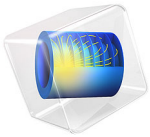

Self-Consistent Schrödinger-Poisson Results for a GaAs Nanowire

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This benchmark model simulates a GaAs nanowire using the self-consistent Schrödinger-Poisson theory to compute the electron density and the confining potential profiles. The predefined Schrödinger-Poisson multiphysics coupling feature is combined with the dedicated Schrödinger-Poisson study type to provide streamlined procedure for model setup and automated creation of self-consistent iterations with tunable parameters for optimizing the convergence under different conditions. The computed electron density and confining potential profiles compare well with the figures in the reference paper, with both profiles reproducing the distinct Friedel-type spatial oscillations at low temperatures.

Introduction

As the semiconductor fabrication technology progresses to miniaturize devices, the effect of quantum confinement becomes more and more important. This tutorial follows the Schrödinger-Poisson theory described in Ref. 1 to compute the self-consistent electron density distribution and confining potential profile for a GaAs nanowire.

Model Definition

The nanowire is assumed to be infinitely long and axially symmetric by the authors of Ref. 1. Thus a 1D axisymmetric geometry is used. Not all simulation parameters are detailed in the paper, especially the material properties. When a parameter is not available, a typical value found in the literature is used in the model.

The radius of the nanowire is assumed to be 50 nm. The electron effective mass is assumed to be 0.067 times free electron mass (as suggested by the Fermi temperature computation result shown in the paper), and the dielectric constant is assumed to be 12.9. The Fermi energy level in the model is set to 0 V and the electric potential at the wall to –0.7 V, to be consistent with the Fermi level pinning boundary condition described in the paper.

We model the case of $2{\cdot}10^{18}$ cm^{-3} uniform ionized dopants at the temperature of 10 K, to compare with the Fig. 2 and 3 in the paper.

The numbers above are entered as global parameters in the model.

Following the approach of the paper, we first solve for the Thomas-Fermi approximate solution. Then use it as the initial condition for the fully coupled Schrödinger-Poisson equation.

See the comments in the section Modeling Instructions for more discussions on the model construction, solution process, and result visualization.

Figure 1 and Figure 2 show the electron density and confining potential, which compare well with Fig. 2 (lower panel) and 3 in Ref. 1, respectively.

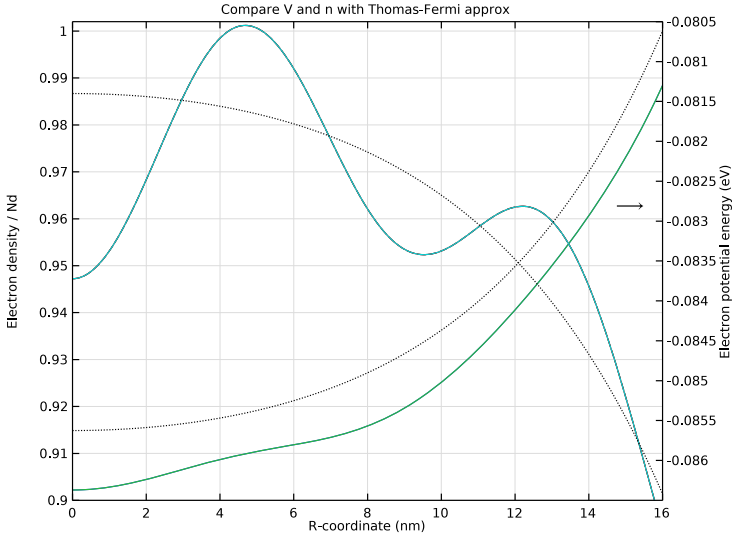


Figure 1: Zoomed-in plot to show the Friedel-type spatial oscillations.

