603, 2002.
3. S. Choi, S.A. Morgan, and K. Burnett, “Phenomenological damping in trapped atomic Bose-Einstein condensates,” *Phys. Rev. A*, vol. 57, p. 4057, 1998.

Application Library path: Semiconductor_Module/Quantum_Systems/
vortex_lattice_formation_in_a_rotating_bose_einstein_condensate




Modeling Instructions

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

NEW

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

MODEL WIZARD

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


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 .

Define a step function to smoothly ramp up and down the ellipticity parameter ε for the time-dependent study.

GLOBAL DEFINITIONS

Step 1 (step1)

- 1 In the **Home** toolbar, click  **Functions** and choose **Global>Step**.
- 2 In the **Settings** window for **Step**, locate the **Parameters** section.
- 3 In the **Location** text field, type 0.5.
- 4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type 0.95.

Following the experimental paper [Ref. 1](#), enter the model parameters.

Parameters 1

- 1 In the **Model Builder** window, 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
a	5.5[nm]	5.5E-9 m	Scattering length
m	86.909[g/mol]/ N_A_const	1.4432E-25 kg	Atomic mass
g	4*pi*hbar_const^2* a/m	5.3261E-51 J·m³	Coupling constant

According to Bretin's thesis, the stirring laser field was turned on instantaneously, with the ellipticity parameter ε ramped up in 20 ms. Therefore in the model we can make the stirring laser field always on, and make the ellipticity parameter ε time dependent. To share the same formulas between time-dependent and stationary studies, define a time parameter using the same name t as the built-in time parameter for time-dependent studies. Then use the step function defined earlier to ramp up and down the ellipticity parameter ε , assuming the same ramp down time period of 20 ms. The formula is set up such that the ramp up starts at -20 ms and finishes at time $t=0$. The magnitude of ε is set to 0.032, which is based on the text in both the experimental paper and Bretin's thesis, even though the caption of Fig. 3 in the paper gave an inconsistent value of 0.025, which presumably is a typo.

4 In the table, enter the following settings:

Name	Expression	Value	Description
tau	20[ms]	0.02 s	Ramp duration
t	-tau	-0.02 s	Time parameter
t_off	300[ms]	0.3 s	Off time
epst	0.032*step1((t+tau)/ tau)*(1-step1((t- t_off)/tau))	0	Ellipticity parameter

It is not clear from the paper how exactly the semimajor and semiminor axes vary with the ellipticity parameter ε . However it seems reasonable to assume that the area of the ellipse remains constant during the ramp. Thus we obtain the following formulas for the ε_X and ε_Y parameters for the optical potential from the stirring laser field. The reference values of 0.03 and 0.09 are based on an earlier experimental paper by the same group as cited by the theoretical paper [Ref. 2](#).

5 In the table, enter the following settings:

Name	Expression	Value	Description
epsX	$(\text{epst} + \sqrt{0.03 \cdot 0.09 + \text{epst}^2 - 0.03 \cdot 0.09 \cdot \text{epst}^2}) / (1 - \text{epst})$	0.051962	Optical potential parameter
epsY	$(-\text{epst} + \sqrt{0.03 \cdot 0.09 + \text{epst}^2 - 0.03 \cdot 0.09 \cdot \text{epst}^2}) / (1 + \text{epst})$	0.051962	Optical potential parameter

With the ellipticity related parameters ε_X and ε_Y ready, we can now enter the trap parameters. The aspect ratio parameter λ is set to 9.2 as shown in the caption of Fig. 3 in the experimental paper. For the trap frequencies, ω_t is without the stirring laser field, while ω_X and ω_Y are with the laser on.

6 In the table, enter the following settings:

Name	Expression	Value	Description
wz	$2 \cdot \pi \cdot 11.8 [\text{Hz}]$	74.142 Hz	Longitudinal trap frequency
lambda	9.2	9.2	Trap aspect ratio
wt	$\text{lambda} \cdot \text{wz}$	682.1 Hz	Transverse trap frequency
wX2	$\text{wt}^2 \cdot (1 + \text{epsX})$	4.8944E5 1/s ²	Transverse trap frequency squared
wY2	$\text{wt}^2 \cdot (1 + \text{epsY})$	4.8944E5 1/s ²	Transverse trap frequency squared
wbar	$\text{wt} \cdot \sqrt{(1.03 + 1.09) / 2}$	702.27 Hz	Average transverse trap frequency

The stirring frequency Ω is scaled with the average transverse trap frequency $\bar{\omega}$ by a constant factor of 0.7 in the experiment. To keep Ω constant (independent of the time-varying ellipticity parameter ε), the average transverse trap frequency $\bar{\omega}$ has been fixed at a constant value using the reference values of 0.03 and 0.09 in the formula above, instead of using the time-varying ω_X and ω_Y as in the experimental paper which would have caused a slight change in Ω when ε is ramped up and down.

7 In the table, enter the following settings:

Name	Expression	Value	Description
Omega	$0.7 \cdot \omega_{\text{bar}}$	491.59 Hz	Stirring frequency

The ellipticity parameter α is expressed in terms of the stirring frequency and the condensate size parameters R_X and R_Y , which will be computed as fitting parameters to the time-dependent simulation result. For the initial stationary solution, we can compute the Thomas–Fermi values for comparison. The number of atoms in the condensate is chosen to be $1.5e5$, which is within the range of the experiment and fits best the number of vortices in the experiment.

