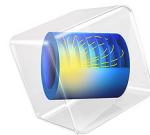


Created in COMSOL Multiphysics 6.2



# A Silicon Quantum Dot in a Uniform Magnetic Field

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This tutorial model solves a two-component Schrödinger equation for the eigenstates of a simple silicon quantum dot in a uniform magnetic field, based on the paper by Jock and others ([Ref. 1](#)) on the topic of spin-orbit qubits. The built-in domain condition Lorentz Force for the Schrödinger Equation interface is used to account for the contribution to the kinetic momentum from the vector potential. The coupling of the spin-up and spin-down components is implemented using the built-in domain condition Zeroth Order Hamiltonian. Together with the benchmark model [k·p Method for Strained Wurtzite GaN Band Structure](#), these examples show how to set up multiple wave-function components with the Schrödinger Equation interface. The computed probability density and kinetic momentum density of the ground state compare well with Supplementary Figure 1 in the paper. In addition, the computed energy difference between the first two eigenstates agrees well with the expected value from an intuitive analytic calculation.

### *Introduction*

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Quantum dots are an essential ingredient in nanotechnology, with potential applications in solar cells, LEDs, displays, photodetectors, and quantum computing. One of the papers on the last application area is published by Jock and others ([Ref. 1](#)). In the Supplementary Note 1 of the paper, the authors provided the formulation describing a silicon quantum dot and showed the numerical solution in Supplementary Figure 1, which will be reproduced by this model.

### *Model Definition*

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Equation (1) in the Supplementary Note 1 of [Ref. 1](#) gives the single-electron Hamiltonian for a silicon quantum dot in a uniform magnetic field  $\mathbf{B}$ , without including spin-orbit coupling

$$H = \frac{P_x^2}{2m_{\perp}} + \frac{P_y^2}{2m_{\perp}} + \frac{P_z^2}{2m_z} + V(\mathbf{r}) + \mu_B \mathbf{B} \cdot \boldsymbol{\sigma} \quad (1)$$

where the g-tensor is assumed to be a scalar of value 2 following the paper, and the kinetic momentum  $\mathbf{P}$  is given by

$$\mathbf{P} = i \hbar \nabla + e\mathbf{A}(\mathbf{r}) \quad (2)$$

Note that there is no minus sign in front of the imaginary unit  $i$  because of the engineering sign convention adopted by all COMSOL physics interfaces: a plane wave is  $\exp(-ikx + i\omega t)$ , not  $\exp(ikx - i\omega t)$ .

The confinement potential energy term  $V(\mathbf{r})$  is given by Eq (9) in the paper:

$$V(\mathbf{r}) = \frac{1}{2}m_{\perp}\omega_x^2x^2 + \frac{1}{2}m_{\perp}\omega_y^2y^2 + qF_zz + U_0\Theta(z) \quad (3)$$

This represents an anisotropic harmonic trapping potential in the lateral directions, an electric field in the  $z$  direction, and a potential barrier at the silicon–oxide interface at  $z = 0$ .

In the model, the confinement potential energies in [Equation 3](#) are implemented using **Electron Potential Energy** domain conditions. The contribution to the kinetic momentum from the vector potential (the second term in [Equation 2](#)) is implemented using the **Lorentz Force** domain condition, and the magnetic coupling of the spin-up and spin-down components (the last term in [Equation 1](#)) is implemented with the **Zeroth Order Hamiltonian** domain condition.

See the [Modeling Instructions](#) section for more detailed explanations on the model setup.

## Results and Discussion

Figure 1 and Figure 2 show the real and imaginary parts of the spin-up component of the ground state wave function, respectively. They have the same shape and magnitude.

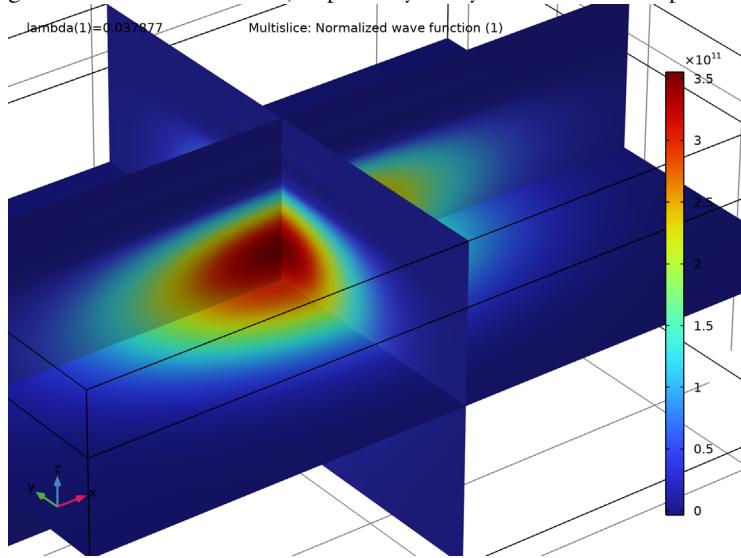


Figure 1: Real part of the spin-up component of the ground state wave function.