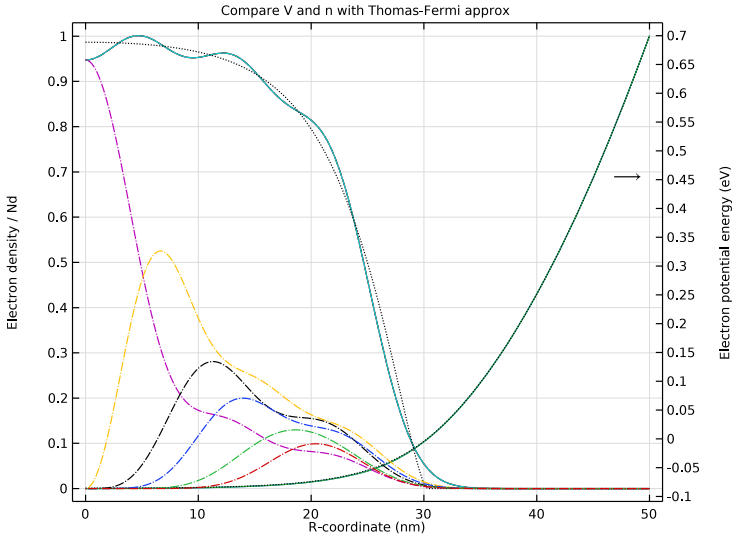


Figure 2: Zoomed-out plot with partial contributions from azimuthal quantum numbers.

Reference

1. J.H. Luscombe, A.M. Bouchard, and M. Luban, "Electron confinement in quantum nanostructures: Self-consistent Poisson-Schrödinger theory," *Phys. Rev. B*, vol. 46, no. 16, p. 10262, 1992.

Application Library path: `Semiconductor_Module/Quantum_Systems/schrodinger_poisson_nanowire`

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 **1D Axisymmetric**.

2 In the **Select Physics** tree, select **Semiconductor>Schrödinger-Poisson Equation**.

3 Click **Add**.

4 Click **Study**.

Since we will first solve for the Thomas-Fermi approximate solution, select the **Stationary** study type. We will add the dedicated **Schrödinger-Poisson** study later.

5 In the **Select Study** tree, select **General Studies>Stationary**.

6 Click **Done**.

GEOMETRY 1

The Model Wizard starts the COMSOL Desktop at the **Geometry** node. Use this chance 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 **nm**.

Load global parameters and local (spatially dependent) variables from files.

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 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `schrodinger_poisson_nanowire_param.txt`.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `schrodinger_poisson_nanowire_var.txt`.

The cross section of the nanowire is a simple radial line segment in the 1D axisymmetric geometry.

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (nm)
0
R0

Create a blank material and enter the dielectric constant of GaAs defined as a global parameter previously.

MATERIALS

Material 1 (mat1)

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.
2. In the **Settings** window for **Material**, locate the **Material Contents** section.
3. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	epsr	1	Basic

Enter the global parameter `m` for the azimuthal quantum number into the corresponding input field in the Schrödinger Equation physics node, so that later we can use the Auxiliary sweep option in the study settings to solve for multiple values of the quantum number.

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. In the m text field, type `m`.

Enter the global parameter `meff` for the effective mass.

Effective Mass 1

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

Since the electron potential energy will be provided by the Schrödinger-Poisson multiphysics coupling, set it to zero in the physics feature.

Electron Potential Energy 1

1. In the **Model Builder** window, click **Electron Potential Energy 1**.
2. In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

3 From the V_e list, choose **User defined**. In the associated text field, type `0`.

Set up the boundary condition for the electrostatics physics at the wall of the nanowire given by the Fermi level pinning at 0.7 V as discussed in the reference paper. Enable Advanced Physics Options to choose the **Use weak constraints** option to obtain accurate displacement field computation for the electrical neutrality check later after solving.