8 In the table, enter the following settings:

Name	Expression	Value	Description
N	$1.5e5$	$1.5E5$	Number of atoms
RrTF	$(15 \cdot g \cdot \omega_z \cdot N / (4 \cdot \pi \cdot m \cdot \omega_{\text{bar}}^3))^{\wedge 0.2}$	$4.267E-6$ m	Transverse size of condensate (T-F)
RzTF	$(15 \cdot g \cdot \omega_{\text{bar}}^2 \cdot N / (4 \cdot \pi \cdot m \cdot \omega_z^4))^{\wedge 0.2}$	$4.0417E-5$ m	Longitudinal size of condensate (T-F)
rho0TF	$15 \cdot N / (8 \cdot \pi \cdot R_{\text{rTF}}^2 \cdot R_{\text{zTF}})$	$1.2165E20$ 1/m ³	Peak density of condensate (T-F)

The Thomas–Fermi approximation also helps to compute a reasonable out-of-plane thickness for the 2D model. If the criterion for the out-of-plane thickness is such that the peak density in the 2D model matches the Thomas–Fermi peak density in 3D, the following formula applies:

9 In the table, enter the following settings:

Name	Expression	Value	Description
L	$N / \rho_{\text{ho0TF}} / (\pi \cdot R_{\text{rTF}}^2 / 2)$	$4.3112E-5$ m	Out-of-plane thickness

Finally, to estimate the parameter γ for the phenomenological damping, the Thomas–Fermi approximation can also help. The formula below is based on the theoretical paper [Ref. 3](#) as cited by [Ref. 2](#). The experimental paper only gives a rough indication of the temperature of 100 nK, which will be used here.



10 In the table, enter the following settings:

Name	Expression	Value	Description
kT	k_B_const*100[nK]	1.3806E-30 J	Thermal energy
muTF	rho0TF*g	6.4795E-31 J	Chemical potential (T-F)
gamma	$4*m*(a*kT)^2/\pi/\hbar_{const}^3*\exp(2*\mu_{TF}/kT)*\mu_{TF}/kT*besselk(1,\mu_{TF}/kT)/wt$	0.028521 rad	Damping parameter
t_damp	$(1+gamma^2)/gamma/wt$	0.051444 s	Damping time scale
t_trap	$2*\pi*(1+gamma^2)/wt$	0.009219 s	Transverse trap time scale

Draw a circle for the modeling domain, using the condensate radius from the Thomas–Fermi approximation as a guide for the domain size.

GEOMETRY I

Circle I (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 $1.6*RrTF$.
- 4 Click  **Build All Objects**.

Set up the physics, first for the eigenvalue study for the ground state of noninteracting atoms, to be used as the initial condition of the subsequent stationary study. Use the transverse trap energy for the eigenvalue scale.

SCHRÖDINGER EQUATION (SCHR)

- 1 In the **Model Builder** window, under **Component I (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 $\hbar_{const}*wt$.

Enter the atomic mass, the trap potential energy, and the optical potential energy from the stirring laser field.


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 $m_{\text{eff},e,11}$ text field, type m .

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 $m*wt^2*(X^2+Y^2)/2$.

Optical Potential Energy

- 1 In the **Physics** toolbar, click  **Domains** and choose **Electron Potential Energy**.
- 2 In the **Settings** window for **Electron Potential Energy**, type Optical Potential Energy in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.
- 4 Locate the **Electron Potential Energy** section. From the V_e list, choose **User defined**. In the associated text field, type $m*wt^2*(\text{epsX}*X^2+\text{epsY}*Y^2)/2$.

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


Create a mesh with finer elements at the central part of the domain, using the condensate radius from the Thomas–Fermi approximation as a guide for the element size.

MESH 1

Size Expression 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Size Expression**.
- 2 In the **Settings** window for **Size Expression**, locate the **Element Size Expression** section.
- 3 In the **Size expression** text field, type $\text{if}(X^2+Y^2 < (\text{RrTF}*1.3)^2, \text{RrTF}/10, \text{RrTF}/7)$.

Free Triangular 1

- 1 In the **Mesh** toolbar, click  **Free Triangular**.
- 2 In the **Settings** window for **Free Triangular**, click to expand the **Tessellation** section.

3 From the **Method** list, choose **Delaunay**.

4 Click  **Build All**.

Set up and compute the eigenvalue study for the noninteracting particle ground state.

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.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

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 **Search for eigenvalues around shift** text field, type 1.

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

Now we can add the interaction term using the coupling constant g multiplied by the particle density. In this model we use the normalization convention that the probability density schr.Pr integrates to the total number of atoms N . Thus the number of atoms N does not appear in the formula. Since this is a 2D model, the probability density schr.Pr is divided by the out-of-plane thickness L to give the correct density in 3D.

SCHRÖDINGER EQUATION (SCHR)

Interaction Energy

1 In the **Physics** toolbar, click  **Domains** and choose **Electron Potential Energy**.

2 In the **Settings** window for **Electron Potential Energy**, locate the **Domain Selection** section.


3 From the **Selection** list, choose **All domains**.

4 Locate the **Electron Potential Energy** section. From the V_e list, choose **User defined**. In the associated text field, type $g \cdot \text{schr.Pr} / L$.