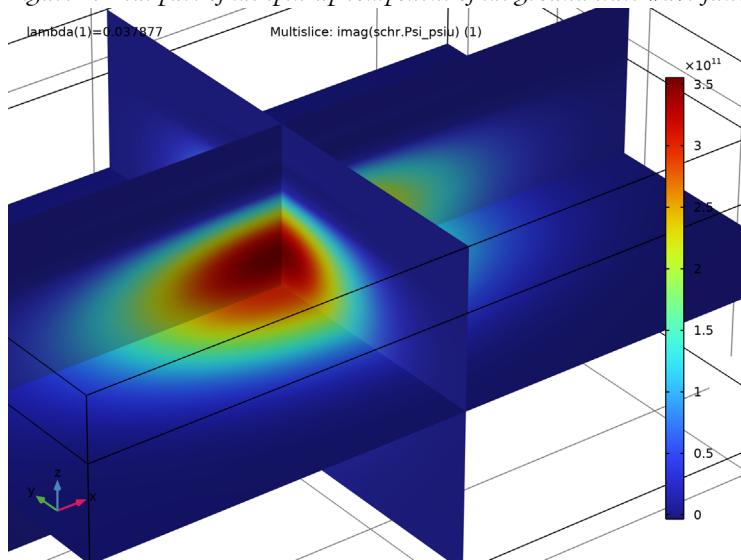
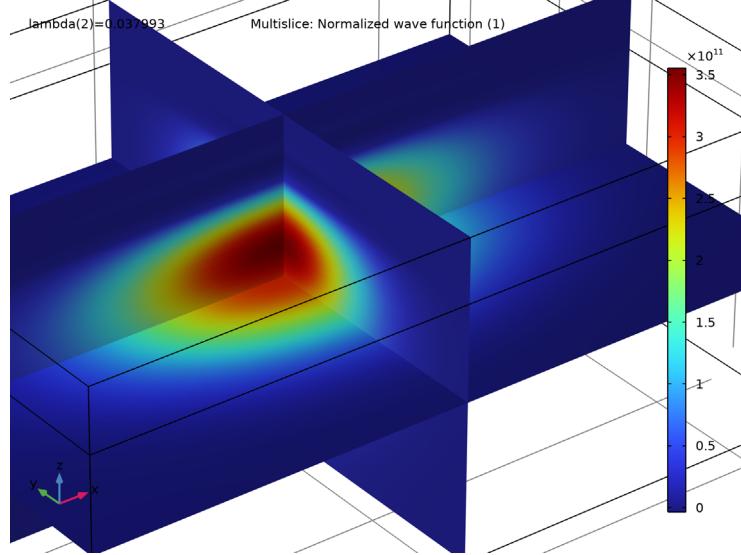
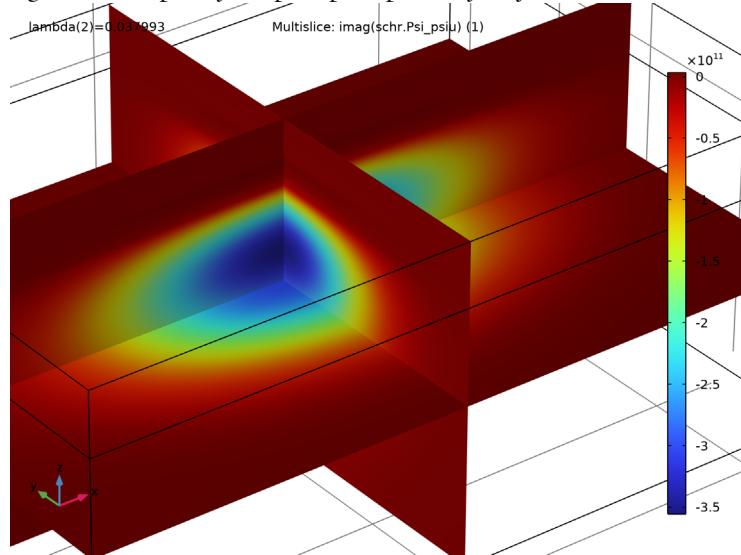


Figure 2: Imaginary part of the spin-up component of the ground state wave function.

[Figure 3](#) and [Figure 4](#) show the real and imaginary parts of the spin-up component of the first excited state wave function, respectively. They have the same shape and magnitude but differ in sign.