ELECTROSTATICS (ES)

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

Electric Potential 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Potential**.
2 Select Boundary 2 only.
3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.
4 In the V_0 text field, type `V_R0`.
5 Click the **Show More Options** button in the **Model Builder** toolbar.
6 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Advanced Physics Options**.
7 Click **OK**.
8 In the **Settings** window for **Electric Potential**, click to expand the **Constraint Settings** section.
9 Select the **Use weak constraints** check box.

Add the space charge density contribution from the uniform distribution of ionized dopants.

Space Charge Density 1: Ionized dopants

1 In the **Physics** toolbar, click **Domains** and choose **Space Charge Density**.
2 In the **Settings** window for **Space Charge Density**, type `Space Charge Density 1: Ionized dopants` in the **Label** text field.
3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.
4 Locate the **Space Charge Density** section. In the ρ_v text field, type `e_const*Nd`.

Add the space charge density contribution from the electrons under the Thomas-Fermi approximation. This contribution will be replaced by a statistically weighted sum of the probability densities of the eigenstates when solving the coupled Schrödinger-Poisson equation.

Space Charge Density 2: Thomas Fermi

1 In the **Physics** toolbar, click **Domains** and choose **Space Charge Density**.

2 In the **Settings** window for **Space Charge Density**, type `Space Charge Density 2: Thomas Fermi` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Space Charge Density** section. In the ρ_v text field, type `rho_TF`.

For the **Particle Density Computation** section, the default option of Fermi-Dirac statistics with parabolic band approximation is suitable to compute the statistically weighted sum of the probability densities of the eigenstates for the electrons in the nanowire. Enter the previously defined global parameters for the temperature, Fermi energy level, and effective mass. To take into account the pairs of degenerate azimuthal quantum numbers, use the formula `1+(m>0)` for the degeneracy factor, which evaluates to `1` for `m=0` and `2` for `m>0`.

MULTIPHYSICS

Schrödinger-Poisson Coupling 1 (schrp1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Schrödinger-Poisson Coupling 1 (schrp1)**.

2 In the **Settings** window for **Schrödinger-Poisson Coupling**, locate the **Model Input** section.

3 In the T text field, type `T`.

4 Locate the **Particle Density Computation** section. In the E_f text field, type `Ef`.

5 In the m_d text field, type `meff`.

6 In the g_i text field, type `1+(m>0)`.

For the **Charge Density Computation** section, leave the charge number at the default of `-1`, appropriate for electrons. The formula for the **Modified Gummel iteration** is based on the limiting case of high temperature, nondegenerate systems. For systems at lower temperatures, convergence of the iteration can be accelerated with a judicious increase of the tuning parameter α. The default expression for the global error variable `(schrp1.max(abs(V-schrp1.V_old)))/1[V]` computes the max difference between the electric potential fields from the two most recent iterations, in the unit of V.

7 Locate the **Charge Density Computation** section. In the α text field, type `4`.

Create a reasonably fine mesh.

MESH 1

Edge 1

In the **Mesh** toolbar, click  **Edge**.

Distribution 1

1 Right-click **Edge 1** and choose **Distribution**.

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

3 In the **Number of elements** text field, type `200`.

The first study solves for the Thomas-Fermi approximate solution, which is fully configured in the Electrostatics physics interface, so we clear the check boxes for the Schrödinger Equation and the Schrödinger-Poisson Coupling in the study settings.

STUDY 1: THOMAS-FERMI

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

2 In the **Settings** window for **Study**, type `Study 1: Thomas-Fermi` in the **Label** text field.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1: Thomas-Fermi** click **Step 1: Stationary**.

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

3 In the table, clear the **Solve for** check box for **Schrödinger Equation (schr)**.

4 In the table, clear the **Solve for** check box for **Schrödinger-Poisson Coupling 1 (schrp1)**.

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

RESULTS

Electric Potential (es)

Now add the dedicated Schrödinger-Poisson study.

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 **Preset Studies for Selected Multiphysics>Schrödinger-Poisson**.