5 In the **Label** text field, type Interaction Energy.

In order for the stationary study to solve the nonlinear eigenvalue problem, we need to set up a global normalization equation for the wave function. First enable the equation-based options if you have not done so. Then set up a global equation to enforce the normalization that the probability density schr.Pr integrates to the total number of

atoms N by adjusting a unitless number E_0 . The number E_0 is then used to scale the total energy of the system with the Thomas–Fermi chemical potential μ_{TF} , which is a convenient constant to use with the appropriate magnitude to make E_0 close to unity for the global equation. The eigenenergy is found when E_0 is such that the global equation for normalization is satisfied.

- 6 Click the  **Show More Options** button in the **Model Builder** toolbar.
- 7 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Equation-Based Contributions**.
- 8 Click **OK**.

Global Equations - Normalization for Stationary Study

- 1 In the **Physics** toolbar, click  **Global** and choose **Global Equations**.
- 2 In the **Settings** window for **Global Equations**, type Global Equations - Normalization for Stationary Study in the **Label** text field.
- 3 Locate the **Global Equations** section. In the table, enter the following settings:

Name	$f(u, ut, utt, t)$ (I)	Initial value (u_0) (I)	Initial value (u_{t0}) (I/s)	Description
E_0	<code>schr.int(schr.Pr)/N-1</code>	0	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 $E_0 \cdot \mu_{TF}$.
Create a node group for the physics features that are only used in the Stationary study. Set up an initial condition node to inherit the normalized wave function `schr.Psi` of the noninteracting particle ground state from the eigenvalue study. Note that this has to be combined with the **Initial expression** option in the study settings as detailed below.
- 7 In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation (schr)** right-click **Global Equations - Normalization for Stationary Study (ODE1)** and choose **Group**.

Stationary Study

In the **Settings** window for **Group**, type Stationary Study in the **Label** text field.



Initial Values 2

- 1 In the **Physics** toolbar, click  **Domains** and choose **Initial Values**.
- 2 In the **Settings** window for **Initial Values**, locate the **Domain Selection** section.

- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Initial Values** section. In the *psi* text field, type `schr.Psi`.

Now we can set up a stationary study to solve for the condensate. Use the **Initial expression** option to enable the **Initial Values 2** node that we just configured. Use the **Auxiliary sweep** to ramp the number of atoms from 1 up to N.

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

- 1 In the **Settings** window for **Stationary**, click to expand the **Results While Solving** section.
- 2 From the **Probes** list, choose **None**.
- 3 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
- 4 From the **Study** list, choose **Study 1 - Eigenvalue for Initial Condition, Eigenvalue**.
- 5 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
- 6 Click **+ Add**.
- 7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
N (Number of atoms)	1 10 N	

- 8 In the **Model Builder** window, click **Study 2**.
- 9 In the **Settings** window for **Study**, type `Study 2 - Stationary for Condensate` in the **Label** text field.
- 10 Locate the **Study Settings** section. Clear the **Generate default plots** check box.
- 11 In the **Home** toolbar, click  **Compute**.


Plot the particle density profile along the X direction to compare with the Thomas–Fermi approximation. Again the probability density schr.Pr is divided by the out-of-plane thickness L to give the correct density in 3D to compare with the Thomas–Fermi result.

RESULTS

Cut Line 2D I

- 1 In the **Model Builder** window, expand the **Results** node.
- 2 Right-click **Results>Datasets** and choose **Cut Line 2D**.
- 3 In the **Settings** window for **Cut Line 2D**, locate the **Data** section.
- 4 From the **Dataset** list, choose **Study 2 - Stationary for Condensate/Solution 2 (sol2)**.
- 5 Locate the **Line Data** section. Clear the **Bounded by points** check box.

Stationary Profile - Compare with T-F Approx.

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Stationary Profile - Compare with T-F Approx. in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D I**.
- 4 From the **Parameter selection (N)** list, choose **Last**.

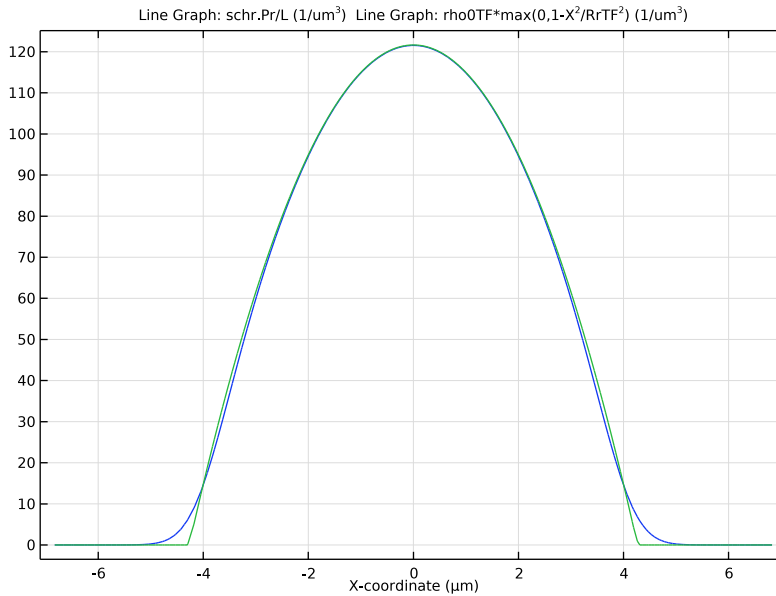
Numerical Solution

- 1 Right-click **Stationary Profile - Compare with T-F Approx.** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, type Numerical Solution in the **Label** text field.
- 3 Locate the **y-Axis Data** section. In the **Expression** text field, type $\text{schr.Pr}/L$.
- 4 In the **Unit** field, type $1/\mu\text{m}^3$.
- 5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 6 In the **Expression** text field, type X .
- 7 Right-click **Numerical Solution** and choose **Duplicate**.