*Figure 3: Real part of the spin-up component of the first excited state wave function.*



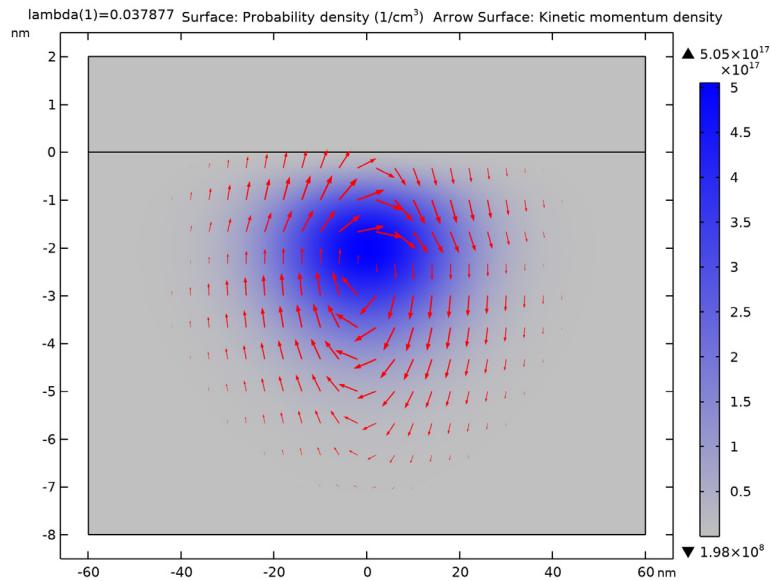
*Figure 4: Imaginary part of the spin-up component of the first excited state wave function.*

A similar relationship can be found among the spin-down components of the first two eigenstates, and between the spin-up and spin-down components. To understand this observation, we evaluate the wave function components near the peak density point. We find that for the ground state, up to an overall scaling factor of about  $3.6 \times 10^{11}$ , the amplitude of the spin-up component is  $1+i = (1)(1+i)$ , and the amplitude of the spin-down component is  $1-i = (-i)(1+i)$ . Therefore, the vector formed by the two components is proportional to  $(1, -i)$ , which is recognized as the spin-down eigenstate of the  $y$ -spin operator  $S_y$ . This is consistent with the intuitive picture that the lower energy state of an electron in a magnetic field has its spin magnetic moment parallel to the magnetic field and thus the spin is anti-parallel to the magnetic field.

Similarly for the first excited state, up to an overall scaling factor of about  $3.6 \times 10^{11}$ , the amplitude of the spin-up component is seen to be  $1-i = (1)(1-i)$ , and the amplitude of the spin-down component is  $1+i = (+i)(1-i)$ . Therefore the vector formed by the two components is proportional to  $(1, +i)$ , which is recognized as the spin-up eigenstate of the  $y$ -spin operator  $S_y$ . This is consistent with the intuitive picture that the higher energy state of an electron in a magnetic field has its spin magnetic moment anti-parallel to the magnetic field and thus the spin is parallel to the magnetic field.

This observation can be further confirmed by comparing the energy difference between the two computed eigenstates with the expected energy difference between a spin-up and a spin-down electron in a uniform magnetic field, using global evaluations. We see a very good agreement of the computed and the expected energy difference between the first two eigenstates – both evaluate to the same value of 0.116 meV.

**Figure 5** shows the probability density and kinetic momentum density of the ground state. It compares well with Supplementary Figure 1 in the paper.



*Figure 5: Probability density and kinetic momentum density of the ground state.*

### Reference

- 
1. R.M. Jock and others, “A silicon metal-oxide-semiconductor electron spin-orbit qubit”, *Nature Communications*, vol. 9, p. 1768, 2018.
- 

**Application Library path:** Semiconductor\_Module/Quantum\_Systems/  
si\_quantum\_dot\_in\_uniform\_magnetic\_field

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### Modeling Instructions

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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**.

In this model we use two wave-function components for the spin-up and spin-down states. Set the variable names accordingly: **psi<sub>u</sub>** for spin-up and **psi<sub>d</sub>** for spin-down.

- 4 In the **Number of wave function components** text field, type 2.

- 5 In the **Wave functions (I)** table, enter the following settings:

<u>psi<sub>u</sub></u>
<u>psi<sub>d</sub></u>

- 6 Click  **Study**.
- 7 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Eigenvalue**.
- 8 Click  **Done**.

## GEOMETRY I

Set the length unit to nm. Create a simple block for the modeling domain. To compare with Supplementary Figure 1 of the reference paper, align the z=0 plane with the interface between the silicon and the oxide.