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: Schrödinger-Poisson

For a completely new problem, it is often necessary to use the default **Manual** search option to find the range of the eigenenergies. Once the range is found, switch to the **Region** search option with appropriate settings for the range and number of eigenvalues, in order to ensure that all significant eigenstates are found by the solver. Here the estimated energy range is between `-0.15` and `0.05` eV. Disable the contribution to the charge density from the Thomas-Fermi approximation as discussed earlier.

1. In the **Settings** window for **Schrödinger-Poisson**, locate the **Study Settings** section.
2. From the **Eigenvalue search method** list, choose **Region**.
3. Find the **Search region** subsection. In the **Smallest real part** text field, type `-0.15`.
4. In the **Largest real part** text field, type `0.05`.
5. Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.
6. In the tree, select **Component 1 (comp1)>Electrostatics (es)> Space Charge Density 2: Thomas Fermi**.
7. Click **Disable**.

   The default iteration method **Minimization of global variable** updates a table displaying the history of a global error variable after each iteration during the solution process. The built-in global error variable `schrp1.global_err` computes the max difference between the electric potential fields from the two most recent iterations, in the unit of V, as already configured in the Schrödinger-Poisson Coupling multiphysics node earlier. (Note that the prefix for the variable, in this case **schrp1**, should match the **Name** input field of the Schrödinger-Poisson Coupling multiphysics node.) Setting the tolerance to `1e-6` thus means the iteration ends after the max difference is less than 1 uV. Use the Thomas-Fermi approximate solution as the initial condition for this study.
8. 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**.
9. From the **Method** list, choose **Solution**.
10. From the **Study** list, choose **Study 1: Thomas-Fermi, Stationary**.

    Use the Auxiliary sweep functionality to solve for a list of nonnegative azimuthal quantum numbers. The negative ones are taken into account using the formula `1+(m>0)` for the degeneracy factor as discussed earlier. The dedicated solver sequence

automatically performs the statistically weighted sum of the probability densities of all the eigenstates.

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

12 Click + **Add**.

13 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
m (Azimuthal quantum number)	0 1 2 3 4 5 6	

Get initial value to generate default plots to be modified and plotted while solving.

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

15 In the **Settings** window for **Study**, type `Study 2: Schrödinger-Poisson` in the **Label** text field.

16 In the **Study** toolbar, click **Get Initial Value**.

RESULTS

Probability Density (schr)

For the plot group **Probability Density (schr)** to show the probability density of each eigenstate, point the dataset to the solution that stores the wave functions.

1 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

2 From the **Dataset** list, choose **Study 2: Schrödinger-Poisson/ Solution Store: Store Wave Function (sol4)**.

3 In the **Probability Density (schr)** toolbar, click **Plot**.

Modify the plot group **Compare n and V with Previous Iteration (schrp1)** to be compared with the figures in the reference paper: Change the generic labels to be more specific to this model. Normalize the electron density with the ionized dopant concentration `Nd`.

Compare V and n with Thomas-Fermi approx

1 In the **Model Builder** window, right-click **Compare n and V with Previous Iteration (schrp1)** and choose **Move Up** four times.

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

3 Click to expand the **Title** section. In the **Title** text area, type `Compare V and n with Thomas-Fermi approx`.

4 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Electron density / Nd`.

5 In the **Secondary y-axis label** text field, type `Electron potential energy (eV)`.

Electron Potential Energy

1 In the **Model Builder** window, expand the **Compare V and n with Thomas-Fermi approx** node, then click **Potential Energy**.

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

3 Locate the **y-Axis Data** section.

4 Select the **Description** check box. In the associated text field, type `Electron Potential Energy`.

Electron Potential Energy from Previous Iteration

1 In the **Model Builder** window, under **Results>Compare V and n with Thomas-Fermi approx** click **Potential Energy from Previous Iteration**.

2 In the **Settings** window for **Line Graph**, type `Electron Potential Energy from Previous Iteration` in the **Label** text field.