T-F Approx.

- 1 In the **Model Builder** window, under **Results>Stationary Profile - Compare with T-F Approx.** click **Numerical Solution I**.
- 2 In the **Settings** window for **Line Graph**, type T-F Approx. in the **Label** text field.
- 3 Locate the **y-Axis Data** section. In the **Expression** text field, type $\rho_0 0TF \cdot \max(0, 1 - X^2/RrTF^2)$.


4 In the **Stationary Profile - Compare with T-F Approx.** toolbar, click  **Plot**.



With the stationary condensate solution ready, we can now set up the physics for time evolution under the influence of the stirring laser field. First add a **Rotating Frame** feature to solve the model in the rotating frame. Put it under a node group for the time-dependent study.

SCHRÖDINGER EQUATION (SCHR)

Rotating Frame I


- 1 In the **Physics** toolbar, click  **Domains** and choose **Rotating Frame**.
- 2 In the **Settings** window for **Rotating Frame**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Rotating Frame** section. In the Ω text field, type Omega.
- 5 Right-click **Rotating Frame I** and choose **Group**.

Transient Study

In the **Settings** window for **Group**, type Transient Study in the **Label** text field.


Add phenomenological damping, which is crucial for the system to relax into the low-energy state of vortex lattices.

Dissipation 1


- 1 In the **Physics** toolbar, click  **Domains** and choose **Dissipation**.
- 2 In the **Settings** window for **Dissipation**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Dissipation** section. In the γ text field, type gamma.

Following the theoretical paper by [Ref. 2](#), use a global equation to adjust the chemical potential in order to maintain the same number of condensate atoms N . As in the global equation for the Stationary study, here we also use a unitless number μ multiplied by the Thomas–Fermi energy μ_{TF} , with the latter having the appropriate magnitude such that the scale of μ is close to unity for the global equation. Use the solution for E_0 from the Stationary study as the initial condition for μ .

Chemical Potential

- 1 In the **Physics** toolbar, click  **Domains** and choose **Electron Potential Energy**.
- 2 In the **Settings** window for **Electron Potential Energy**, type Chemical Potential in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.
- 4 Locate the **Electron Potential Energy** section. From the V_e list, choose **User defined**. In the associated text field, type $-\mu \cdot \mu_{TF}$.


Global Equations 2 (ODE2)

- 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
μ	<code>schr.int(schr.Pr)/N-1</code>	<code>withsol('sol2',E0, setind(N, -1))</code>	0	

Finally set up the initial value to use the solution for the dependent variable ψ from the Stationary study. Note that this has to be combined with the **Initial expression** option in the study settings as detailed below.

Initial Values 3

- 1 In the **Physics** toolbar, click  **Domains** and choose **Initial Values**.
- 2 In the **Settings** window for **Initial Values**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Initial Values** section. In the ψ text field, type ψi .

Now set up a time-dependent study to simulate the transient behavior. To save time, choose a slightly loose relative tolerance. Disable the physics node group for the Stationary study. Use the **Initial expression** option to enable the **Initial Values 3** node that we just configured.

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>Time Dependent**.

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

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

STUDY 3

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 From the **Time unit** list, choose **ms**.

3 In the **Output times** text field, type `range(-tau,5[ms],250[ms]) range(252[ms],2[ms],450[ms]) range(455[ms],5[ms],600[ms])`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type $5e-4$.

6 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

7 In the tree, select **Component 1 (comp1)>Schrödinger Equation (schr)>Stationary Study**.

8 Click  **Disable**.

9 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

10 From the **Study** list, choose **Study 2 - Stationary for Condensate, Stationary**.


11 From the **Parameter value (N)** list, choose **Last**.

12 In the **Model Builder** window, click **Study 3**.

- 13** In the **Settings** window for **Study**, type Study 3 - Transient for Vortex Lattice Formation in the **Label** text field.

The system goes through a time period of dynamical instability before settling down to the low-energy vortex lattice state. The stochastic nature of this physical process leads to a significant variation in the simulated time history from run to run. To improve numerical convergence, some adjustments to the solver settings are made. Since the initial condition is a physical solution from the stationary study, consistent initialization can be turned off. It often helps to exclude algebraic states from the error control. The automatic Newton method with large number of iterations helps go through the unstable period when the nonlinearity is severe.

Solution 3 (sol3)

- 1** In the **Study** toolbar, click  **Show Default Solver**.
- 2** In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Time-Dependent Solver I**.
- 3** In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.
- 4** From the **Maximum step constraint** list, choose **Expression**.
- 5** In the **Maximum step** text field, type $t_{\text{trap}}/9$.
- 6** Find the **Algebraic variable settings** subsection. From the **Consistent initialization** list, choose **Off**.
- 7** From the **Error estimation** list, choose **Exclude algebraic**.
- 8** In the **Model Builder** window, expand the **Study 3 - Transient for Vortex Lattice Formation>Solver Configurations>Solution 3 (sol3)>Time-Dependent Solver I** node, then click **Fully Coupled I**.
- 9** In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.
- 10** From the **Nonlinear method** list, choose **Automatic (Newton)**.
- 11** In the **Maximum number of iterations** text field, type 100.

Create a global variable probe to monitor the time evolution of the angular momentum per atom during the solution process.


