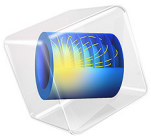
Created in COMSOL Multiphysics 6.2



Solving the Hydrogen Atom

Introduction

In this tutorial model, we take a look at perhaps the most significant exact results of quantum mechanics — the ground state and the first few excited states of the hydrogen atom — and go over how to reproduce these results using COMSOL Multiphysics.

The hydrogen atom with its single electron is described by the time-independent Schrödinger equation (TISE):

$$\hat{H}\psi(r) = -\left(\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}\right)\psi(r) = E\psi(r) \tag{1}$$

Here, $\hbar$, m, e, and ε_0 are the reduced Planck constant, electron mass, elementary charge, and the permittivity of vacuum, respectively. The dependent variable to be solved for, $\psi(r)$, is the wave function: a complex scalar field whose norm, $|\psi(r)|^2$, gives the probability of finding the electron at r. The operator $\hat{H}$, is the Hamiltonian, which corresponds to the total energy of the system. The Laplacian term gives the kinetic energy of the electron, whereas the potential energy is simply given by the Coulomb potential due to the positively charged nucleus at the origin. The TISE is in the form of an eigenvalue problem for the unknown total energy, E, and can be solved exactly by the usual tools of the trade: separation of variables and series expansions. The resulting eigenstates are labeled by three integers: the quantum numbers, n, l, and m, where $n, l \in N$, $l \leq n$ and $m = -l, \ldots, 0, \ldots, l$. Using spherical polar coordinates with θ and ϕ denoting the polar and azimuthal angles, respectively, they can be expressed as

$$\psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \phi) \tag{2}$$

where $R_{nl}(r)$ is the radial wave functions and $Y_l^m(\theta, \phi) \propto P_l^m(\cos\theta)e^{im\phi}$, expressed in terms of the Legendre polynomials $P_l^m(\cos\theta)$, are known as the spherical harmonics. The eigenenergy only depends on the principal quantum number, n:

$$E_n = -\frac{m_e e^4}{2(4\pi\varepsilon_0)^2\hbar^2}\frac{1}{n^2} \equiv R_H\frac{1}{n^2} \tag{3}$$

where $R_H \approx 13.6057$ eV is known as the Rydberg constant.

Model Definition

In the case of the hydrogen atom, the TISE is simply a PDE for a complex-valued scalar field in 3D, thus allowing for a FEM-based solution of the eigenvalue problem. The

Semiconductor Module, an add-on to COMSOL Multiphysics, offers a Schrödinger Equation interface (abbreviated as schr), which we can use for building our hydrogen atom model.

Set up a sphere of radius $A_0 = 15a_0$, where $a_0 = \hbar^2/(m_e e^2) \approx 52.9$ pm is the Bohr radius. In the Schrödinger Equation interface, modify the default nodes (Effective Mass and Electron Potential Energy) so that the effective mass is equal to m_e (this model does not use a periodic lattice) and the electron potential energy is equal to the Coulomb potential of the nucleus. The only boundary condition needed here is $\psi \to 0$ as $r \to \infty$, which corresponds to bound states. Therefore, surround the sphere with a thin layer and define it as an infinite element domain. To improve the computation speed, use a mesh that becomes progressively coarser in the radial direction. Finally, specify the energy scale as eV and estimate –15 eV as the starting point for the eigenvalue search.

Results and Discussion

Table 1 shows the eigenenergies obtained for the first two principal quantum numbers together with their theoretical values.

TABLE 1: EIGENENERGIES OBTAINED FOR THE FIRST TWO PRINCIPAL QUANTUM NUMBERS — ANALYTICAL VALUES VS. MODEL SIMULATION RESULTS.

n	**Analytical method** (R_H/n^2 **(eV))**	**COMSOL** (E_n (eV) from schr)
1	-13.6057	-13.6108
2	-3.4014	-3.4013

Note that the eigenvalues depend on the mesh used, so we always recommend running a mesh refinement study to get reliable results. Figure 1 shows the shape of the eigenstates, or orbitals, plotted using 3D isosurface plots.