- 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**.

### Block 1 (blk1)

- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 120.
- 4 In the **Depth** text field, type 80.
- 5 In the **Height** text field, type 10.
- 6 Locate the **Position** section. From the **Base** list, choose **Center**.
- 7 In the **z** text field, type -3.

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

Layer name	Thickness (nm)
Layer 1	2

- 9 Find the **Layer position** subsection. Clear the **Bottom** check box.

- 10 Select the **Top** check box.

- 11 Click  **Build All Objects**.

Adjust the aspect ratio of the view in the graphics window to shown the layers more clearly.

## DEFINITIONS

In the **Model Builder** window, expand the **Component 1 (compl)>Definitions** node.

### *Camera*

- 1 In the **Model Builder** window, expand the **Component 1 (compl)>Definitions>View 1** node, then click **Camera**.
- 2 In the **Settings** window for **Camera**, locate the **Camera** section.
- 3 From the **View scale** list, choose **Automatic**.
- 4 From the **Automatic** list, choose **Anisotropic**.
- 5 In the **x weight** text field, type **1.2**.
- 6 In the **y weight** text field, type **0.8**.
- 7 In the **z weight** text field, type **0.5**.
- 8 Click  **Update**.

Enter the model parameters. A guess value is entered for the magnetic field, since it is not specified in the reference paper.

## GLOBAL DEFINITIONS

### *Parameters 1*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

- 3** In the table, enter the following settings:

Name	Expression	Value	Description
mxy	0.19*me_const	1.7308E-31 kg	Lateral effective mass
mz	0.98*me_const	8.9272E-31 kg	Vertical effective mass
wx	1[meV]/hbar_const	1.5193E12 rad/s	Trap frequency in the x direction
wy	3*wx	4.5578E12 rad/s	Trap frequency in the y direction
Fz	10[MV/m]	1E7 V/m	Electric field
U0	3[eV]	4.8065E-19 J	Oxide energy barrier
uB	e_const*hbar_const/2/me_const	9.274E-24 m^2·A	Bohr magneton
B	1[T]	1 T	Magnetic field

Following the reference paper, enter the components of the vector potential **A** as variables, given by one half of the cross product of the uniform magnetic field **B** and the position vector **r**.

#### DEFINITIONS

Variables /

- In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- In the **Settings** window for **Variables**, locate the **Variables** section.
- In the table, enter the following settings:

Name	Expression	Unit	Description
Ax	z*B/2	Wb/m	Vector potential
Ay	0[Wb/m]	Wb/m	Vector potential
Az	-x*B/2	Wb/m	Vector potential

Enter the lateral effective mass for the x and y directions and the vertical effective mass for the z directions. Even though in this model the two wave-function components share the same effective masses, the user interface allows different values for different wave-function components for general cases.

## SCHRÖDINGER EQUATION (SCHR)

### *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 From the list, choose **Diagonal**.
- 4 In the  $\mathbf{m}_{\text{eff},e,11}$  table, enter the following settings:

mxy	0	0
0	mxy	0
0	0	mz

- 5 From the list, choose **Diagonal**.
- 6 In the  $\mathbf{m}_{\text{eff},e,22}$  table, enter the following settings:

mxy	0	0
0	mxy	0
0	0	mz

The quantum dot is assumed to be confined laterally by an anisotropic harmonic potential. Use the default **Electron Potential Energy** feature for this.

### *Electron Potential Energy 1 - Lateral harmonic confinement*

- 1 In the **Model Builder** window, click **Electron Potential Energy 1**.
- 2 In the **Settings** window for **Electron Potential Energy**, type **Electron Potential Energy 1 - Lateral harmonic confinement** in the **Label** text field.
- 3 Locate the **Electron Potential Energy** section. In the  $V_{e,11}$  text field, type  $0.5*mxy*(wx^2*x^2+wy^2*y^2)$ .
- 4 In the  $V_{e,22}$  text field, type  $0.5*mxy*(wx^2*x^2+wy^2*y^2)$ .

The vertical confinement is via the combination of a uniform vertical electric field **Fz** and an interface energy offset **U0**. This can be done with two additional **Electron Potential Energy** features, which are accumulative ("contributing" in COMSOL language).

### *Electron Potential Energy 2 - E field*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Electron Potential Energy**.
- 2 In the **Settings** window for **Electron Potential Energy**, type **Electron Potential Energy 2 - E field** 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. In the  $V_{e,11}$  text field, type `schr.q*Fz*z.`
- 5 In the  $V_{e,22}$  text field, type `schr.q*Fz*z.`

*Electron Potential Energy 3 - Oxide energy barrier*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Electron Potential Energy**.
- 2 In the **Settings** window for **Electron Potential Energy**, type **Electron Potential Energy 3 - Oxide energy barrier** in the **Label** text field.
- 3 Select Domain 2 only.
- 4 Locate the **Electron Potential Energy** section. In the  $V_{e,11}$  text field, type `U0.`
- 5 In the  $V_{e,22}$  text field, type `U0.`

The **Lorentz Force** domain condition accounts for the additional term in the kinetic momentum from the vector potential that contributes to the Hamiltonian.