DEFINITIONS

Global Variable Probe I - Lz

- 1** In the **Definitions** toolbar, click  **Probes** and choose **Global Variable Probe**.

- 2 In the **Settings** window for **Global Variable Probe**, type Global Variable Probe 1 - Lz in the **Label** text field.
- 3 In the **Variable name** text field, type Lz_probe.
- 4 Locate the **Expression** section. In the **Expression** text field, type $\text{schr.L_avZ}/\text{hbar_const}/N$.
- 5 Select the **Description** check box. In the associated text field, type Angular momentum per atom.

STUDY 3 - TRANSIENT FOR VORTEX LATTICE FORMATION

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

Modify the color scheme of the default plot for the particle density to compare with Fig. 3 of Ref. 1 and Fig. 1 of the theoretical paper Ref. 2.

RESULTS


Wave Function (schr)

In the **Model Builder** window, expand the **Results>Wave Function (schr)** node.

Height Expression 1



- 1 In the **Model Builder** window, expand the **Results>Wave Function (schr)>Real Part** node.
- 2 Right-click **Height Expression 1** and choose **Disable**.

Real Part

- 1 In the **Model Builder** window, click **Real Part**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 Click  **Change Color Table**.
- 4 In the **Color Table** dialog box, select **Linear>GrayScale** in the tree.
- 5 Click **OK**.

Make a movie to savor the rich transitions shown in the time evolution of the particle density profile.


Animation 1

- 1 In the **Results** toolbar, click  **Animation** and choose **Player**.
- 2 In the **Settings** window for **Animation**, locate the **Scene** section.
- 3 From the **Subject** list, choose **Wave Function (schr)**.
- 4 Locate the **Frames** section. From the **Frame selection** list, choose **All**.
- 5 Click the  **Play** button in the **Graphics** toolbar.

Next we use the optimization functionality to compute the ellipticity parameter α and compare with the experimental paper. Define the fitting parameters and an index parameter to point to each time step of the time-dependent solution. Define the final output of the ellipticity parameter $|\tilde{\alpha}|$ as a function of the fit major and minor axes according to the experimental paper.

GLOBAL DEFINITIONS

Parameters 2 - Optimization


- 1 In the **Home** toolbar, click  **Parameters** and choose **Add>Parameters**.
- 2 In the **Settings** window for **Parameters**, type Parameters 2 - Optimization in the **Label** text field.
- 3 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
index	1	1	Solution index
RXfit	RrTF	4.267E-6 m	First major/minor axis to fit
RYfit	RrTF	4.267E-6 m	Second major/minor axis to fit
thetafit	0[rad]	0 rad	Tilt angle to fit
rho0fit	rho0TF	1.2165E20 1/m ³	Peak density to fit
alphafit	abs(Omega*(RXfit^2-RYfit^2)/(RXfit^2+RYfit^2)/wbar)	0	Ellipticity parameter

Use the Thomas–Fermi density profile as the fit function, and define a variable for the difference between the computed data and the fit function to serve as the objective to be minimized by the optimization study. Define an average operator to average the difference over the simulation domain. Scale the difference by the Thomas–Fermi peak density so that the magnitude of the objective does not become too large for the optimizer to handle.

DEFINITIONS

Average I (aveopI)

- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Average**.
- 2 In the **Settings** window for **Average**, locate the **Source Selection** section.
- 3 From the **Selection** list, choose **All domains**.



Variables I

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 In the table, enter the following settings:

Name	Expression	Unit	Description
fit_fn	$\max(0, 1 - (\cos(\text{thetafit}) * X + \sin(\text{thetafit}) * Y)^2 / R_{X\text{fit}}^2 - (\cos(\text{thetafit}) * Y - \sin(\text{thetafit}) * X)^2 / R_{Y\text{fit}}^2) * \rho_{0\text{fit}}$	l/m ³	Fit function based on T-F density profile
residual	$\text{realdot}(\psi, \psi) [m^{-2}] / L - \text{fit_fn}$	l/m ³	Difference between fit function and computed data
q0	$\text{aveop1}(\text{realdot}(\text{residual}, \text{residual}) / \rho_{0TF}^2)$		Objective - scaled and averaged difference between fit function and computed data

Now set up the Optimization study to fit the computed density profiles at each time point, using Parametric Sweep and the index parameter to pick out the solution at each time step. Use a dummy Stationary study step to pick out the solution by setting up the **Values of variables not solved for** section.

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 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Schrödinger Equation (schr)**.
- 5 Click **Add Study** in the window toolbar.
- 6 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 4

Step 1: Stationary

- 1 In the **Settings** window for **Stationary**, locate the **Values of Dependent Variables** section.
- 2 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.
- 3 From the **Method** list, choose **Solution**.
- 4 From the **Study** list, choose **Study 3 - Transient for Vortex Lattice Formation, Time Dependent**.
- 5 From the **Time (ms)** list, choose **Manual**.
- 6 In the **Index** text field, type index.
- 7 In the **Model Builder** window, click **Study 4**.
- 8 In the **Settings** window for **Study**, type Study 4 - Optimization for Parameter Estimation in the **Label** text field.

Parametric Sweep

- 1 In the **Study** toolbar, click  **Parametric Sweep**.
- 2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
- 3 Click  **Add**.
- 4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
index (Solution index)	range (1 , 185)	

- 5 In the table, click to select the cell at row number 1 and column number 3.