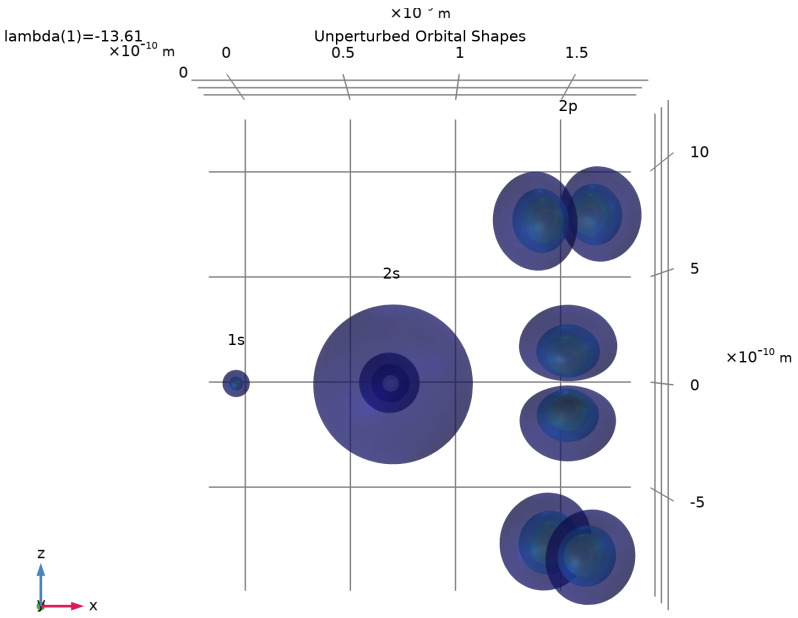


Figure 1: Orbital shapes of unperturbed hydrogen, visualized using a series of displaced 3D isosurface plots.

Adopt the labeling used extensively in atomic physics: 1s, 2s, $2p_x$, …. It is clear from the figure that the s-states are radially symmetric, whereas each of the p-states has cylindrical symmetry along one of three mutually perpendicular axes. For the spherically symmetric s-states, the radial probability density has the simple analytical form

$$P(r) = \iint \sin\theta d\theta d\phi r^2 |\psi(r)|^2 = 4\pi r^2 |\psi(r)|^2 \tag{4}$$

Figure 2 and Figure 3 show a comparison between the analytical and simulated results.

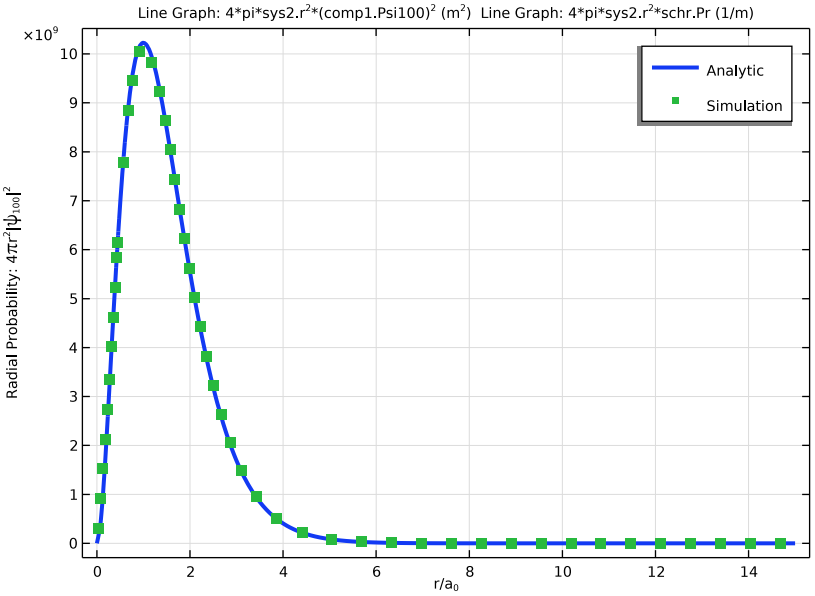


Figure 2: Radial probability of the 1s state (ground state). Analytical results are shown using solid lines, while numerical result obtained in COMSOL Multiphysics are shown using point markers.