*Lorentz Force I*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Lorentz Force**.
- 2 In the **Settings** window for **Lorentz Force**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Lorentz Force** section. Specify the **A** vector as

Ax	X
Ay	Y
Az	Z

Finally the **Zeroth Order Hamiltonian** domain condition takes into account the interaction between the magnetic field and the electron spin (last term in Eq. (1) in the SUPPLEMENTARY NOTE 1 of the reference paper). Remember to compensate for the factor of  $(\hbar^2/2m_e)$  that is inherent in all of this type of Hamiltonian features.

*Zeroth Order Hamiltonian I - Spin*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Zeroth-Order Hamiltonian**.
- 2 In the **Settings** window for **Zeroth-Order Hamiltonian**, type **Zeroth Order Hamiltonian 1 - Spin** in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

- 4** Locate the **Hamiltonian** section. In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Zeroth-order Hamiltonian parameter ( $\text{J/m}^2$ )	Description
1	2	$-\text{i}^*\text{uB}^*\text{B}/(\text{hbar\_const}^2/2/\text{me\_const})$	H12

- 5** Click  **Add**.

- 6** In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Zeroth-order Hamiltonian parameter ( $\text{J/m}^2$ )	Description
2	1	$+\text{i}^*\text{uB}^*\text{B}/(\text{hbar\_const}^2/2/\text{me\_const})$	H21

For the simple geometry of this model, it is efficient to use the brick type mesh elements by first creating a mapped mesh on the top surface, and then sweeping it in the vertical direction to create the bricks.

## MESH 1

### Mapped 1

- 1** In the **Mesh** toolbar, click  **More Generators** and choose **Mapped**.

- 2** Select Boundary 7 only.

### Distribution 1

- 1** Right-click **Mapped 1** and choose **Distribution**.
- 2** In the **Settings** window for **Distribution**, locate the **Edge Selection** section.
- 3** From the **Selection** list, choose **All edges**.
- 4** Locate the **Distribution** section. In the **Number of elements** text field, type 20.

### Swept 1

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

### Distribution 1

- 1** Right-click **Swept 1** and choose **Distribution**.
- 2** Select Domain 2 only.

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

**4** In the **Number of elements** text field, type 2.

#### *Distribution 2*

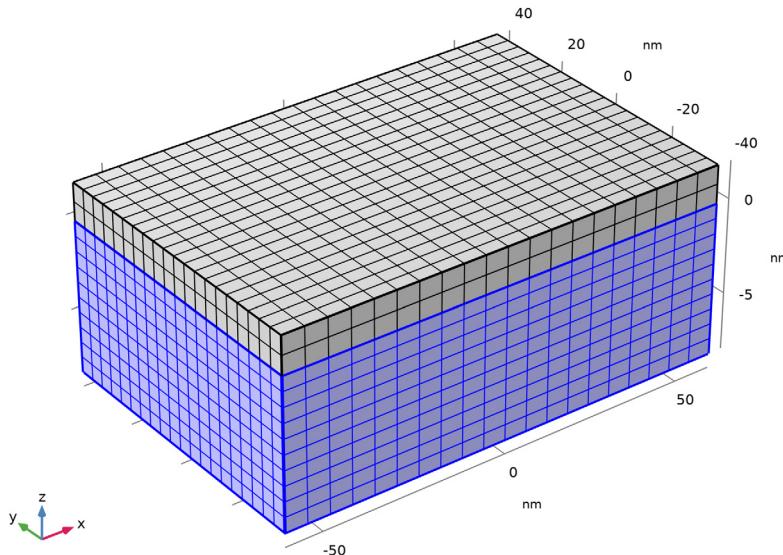
**1** In the **Model Builder** window, right-click **Swept 1** and choose **Distribution**.

**2** Select Domain 1 only.

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

**4** In the **Number of elements** text field, type 10.

**5** In the **Mesh** toolbar, click  **Build Mesh**.



Adjust the eigenvalue search value to close to the ground state energy. (For a new problem, some trial and error will be needed to find a good value.) The **Eigenvalue scale** input of the Schrödinger Equation interface by default is 1[eV]. Therefore a search value of 0.03 entered here means to search for eigenenergies close to 0.03 eV.