Use the variable and parameters defined earlier to set up the objective and the fitting parameters for the optimization study step. The objective variable is already scaled appropriately by its definition. For the fitting parameters, use the Thomas–Fermi approximation values to provide good initial guesses and scales. Turn off the angular momentum probe.

STUDY 3 - TRANSIENT FOR VORTEX LATTICE FORMATION

In the **Model Builder** window, collapse the **Study 3 - Transient for Vortex Lattice Formation** node.

STUDY 4 - OPTIMIZATION FOR PARAMETER ESTIMATION

Optimization

- 1 In the **Study** toolbar, click  **Optimization** and choose **Optimization**.
- 2 In the **Settings** window for **Optimization**, locate the **Optimization Solver** section.
- 3 From the **Method** list, choose **IPOPT**.
- 4 Click **Add Expression** in the upper-right corner of the **Objective Function** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>comp1.q0 - Objective - scaled and averaged difference between fit function and computed data - 1**.
- 5 Locate the **Control Variables and Parameters** section. Click  **Add** four times.
- 6 In the table, enter the following settings:

Parameter name	Initial value	Scale	Lower bound	Upper bound
RXfit (First major/minor axis to fit)	RrTF	RrTF	RrTF/4	RrTF*4
RYfit (Second major/minor axis to fit)	RrTF	RrTF	RrTF/4	RrTF*4
thetafit (Tilt angle to fit)	0 [rad]	pi	-pi	pi
rho0fit (Peak density to fit)	rho0TF	rho0TF	rho0TF/8	rho0TF*3


- 7 Locate the **Output While Solving** section. From the **Probes** list, choose **None**.

- 8 In the **Study** toolbar, click  **Compute**.

Make a plot of the final output of the ellipticity parameter $|\tilde{\alpha}|$ to compare with Fig. 3 in the experimental paper. For the horizontal axis, use the `withsol` operator to pick out the time point from the transient solution. The time scale of the initial oscillation of $|\tilde{\alpha}|$ compares well with the experimental data. Due to the stochastic nature of the physical process, the time scale of the collapse of $|\tilde{\alpha}|$ can vary, both physically and numerically. Nevertheless the match between simulation and experiment in this case is reasonably good.

RESULTS

Ellipticity Parameter and Angular Momentum


- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Ellipticity Parameter and Angular Momentum in the **Label** text field.

- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 4 - Optimization for Parameter Estimation/Parametric Solutions 1 (sol5)**.
- 4 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Global 1

- 1 Right-click **Ellipticity Parameter and Angular Momentum** and choose **Global**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
alphafit	1	Ellipticity parameter

- 4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 5 In the **Expression** text field, type `withsol('sol3',t,setind(t,index))`.
- 6 From the **Unit** list, choose **ms**.
- 7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.
- 8 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.
- 9 In the **Ellipticity Parameter and Angular Momentum** toolbar, click  **Plot**.

Add the plot of angular momentum to compare with Fig. 3 in the theoretical paper [Ref. 2](#). The general trend agrees well: an initial oscillation followed by the buildup of an angular momentum plateau corresponding to the formation process of the vortex lattice. The time scales in this model agree better with the experiment, because the choice of simulation parameters is more consistent with the experimental condition.

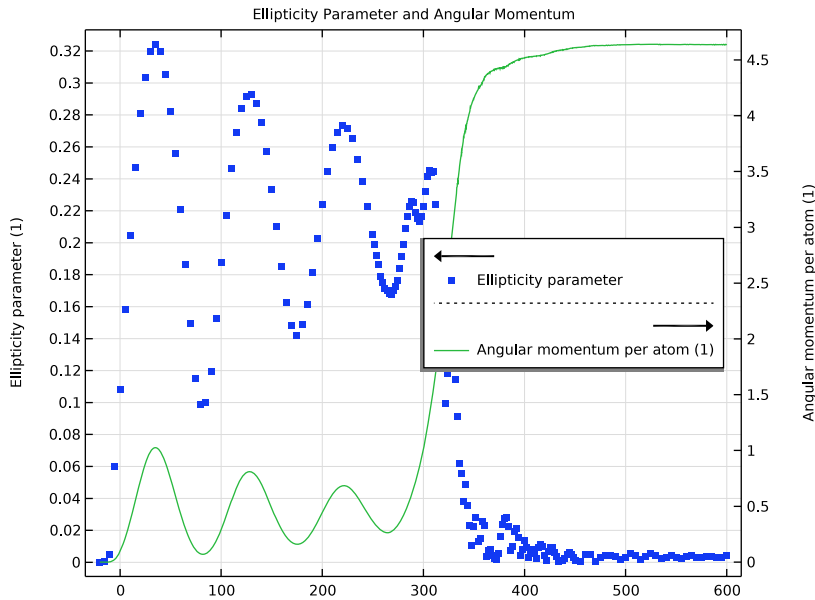
Probe Table Graph 1

- 1 In the **Model Builder** window, expand the **Results>Probe Plot Group 2** node.
- 2 Right-click **Probe Table Graph 1** and choose **Copy**.

Ellipticity Parameter and Angular Momentum

- 1 In the **Model Builder** window, under **Results** right-click **Ellipticity Parameter and Angular Momentum** and choose **Paste Table Graph**.
- 2 In the **Model Builder** window, click **Ellipticity Parameter and Angular Momentum**.
- 3 In the **Settings** window for **ID Plot Group**, click to expand the **Title** section.
- 4 From the **Title type** list, choose **Label**.
- 5 Locate the **Plot Settings** section. Select the **Two y-axes** check box.
- 6 In the table, select the **Plot on secondary y-axis** check box for **Probe Table Graph 1**.