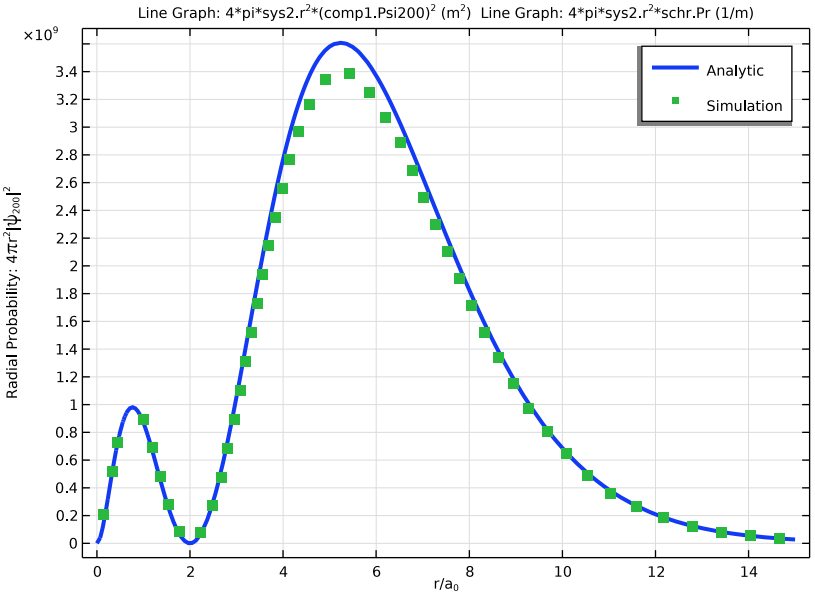


Figure 3: Radial probability of the 2s state (first excited state). Analytical results are shown using solid lines, while numerical result obtained in COMSOL Multiphysics are shown using point markers.

STARK EFFECT

In the hydrogen atom, the Stark effect can be observed as a possible shift of the energy levels, when an external electric field is applied.The perturbation can be represented by the Hamiltonian $V_{\text{Stark}} = e\varepsilon_{\text{ext}}z$. To implement the Stark effect in COMSOL Multiphysics, simply add another Electron Potential Energy node to the model. Then, the split energy levels and the corresponding orbital shapes can readily be obtained. To make the effect clearly visible, use an extremely high external field of ~ 2×10^8 V/m.

See the Modeling Instructions section for more detailed explanations on the model setup.

Application Library path: `Semiconductor_Module/Quantum_Systems/solving_hydrogen_atom`

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

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**.

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 `solving_hydrogen_atom_parameters.txt`.

GEOMETRY 1

Sphere 1 (sph1)

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

2 In the **Settings** window for **Sphere**, locate the **Size** section.

3 In the **Radius** text field, type `A0+0.1*A0`.

4 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	0.1*A0

Point 1 (pt1)

In the **Geometry** toolbar, click **More Primitives** and choose **Point**.

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 In the table, enter the following settings:

Name	Expression	Unit	Description
Psi100	exp(-sys2.r/a0_const)/(sqrt(pi*a0_const^3))		Ground state
Psi200	0.25*(2-sys2.r/a0_const)/(sqrt(2*pi*a0_const^3))*exp(-sys2.r/a0_const/2)		n=2, l,m=0 eigenstate

Simulation domain

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Simulation domain` in the **Label** text field.

3 Select Domain 5 only.

Infinite element domain

1 In the **Definitions** toolbar, click **Complement**.

2 In the **Settings** window for **Complement**, type `Infinite element domain` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to invert**, click **Add**.

4 In the **Add** dialog box, select **Simulation domain** in the **Selections to invert** list.

5 Click **OK**.

Exterior boundary

1 In the **Definitions** toolbar, click **Adjacent**.

2 In the **Settings** window for **Adjacent**, type `Exterior boundary` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Input selections**, click **Add**.

4 In the **Add** dialog box, in the **Input selections** list, choose **Simulation domain** and **Infinite element domain**.

5 Click **OK**.

Interior boundary

1 In the **Definitions** toolbar, click **Adjacent**.

2 In the **Settings** window for **Adjacent**, type `Interior boundary` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Input selections**, click + **Add**.

4 In the **Add** dialog box, select **Simulation domain** in the **Input selections** list.

5 Click **OK**.

Spherical System 2 (sys2)

In the **Definitions** toolbar, click **Coordinate Systems** and choose **Spherical System**.

Infinite Element Domain 1 (ie1)

1 In the **Definitions** toolbar, click **Infinite Element Domain**.

2 In the **Settings** window for **Infinite Element Domain**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Infinite element domain**.

4 Locate the **Geometry** section. From the **Type** list, choose **Spherical**.

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 **Stationary study** subsection. In the E text field, type `-15[eV]`.

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 `me_const`.

Nucleus

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 `Nucleus` 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 `-kC*e_const^2/sys2.r`.