## **STUDY 1**

### *Step 1: Eigenvalue*

**1** In the **Model Builder** window, under **Study 1** 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 9.
- 4 In the **Search for eigenvalues around shift** text field, type 0.037.
- 5 In the **Home** toolbar, click  **Compute**.

Evaluate the default Global Evaluation to see the list of eigenenergies and to double check the normalization works to make the total probability unity.

## RESULTS

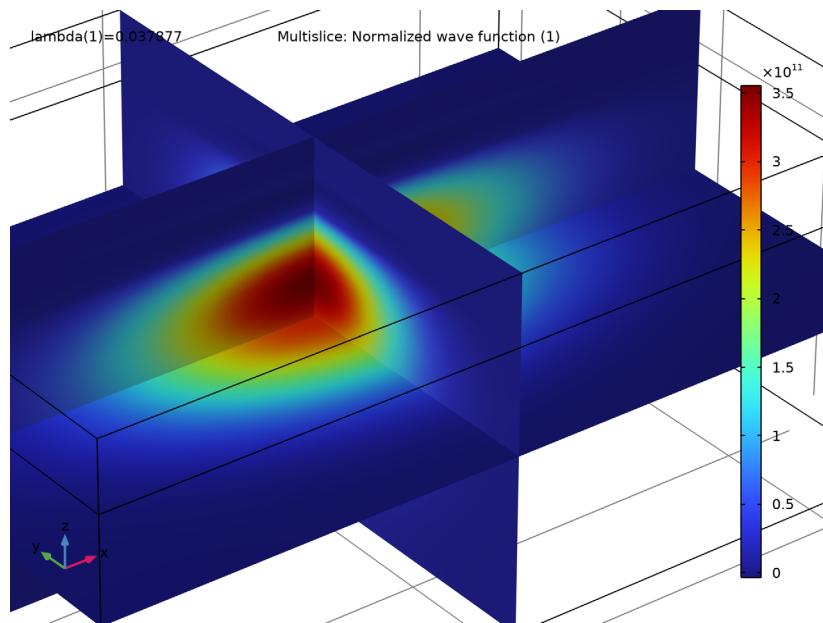
### *Eigenvalue*

- 1 In the **Model Builder** window, expand the **Results>Derived Values** node, then click **Eigenvalue**.
- 2 In the **Settings** window for **Global Evaluation**, click  **Evaluate**.

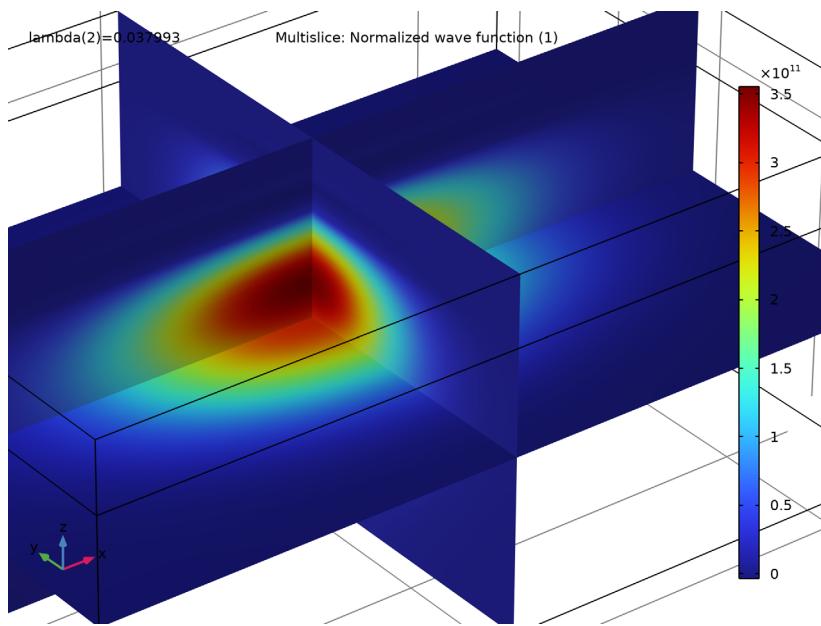
By default only the first wave-function component (in this model: the spin-up component; `schr.Psi_psiu`) is plotted. Take a look at the real part of the first wave-function component for the ground state and the first excited state. We see that they have the same shape except a slight shift in the x direction.