3 Locate the **y-Axis Data** section.

4 Select the **Description** check box. In the associated text field, type `Electron Potential Energy, Previous Iteration`.

Electron Density from Weighted Sum

1 In the **Model Builder** window, under **Results>Compare V and n with Thomas-Fermi approx** click **Particle Density from Weighted Sum**.

2 In the **Settings** window for **Line Graph**, type `Electron Density from Weighted Sum` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `schrp1.n_sum/Nd`.

4 Select the **Description** check box. In the associated text field, type `Electron Density, Weighted Sum`.

Electron Density

1 In the **Model Builder** window, under **Results>Compare V and n with Thomas-Fermi approx** click **Particle Density**.

2 In the **Settings** window for **Line Graph**, type `Electron Density` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `schrp1.rhoq/schrp1.q/Nd`.

4 Select the **Description** check box. In the associated text field, type `Electron Density`.

Electron Density from Previous Iteration

1 In the **Model Builder** window, under **Results>Compare V and n with Thomas-Fermi approx** click **Particle Density from Previous Iteration**.

2 In the **Settings** window for **Line Graph**, type `Electron Density from Previous Iteration` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `schrp1.rhoq_old/schrp1.q/Nd`.

4 Select the **Description** check box. In the associated text field, type `Electron Density, Previous Iteration`.

Add the electron density and potential energy profile from the Thomas-Fermi approximation for comparison. Since two y-axes are used, add an arrow to indicate that the potential energy profile uses the vertical scale on the right hand side.

Electron Density from Thomas-Fermi Approx

1 Right-click **Electron Density from Previous Iteration** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Electron Density from Thomas-Fermi Approx` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1: Thomas-Fermi/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `n_TF/Nd`.

5 In the **Description** text field, type `Electron Density, Thomas-Fermi`.

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

7 From the **Color** list, choose **Black**.

Electron Potential Energy from Thomas-Fermi Approx

1 Right-click **Electron Density from Thomas-Fermi Approx** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Electron Potential Energy from Thomas-Fermi Approx` in the **Label** text field.

3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** check box.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `-V`.

5 In the **Description** text field, type `Electron Potential Energy, Thomas-Fermi`.

Annotation 1

1 In the **Model Builder** window, right-click **Compare V and n with Thomas-Fermi approx** and choose **Annotation**.

2 In the **Settings** window for **Annotation**, locate the **y-Axis** section.

3 Select the **Plot on secondary y-axis** check box.

4 Locate the **Annotation** section. In the **Text** text field, type `$\longrightarrow$`.

5 Locate the **Position** section. In the **r** text field, type `46`.

6 In the **z** text field, type `0.47`.

7 Locate the **Coloring and Style** section. Clear the **Show point** check box.

8 Locate the **Annotation** section. Select the **LaTeX markup** check box.

Add the plot to be plotted while solving, then click compute and watch the progress of the iteration in the plot and in the table of absolute errors.

STUDY 2: SCHRÖDINGER-POISSON

Solver Configurations

In the **Model Builder** window, expand the **Study 2: Schrödinger-Poisson>Solver Configurations** node.

Solution 2 (sol2)

1 In the **Model Builder** window, expand the **Study 2: Schrödinger-Poisson> Solver Configurations>Solution 2 (sol2)>Stationary Solver 2: Solve for Electric Potential** node, then click **Fully Coupled 1**.

2 In the **Settings** window for **Fully Coupled**, click to expand the **Results While Solving** section.

3 Select the **Plot** check box.

4 From the **Plot group** list, choose **Compare V and n with Thomas-Fermi approx**.

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

RESULTS

Compare V and n with Thomas-Fermi approx

Add a zoomed-in version of the plot to compare with Fig. 2 in the reference paper. Move the arrow indicator to a proper position.