Zero Probability 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Zero Probability**.

2 In the **Settings** window for **Zero Probability**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Exterior boundary**.

External field along z-axis

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

2 In the **Settings** window for **Electron Potential Energy**, type `External field along z-axis` 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 `e_const*Eext*z`.

MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size

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

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `10*h0`.

5 In the **Minimum element size** text field, type `0.1*h0`.

Free Tetrahedral 1

1 In the **Model Builder** window, click **Free Tetrahedral 1**.

2 In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Simulation domain**.

Size Expression 1

1 Right-click **Free Tetrahedral 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 `(1+sqrt(x^2+y^2+z^2)*hg)*h0`.

Swept 1

1 In the **Mesh** toolbar, click **Swept**.

2 In the **Settings** window for **Swept**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Infinite element domain**.

5 Click to expand the **Source Faces** section. From the **Selection** list, choose **Interior boundary**.

6 Click to expand the **Destination Faces** section. From the **Selection** list, choose **Exterior boundary**.

Distribution 1

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

NO EXTERNAL FIELD

In the **Settings** window for **Study**, type `No External Field` in the **Label** text field.

Step 1: Eigenvalue

1 In the **Model Builder** window, under **No External Field** 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 `5`.

4 In the **Search for eigenvalues around shift** text field, type `-15`.

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)>Schrödinger Equation (schr)> External field along z-axis**.

7 Click **Disable**.

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

RESULTS

Cut Line 3D 1

1 In the **Results** toolbar, click **Cut Line 3D**.

2 In the **Settings** window for **Cut Line 3D**, locate the **Line Data** section.

3 In row **Point 2**, set **X** to `0`.

4 In row **Point 2**, set **Z** to `A0`.

5 Click to expand the **Advanced** section.

1s Radial Probability

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `1s Radial Probability` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 3D 1**.

4 From the **Eigenvalue selection** list, choose **First**.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `r/a<sub>0</sub>`.

7 Select the **y-axis label** check box. In the associated text field, type `Radial Probability: 4\pi r<sup>2</sup>|\psi<sub>100</sub>|<sup>2</sup>`.

Line Graph 1

1 Right-click **1s Radial Probability** and choose **Line Graph**.

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

3 In the **Expression** text field, type `4*pi*sys2.r^2*(comp1.Psi100)^2`.

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

5 In the **Expression** text field, type `sys2.r/a0_const`.

6 Click to expand the **Coloring and Style** section. From the **Width** list, choose **3**.

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

8 From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
Analytic

10 Click to expand the **Quality** section. From the **Resolution** list, choose **Finer**.

Line Graph 2

1 In the **Model Builder** window, right-click **1s Radial Probability** and choose **Line Graph**.

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

3 In the **Expression** text field, type `4*pi*sys2.r^2*schr.Pr`.

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

5 In the **Expression** text field, type `sys2.r/a0_const`.

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

7 From the **Width** list, choose **3**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.

9 From the **Positioning** list, choose **Interpolated**.

10 In the **Number** text field, type `50`.

11 Locate the **Legends** section. Select the **Show legends** check box.

12 From the **Legends** list, choose **Manual**.

13 In the table, enter the following settings:

Legends
Simulation

14 In the **1s Radial Probability** toolbar, click **Plot**.

1s Radial Probability

Right-click **1s Radial Probability** and choose **Duplicate**.

2s Radial Probability

1 In the **Model Builder** window, under **Results** click **1s Radial Probability 1**.

2 In the **Settings** window for **1D Plot Group**, type `2s Radial Probability` in the **Label** text field.

3 Locate the **Data** section. From the **Eigenvalue selection** list, choose **Manual**.

4 In the **Eigenvalue indices (1-5)** text field, type `2`.

5 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Radial Probability: 4\pi r<sup>2</sup>|\psi<sub>200</sub>|<sup>2</sup>`.

Line Graph 1

1 In the **Model Builder** window, expand the **2s Radial Probability** node, then click **Line Graph 1**.

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

3 In the **Expression** text field, type `4*pi*sys2.r^2*(comp1.Psi200)^2`.

4 In the **2s Radial Probability** toolbar, click **Plot**.

Unperturbed orbital shapes

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Unperturbed orbital shapes` in the **Label** text field.