### *Normalized Wave Function (schr)*

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



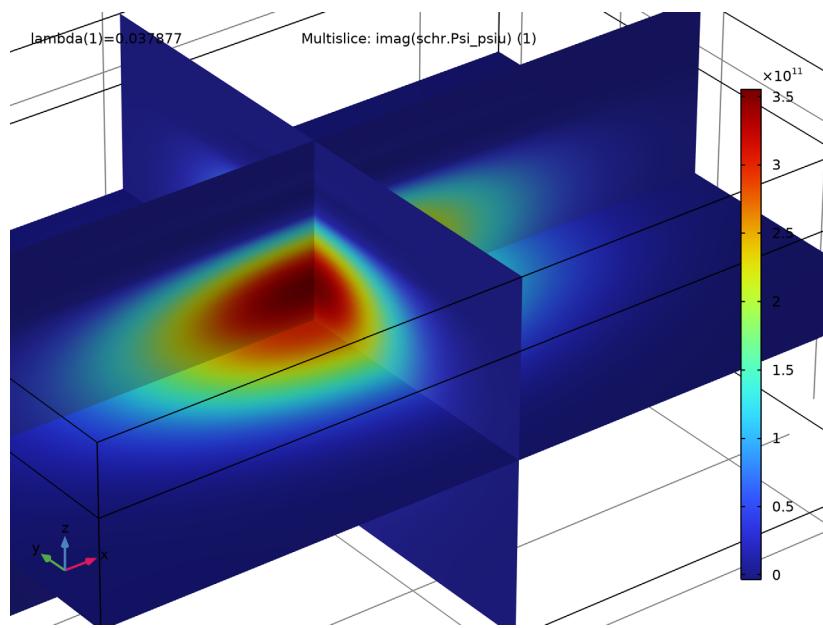
**2** In the **Settings** window for **3D Plot Group**, click  **Plot Next**.



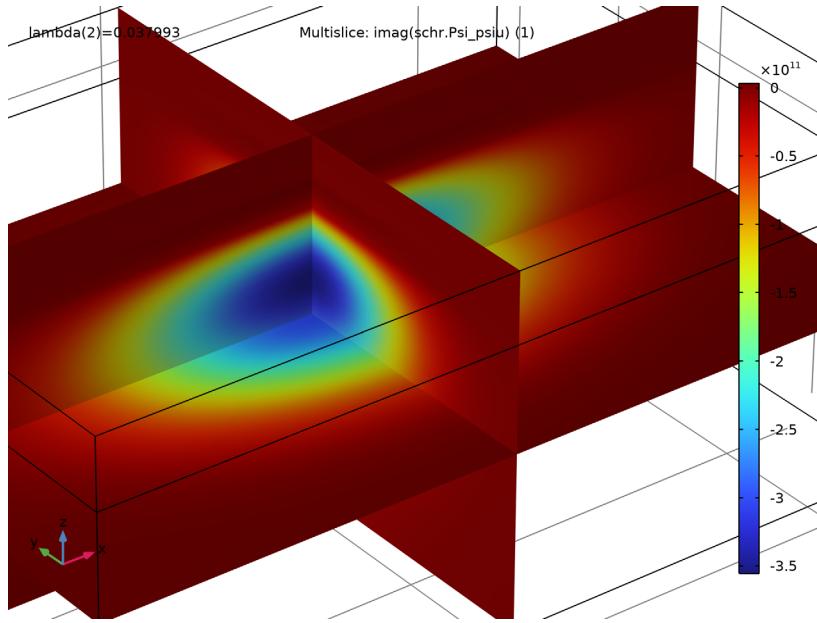
Now take a look at the imaginary part of the first wave-function component for the ground state and the first excited state.

*Normalized Wave Function (schr) I*

I In the **Model Builder** window, click **Normalized Wave Function (schr) I**.



- 2** In the **Settings** window for **3D Plot Group**, click  **Plot Next**.



As the figures show, the imaginary parts have the same shape and magnitude as the real parts and the sign of the imaginary part of the wave function is flipped for the first excited state.

Repeating the procedure for the other wave-function component (spin-down; `schr.Psi_psid`) shows that all real and imaginary parts for the first two eigenstates have the same shape and magnitude among themselves and also as those for the spin-up component, except some slight shift in the x direction and some sign flips.

To understand the meaning of this observation, first create a point dataset to evaluate the wave-function components near the peak density point.

#### *Cut Point 3D 1*

- 1** In the **Results** toolbar, click  **Cut Point 3D**.
- 2** In the **Settings** window for **Cut Point 3D**, locate the **Point Data** section.
- 3** In the **X** text field, type 0.
- 4** In the **Y** text field, type 0.
- 5** In the **Z** text field, type -2.

#### *Evaluation Group 1 - Wave functions*

- 1** In the **Results** toolbar, click  **Evaluation Group**.

- 2 In the **Settings** window for **Evaluation Group**, type **Evaluation Group 1 - Wave functions** in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Cut Point 3D I**.
- 4 From the **Eigenvalue selection** list, choose **Manual**.
- 5 In the **Eigenvalue indices (1-9)** text field, type **1 2**.