7 In the **Ellipticity Parameter and Angular Momentum** toolbar, click  **Plot**.



Create a combo plot to show the time evolution of the particle density profile. Due to the stochastic nature of the physical process, the simulation result may vary from run to run.

Probability Density (schr)

In the **Model Builder** window, right-click **Probability Density (schr)** and choose **Duplicate**.

Probability Density vs. Time

- 1 In the **Model Builder** window, under **Results** click **Probability Density (schr) I**.
- 2 In the **Settings** window for **2D Plot Group**, type Probability Density vs. Time in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **None**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Label**.
- 5 In the **Model Builder** window, expand the **Probability Density vs. Time** node.

Height Expression I

- 1 In the **Model Builder** window, expand the **Results>Probability Density vs. Time>Surface I** node.
- 2 Right-click **Height Expression I** and choose **Delete**.

Surface 1

- 1 In the **Model Builder** window, under **Results>Probability Density vs. Time** click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 3 - Transient for Vortex Lattice Formation/ Solution 3 (sol3)**.
- 4 From the **Time (ms)** list, choose **-20**.
- 5 Locate the **Expression** section. In the **Expression** text field, type schr.Pr/L .
- 6 In the **Unit** field, type $1/\mu\text{m}^3$.

Annotation 1

- 1 In the **Model Builder** window, right-click **Probability Density vs. Time** and choose **Annotation**.
- 2 In the **Settings** window for **Annotation**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 3 - Transient for Vortex Lattice Formation/ Solution 3 (sol3)**.
- 4 From the **Time (ms)** list, choose **-20**.
- 5 Locate the **Annotation** section. In the **Text** text field, type $t=\text{eval}(t,\text{ms}) \text{ ms}$.
- 6 Locate the **Position** section. In the **Y** text field, type $-1.59 \cdot R_{\text{TF}}$.
- 7 Locate the **Coloring and Style** section. Clear the **Show point** check box.
- 8 From the **Anchor point** list, choose **Upper middle**.

Surface 1

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

Surface 2

- 1 In the **Model Builder** window, click **Surface 2**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **30**.
- 4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

Deformation 1

- 1 Right-click **Surface 2** and choose **Deformation**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **X-component** text field, type $3.3 \cdot R_{\text{TF}}$.
- 4 In the **Y-component** text field, type 0.
- 5 Locate the **Scale** section.

- 6 Select the **Scale factor** check box. In the associated text field, type 1.

Annotation 1

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Annotation 1** and choose **Duplicate**.

Annotation 2

- 1 In the **Model Builder** window, click **Annotation 2**.
- 2 In the **Settings** window for **Annotation**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **30**.

Deformation 1

In the **Model Builder** window, under **Results>Probability Density vs. Time>Surface 2** right-click **Deformation 1** and choose **Copy**.

Annotation 2

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Annotation 2** and choose **Paste Deformation**.

Surface 2

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

Surface 3

- 1 In the **Model Builder** window, click **Surface 3**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **300**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Surface 3** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **X-component** text field, type $6.6 \cdot R \cdot T F$.

Annotation 2

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Annotation 2** and choose **Duplicate**.

Annotation 3

- 1 In the **Model Builder** window, click **Annotation 3**.
- 2 In the **Settings** window for **Annotation**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **300**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Annotation 3** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **X-component** text field, type $6.6 \cdot R \cdot T F$.

Surface 3

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Surface 3** and choose **Duplicate**.

Surface 4

- 1 In the **Model Builder** window, click **Surface 4**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **320**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Surface 4** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **X-component** text field, type 0.
- 4 In the **Y-component** text field, type $-3.6 \cdot R \cdot T F$.

Annotation 3

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Annotation 3** and choose **Duplicate**.

Annotation 4

- 1 In the **Model Builder** window, click **Annotation 4**.
- 2 In the **Settings** window for **Annotation**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **320**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Annotation 4** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **X-component** text field, type 0.
- 4 In the **Y-component** text field, type $-3.6 \cdot R \cdot T F$.

Surface 2

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Surface 2** and choose **Duplicate**.

Surface 5

- 1 In the **Model Builder** window, click **Surface 5**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **340**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Surface 5** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **Y-component** text field, type $-3.6 \cdot R \cdot T F$.

Annotation 2

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Annotation 2** and choose **Duplicate**.

Annotation 5

- 1 In the **Model Builder** window, click **Annotation 5**.
- 2 In the **Settings** window for **Annotation**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **340**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Annotation 5** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **Y-component** text field, type $-3.6 \cdot R \cdot T F$.

Surface 3

In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Surface 3** and choose **Duplicate**.

Surface 6

- 1 In the **Model Builder** window, click **Surface 6**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **600**.

Deformation 1

- 1 In the **Model Builder** window, expand the **Surface 6** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **Y-component** text field, type $-3.6 \cdot R \cdot T F$.