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

4 In the **Title** text area, type `Unperturbed Orbital Shapes`.

5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

6 Locate the **Color Legend** section. Clear the **Show legends** check box.

Isosurface 1

1 Right-click **Unperturbed orbital shapes** and choose **Isosurface**.

2 In the **Settings** window for **Isosurface**, locate the **Expression** section.

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

Isosurface 2

1 In the **Model Builder** window, right-click **Unperturbed orbital shapes** and choose **Isosurface**.

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

3 From the **Dataset** list, choose **No External Field/Solution 1 (sol1)**.

4 From the **Eigenvalue** list, choose **-3.4012**.

5 Locate the **Expression** section. In the **Expression** text field, type `schr.Pr`.

6 Locate the **Levels** section. Select the **Interactive** check box.

7 In the **Shift** text field, type `-2.45E28`.

Translation 1

1 Right-click **Isosurface 2** and choose **Translation**.

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

3 In the **x** text field, type `7E-10`.

Isosurface 3

1 In the **Model Builder** window, right-click **Unperturbed orbital shapes** and choose **Isosurface**.

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

3 From the **Dataset** list, choose **No External Field/Solution 1 (sol1)**.

4 From the **Eigenvalue** list, choose **-3.401**.

5 Locate the **Expression** section. In the **Expression** text field, type `schr.Pr`.

Translation 1

1 Right-click **Isosurface 3** and choose **Translation**.

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

3 In the **x** text field, type `15E-10`.

Isosurface 4

1 In the **Model Builder** window, right-click **Unperturbed orbital shapes** and choose **Isosurface**.

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

3 From the **Dataset** list, choose **No External Field/Solution 1 (sol1)**.

4 From the **Eigenvalue** list, choose **-3.401**.

5 Locate the **Expression** section. In the **Expression** text field, type `schr.Pr`.

Translation 1

1 Right-click **Isosurface 4** and choose **Translation**.

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

3 In the **x** text field, type `15E-10`.

4 In the **z** text field, type `7.5E-10`.

Isosurface 5

1 In the **Model Builder** window, right-click **Unperturbed orbital shapes** and choose **Isosurface**.

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

3 From the **Dataset** list, choose **No External Field/Solution 1 (sol1)**.

4 From the **Eigenvalue** list, choose **-3.401**.

5 Locate the **Expression** section. In the **Expression** text field, type `schr.Pr`.

Translation 1

1 Right-click **Isosurface 5** and choose **Translation**.

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

3 In the **x** text field, type `15E-10`.

4 In the **z** text field, type `-7.5E-10`.

Annotation 1

1 In the **Model Builder** window, right-click **Unperturbed orbital shapes** and choose **Annotation**.

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

3 In the **Text** text field, type `1s`.

4 Locate the **Position** section. In the **Z** text field, type `2E-10`.

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

6 From the **Anchor point** list, choose **Center**.

Annotation 2

1 Right-click **Unperturbed orbital shapes** and choose **Annotation**.

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

3 In the **Text** text field, type `2s`.

4 Locate the **Position** section. In the **X** text field, type `7E-10`.

5 In the **Z** text field, type `5E-10`.

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

7 From the **Anchor point** list, choose **Center**.

Annotation 3

1 Right-click **Unperturbed orbital shapes** and choose **Annotation**.

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

3 In the **Text** text field, type `2p`.

4 Locate the **Position** section. In the **X** text field, type `15E-10`.

5 In the **Z** text field, type `12.5E-10`.

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

7 From the **Anchor point** list, choose **Center**.

8 Click the  **Go to XZ View** button in the **Graphics** toolbar.

9 Click the  **Transparency** button in the **Graphics** toolbar.

10 In the **Unperturbed orbital shapes** toolbar, click  **Plot**.

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 Physics Interfaces>Eigenvalue**.

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

STARK EFFECT

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

2 In the **Settings** window for **Study**, type `Stark Effect` in the **Label** text field.

Step 1: Eigenvalue

1 In the **Model Builder** window, under **Stark Effect** 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 `5`.

4 In the **Search for eigenvalues around shift** text field, type `-15`.

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

RESULTS

Unperturbed orbital shapes

In the **Model Builder** window, under **Results** right-click **Unperturbed orbital shapes** and choose **Duplicate**.