Compare V and n with Thomas-Fermi approx 1

1 Right-click **Compare V and n with Thomas-Fermi approx** and choose **Duplicate**.

2 Right-click **Compare V and n with Thomas-Fermi approx 1** and choose **Move Up** four times.

3 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

4 Select the **Manual axis limits** check box.

5 In the **x minimum** text field, type `0`.

6 In the **x maximum** text field, type `16`.

7 In the **y minimum** text field, type `0.9`.

8 In the **y maximum** text field, type `1.002`.

9 In the **Secondary y minimum** text field, type `-86.5e-3`.

10 In the **Secondary y maximum** text field, type `-80.5e-3`.

Annotation 1

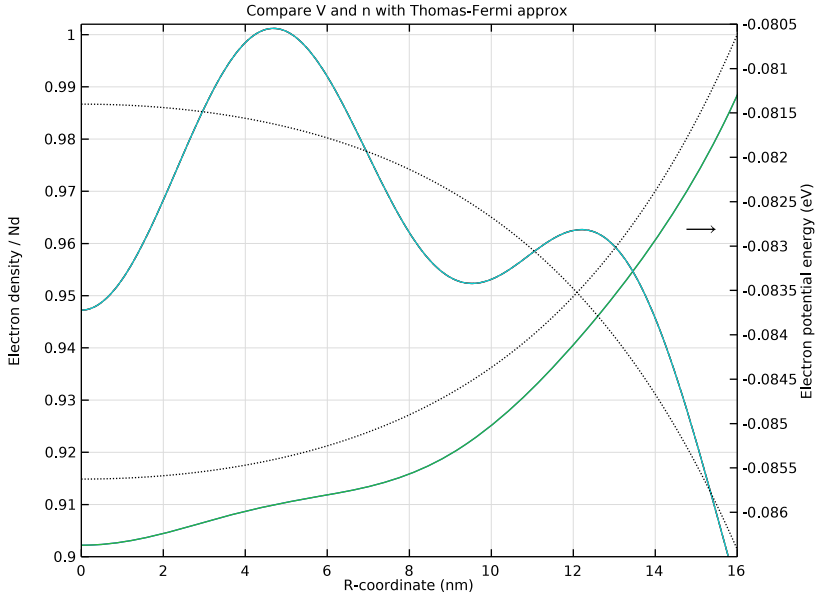
1 In the **Model Builder** window, expand the **Compare V and n with Thomas-Fermi approx 1** node, then click **Annotation 1**.

2 In the **Settings** window for **Annotation**, locate the **Position** section.

3 In the **r** text field, type `14.5`.

4 In the **z** text field, type `-0.0827`.

5 In the **Compare V and n with Thomas-Fermi approx 1** toolbar, click **Plot**.



Optionally, add the contribution to the electron density from each azimuthal quantum number to the original plot, to compare with Fig. 3 in the reference paper. The expression for the plot is slightly complicated but is only needed for visualizing the sub-contributions. Use the solution from the **Solution Store: Store Wave Function (sol4)** node in the solver sequence to provide data for the statistically weighted partial sums. The `sum` operator is used to do the summation and the `withsol` operator is used to select the solutions with the desired quantum number `m` to be summed over the eigenvalue `lambda`. Detailed discussions on the `withsol` operator can be found in the COMSOL Multiphysics Reference Manual.

Electron Density from m=0

1. In the **Model Builder** window, right-click **Electron Density from Thomas-Fermi Approx** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Electron Density from m=0` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `sum(withsol('sol4', schrp1.ni,setval(m,0),setind(lambda,jj)),jj,1,4)/Nd`.
4. In the **Description** text field, type `m=0`.
5. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dash-dot**.
6. From the **Color** list, choose **Cycle**.

Electron Density from m=+/-1

1. Right-click **Electron Density from m=0** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Electron Density from m=+/-1` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `sum(withsol('sol4', schrp1.ni,setval(m,1),setind(lambda,jj)),jj,1,4)/Nd`.
4. In the **Description** text field, type `|m|=1`.