Annotation 3

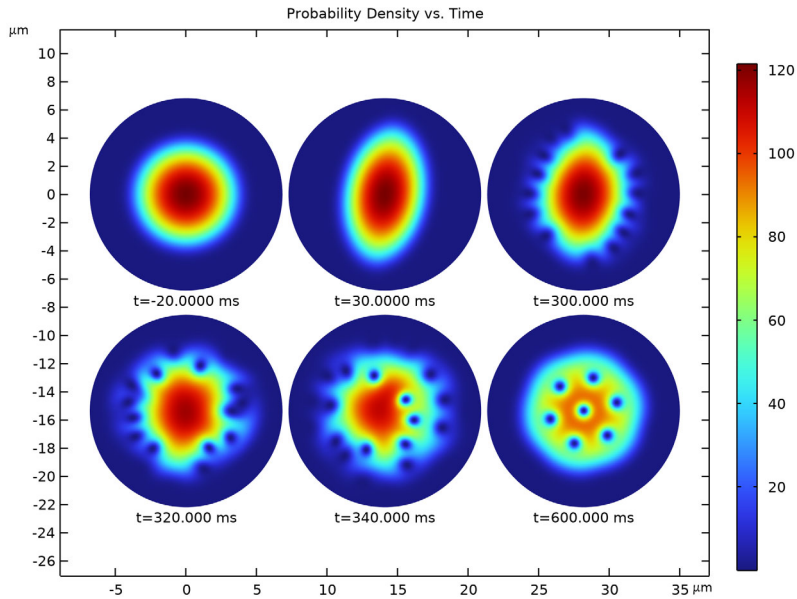
In the **Model Builder** window, under **Results>Probability Density vs. Time** right-click **Annotation 3** and choose **Duplicate**.

Annotation 6

- 1 In the **Model Builder** window, click **Annotation 6**.
- 2 In the **Settings** window for **Annotation**, locate the **Data** section.
- 3 From the **Time (ms)** list, choose **600**.


Deformation 1

- 1 In the **Model Builder** window, expand the **Annotation 6** node, then click **Deformation 1**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 In the **Y-component** text field, type $-3.6 \cdot RrTF$.
- 4 In the **Probability Density vs. Time** toolbar, click  **Plot**.



Optionally use contour plots to check the fit.

Check the Fit

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type Check the Fit in the **Label** text field.


- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 4 - Optimization for Parameter Estimation/Parametric Solutions 1 (sol5)**.
- 4 From the **Parameter value (index)** list, choose **11**.

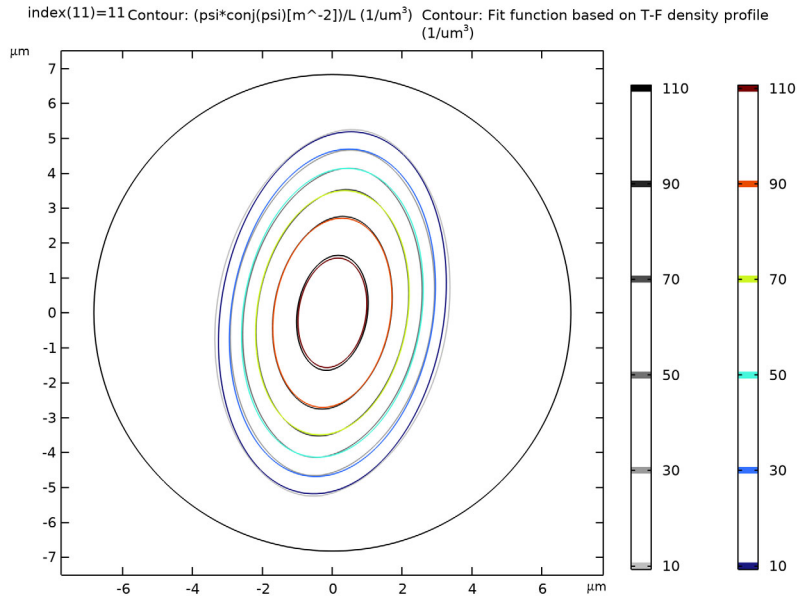
Contour 1 - Data

- 1 Right-click **Check the Fit** and choose **Contour**.
- 2 In the **Settings** window for **Contour**, type Contour 1 - Data in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type $(\psi * \text{conj}(\psi) [m^2]) / L$.
- 4 In the **Unit** field, type $1/\mu m^3$.
- 5 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.
- 6 In the **Levels** text field, type $\text{range}(10, 20, 110)$.
- 7 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Gradient**.
- 8 From the **Top color** list, choose **Black**.
- 9 From the **Bottom color** list, choose **Gray**.
- 10 Right-click **Contour 1 - Data** and choose **Duplicate**.

Contour 2 - Fit

- 1 In the **Model Builder** window, under **Results>Check the Fit** click **Contour 1 - Data 1**.
- 2 In the **Settings** window for **Contour**, type Contour 2 - Fit in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type fit_fn .
- 4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Color table**.




5 In the **Check the Fit** toolbar, click  **Plot**.



Finally disable unused nodes for the eigenvalue and stationary studies, so that in the future they can be recomputed with their intended setup.


STUDY I - EIGENVALUE FOR INITIAL CONDITION

Step 1: Eigenvalue

- 1 In the **Model Builder** window, under **Study I - 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 I (comp1)>Schrödinger Equation (schr)>Interaction Energy**.
- 5 Click  **Disable**.
- 6 In the tree, select **Component I (comp1)>Schrödinger Equation (schr)>Stationary Study**.
- 7 Click  **Disable**.
- 8 In the tree, select **Component I (comp1)>Schrödinger Equation (schr)>Transient Study**.
- 9 Click  **Disable**.

STUDY 2 - STATIONARY FOR CONDENSATE

Step 1: Stationary

- 1 In the **Model Builder** window, under **Study 2 - Stationary for Condensate** click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, 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)>Transient Study**.
- 5 Click  **Disable**.