Stark effect orbital shapes

1. In the **Model Builder** window, under **Results** click **Unperturbed orbital shapes 1**.
2. In the **Settings** window for **3D Plot Group**, type `Stark effect orbital shapes` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Stark Effect/Solution 2 (sol2)**.
4. Locate the **Title** section. In the **Title** text area, type `Stark Effect Orbital Shapes`.
5. In the **Model Builder** window, expand the **Stark effect orbital shapes** node.

Isosurface 2

1. In the **Model Builder** window, expand the **Results>Stark effect orbital shapes>Isosurface 2** node, then click **Isosurface 2**.
2. In the **Settings** window for **Isosurface**, locate the **Data** section.
3. From the **Dataset** list, choose **Stark Effect/Solution 2 (sol2)**.
4. From the **Eigenvalue** list, choose **-3.4013**.
5. Locate the **Levels** section. Clear the **Interactive** check box.

Isosurface 3

1. In the **Model Builder** window, click **Isosurface 3**.
2. In the **Settings** window for **Isosurface**, locate the **Data** section.
3. From the **Dataset** list, choose **Stark Effect/Solution 2 (sol2)**.
4. From the **Eigenvalue** list, choose **-3.4013**.

Isosurface 4

1. In the **Model Builder** window, expand the **Isosurface 3** node, then click **Results> Stark effect orbital shapes>Isosurface 4**.
2. In the **Settings** window for **Isosurface**, locate the **Data** section.
3. From the **Dataset** list, choose **Stark Effect/Solution 2 (sol2)**.
4. From the **Eigenvalue** list, choose **-3.3714**.

Translation 1

1. In the **Model Builder** window, expand the **Isosurface 4** node, then click **Translation 1**.
2. In the **Settings** window for **Translation**, locate the **Translation** section.

3 In the **x** text field, type `11E-10`.

4 In the **z** text field, type `5E-10`.

Isosurface 5

1 In the **Model Builder** window, under **Results>Stark effect orbital shapes** click **Isosurface 5**.

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

3 From the **Dataset** list, choose **Stark Effect/Solution 2 (sol2)**.

4 From the **Eigenvalue** list, choose **-3.4314**.

Translation 1

1 In the **Model Builder** window, expand the **Isosurface 5** node, then click **Translation 1**.

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

3 In the **x** text field, type `11E-10`.

4 In the **z** text field, type `-5E-10`.

Annotation 1

1 In the **Model Builder** window, under **Results>Stark effect orbital shapes** click **Annotation 1**.

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

3 In the **Text** text field, type `1s (no splitting)`.

4 Select the **LaTeX markup** check box.

Annotation 2

1 In the **Model Builder** window, click **Annotation 2**.

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

3 In the **Text** text field, type `2px, 2py \\ (no splitting)`.

4 Select the **LaTeX markup** check box.

5 Locate the **Position** section. In the **X** text field, type `22E-10`.

6 In the **Z** text field, type `0`.

Annotation 3

1 In the **Model Builder** window, click **Annotation 3**.

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

3 In the **Text** text field, type `Hybrid 2s+2pz \\(Stark splitting by +0.03 eV)`.

4 Select the **LaTeX markup** check box.

5 Locate the **Position** section. In the **X** text field, type `11E-10`.

6 In the **Z** text field, type `10E-10`.

Annotation 4

1 In the **Model Builder** window, right-click **Stark effect orbital shapes** and choose **Annotation**.

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

3 In the **Text** text field, type `Hybrid 2s+2pz \\(Stark splitting by -0.03 eV)`.

4 Select the **LaTeX markup** check box.

5 Locate the **Position** section. In the **X** text field, type `11E-10`.

6 In the **Z** text field, type `-10E-10`.

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

8 From the **Anchor point** list, choose **Center**.

9 In the **Stark effect orbital shapes** toolbar, click **Plot**.

Unperturbed eigenenergies

1 In the **Model Builder** window, expand the **Results>Derived Values** node, then click **Eigenvalue**.

2 In the **Settings** window for **Global Evaluation**, type `Unperturbed eigenenergies` in the **Label** text field.

3 Locate the **Data** section. From the **Eigenvalue selection** list, choose **Manual**.

4 In the **Eigenvalue indices (1-5)** text field, type `1,2`.

5 Click **Evaluate**.

Stark effect eigenenergies

1 In the **Model Builder** window, under **Results>Derived Values** click **Eigenvalue 1**.

2 In the **Settings** window for **Global Evaluation**, type `Stark effect eigenenergies` in the **Label** text field.

3 Click **Evaluate**.