Electron Density from m=+/-2

1. Right-click **Electron Density from m=+/-1** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Electron Density from m=+/-2` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `sum(withsol('sol4', schrp1.ni,setval(m,2),setind(lambda,jj)),jj,1,4)/Nd`.
4. In the **Description** text field, type `|m|=2`.

Electron Density from m=+/-3

1. Right-click **Electron Density from m=+/-2** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Electron Density from m=+/-3` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `sum(withsol('sol4', schrp1.ni,setval(m,3),setind(lambda,jj)),jj,1,3)/Nd`.
4. In the **Description** text field, type `|m|=3`.

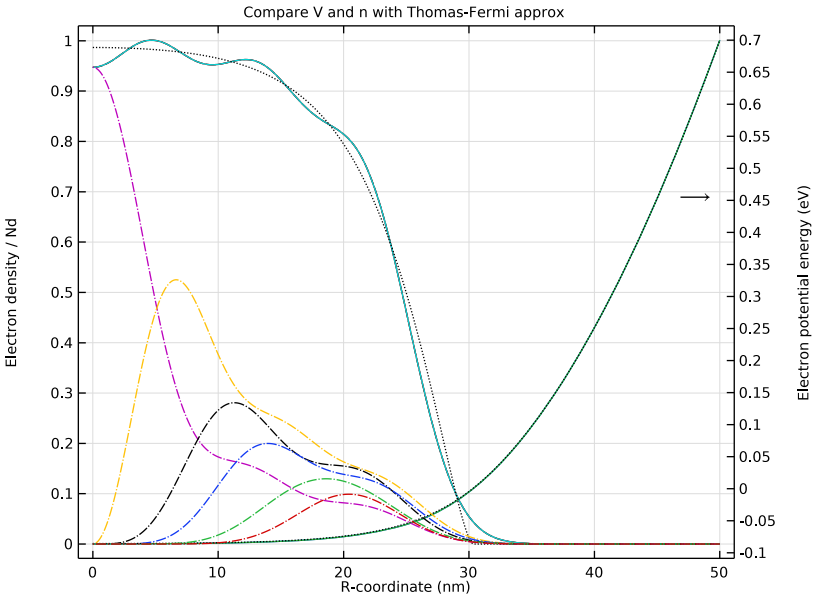
Electron Density from m=+/-4

1. Right-click **Electron Density from m=+/-3** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Electron Density from m=+/-4` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `sum(withsol('sol4', schrp1.ni,setval(m,4),setind(lambda,jj)),jj,1,3)/Nd`.
4. In the **Description** text field, type `|m|=4`.

Electron Density from m=+/-5

1. Right-click **Electron Density from m=+/-4** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Electron Density from m=+/-5` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `sum(withsol('sol4', schrp1.ni,setval(m,5),setind(lambda,jj)),jj,1,2)/Nd`.
4. In the **Description** text field, type `|m|=5`.

5 In the **Compare V and n with Thomas-Fermi approx** toolbar, click **Plot**.



Finally check the charge neutrality as discussed in the reference paper. The built-in integration operator `schrp1.int` is used to compute the number of electrons per unit length inside the nanowire. This number is added to the contribution from the surface charge density given by the electric displacement field at the nanowire surface. The sum is then divided by the total number of ionized dopants per unit length. The ratio is subtracted by 1 to obtain the relative error.

Point Evaluation 1: check charge neutrality

1 In the **Results** toolbar, click **Point Evaluation**.

2 In the **Settings** window for **Point Evaluation**, type `Point Evaluation 1: check charge neutrality` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Schrödinger-Poisson/ Solution 2 (sol2)**.

4 Select Boundary 2 only.

5 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`(schrp1.int(2*pi*R*schrp1.n_sum)-2*pi*R*es.nD/e_const)/(pi*R^2*Nd)-1`	1	`Relative error`

6 Click **Evaluate**.

We see that the relative error for charge neutrality is less than 1e-6.