#### *Point Evaluation I*

- 1 Right-click **Evaluation Group I - Wave functions** and choose **Point Evaluation**.
- 2 In the **Settings** window for **Point Evaluation**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
schr.Psi_psiu/3.56575008131e11	1	up
schr.Psi_psid/3.56575008131e11	1	down

- 4 In the **Evaluation Group I - Wave functions** toolbar, click  **Evaluate**.

We see that for the ground state, up to an overall scaling factor of about 3.6e11, the amplitude of the spin-up component is  $1+i = (1)(1+i)$ , and the amplitude of the spin-down component is  $1-i = (-i)(1+i)$ . Therefore the vector formed by the two components is proportional to  $(1,-i)$ , which is recognized as the spin-down eigenstate of the y-spin operator  $S_y$ . This is consistent with the intuitive picture that the lowest energy state of an electron in a magnetic field has its spin magnetic moment parallel to the magnetic field and thus the spin is anti-parallel to the magnetic field.

#### **EVALUATION GROUP I - WAVE FUNCTIONS**

- 1 Go to the **Evaluation Group I - Wave functions** window.

Similarly for the first excited state, up to an overall scaling factor of about 3.6e11, the amplitude of the spin-up component is seen to be  $1-i = (1)(1-i)$ , and the amplitude of the spin-down component is  $1+i = (+i)(1-i)$ . Therefore the vector formed by the two components is proportional to  $(1,+i)$ , which is recognized as the spin-up eigenstate of the y-spin operator  $S_y$ . This is consistent with the intuitive picture that the higher energy state of an electron in a magnetic field has its spin magnetic moment anti-parallel to the magnetic field and thus the spin is parallel to the magnetic field.

This observation can be further confirmed by comparing the energy difference between the two computed eigenstates with the expected energy difference between a spin-up and a spin-down electron in a uniform magnetic field, using global evaluations. Choose the

ground state as the evaluation dataset, and use the `withsol` operator to pick up the eigenenergy of the first excited state.

## RESULTS

### Evaluation Group 2 - Compare energy difference

- 1 In the **Results** toolbar, click  **Evaluation Group**.
- 2 In the **Settings** window for **Evaluation Group**, type **Evaluation Group 2 - Compare energy difference** in the **Label** text field.
- 3 Locate the **Data** section. From the **Eigenvalue selection** list, choose **First**.

### Global Evaluation 1

- 1 Right-click **Evaluation Group 2 - Compare energy difference** and choose **Global Evaluation**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
<code>withsol('sol1',schr.Ei, setind(lambda,2))-schr.Ei</code>	meV	Computed energy difference
<code>2*uB*B</code>	meV	Expected energy difference

- 4 In the **Evaluation Group 2 - Compare energy difference** toolbar, click  **Evaluate**.

We see a very good agreement of the computed and the expected energy difference between the first two eigenstates.

Next, create a cut plane dataset and a 2D plot to compare with Supplementary Figure 1 of the reference paper. Use automatic view scale for the 2D plot to magnify the vertical direction.

### Cut Plane 1

- 1 In the **Results** toolbar, click  **Cut Plane**.
- 2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.
- 3 From the **Plane** list, choose **XZ-planes**.

### Supplementary Figure 1

- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type **Supplementary Figure 1** in the **Label** text field.

- 3** Locate the **Color Legend** section. Select the **Show maximum and minimum values** check box.

#### *Surface 1*

- 1** Right-click **Supplementary Figure 1** and choose **Surface**.
- 2** In the **Settings** window for **Surface**, locate the **Expression** section.
- 3** In the **Expression** text field, type `schr.Pr.`
- 4** In the **Unit** field, type  $1/\text{cm}^3$ .
- 5** Locate the **Coloring and Style** section. From the **Coloring** list, choose **Gradient**.
- 6** From the **Top color** list, choose **Blue**.
- 7** From the **Bottom color** list, choose **Gray**.

#### *Arrow Surface 1*

- 1** In the **Model Builder** window, right-click **Supplementary Figure 1** and choose **Arrow Surface**.
- 2** In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (compl)> Schrödinger Equation>schr.PiX,...,schr.PiZ - Kinetic momentum density**.
- 3** Locate the **Arrow Positioning** section. Find the **x grid points** subsection. In the **Points** text field, type 30.
- 4** Locate the **Coloring and Style** section. From the **Arrow length** list, choose **Logarithmic**.
- 5** Select the **Scale factor** check box. In the associated text field, type  $1e5$ .
- 6** In the **Model Builder** window, expand the **Results>Views** node.

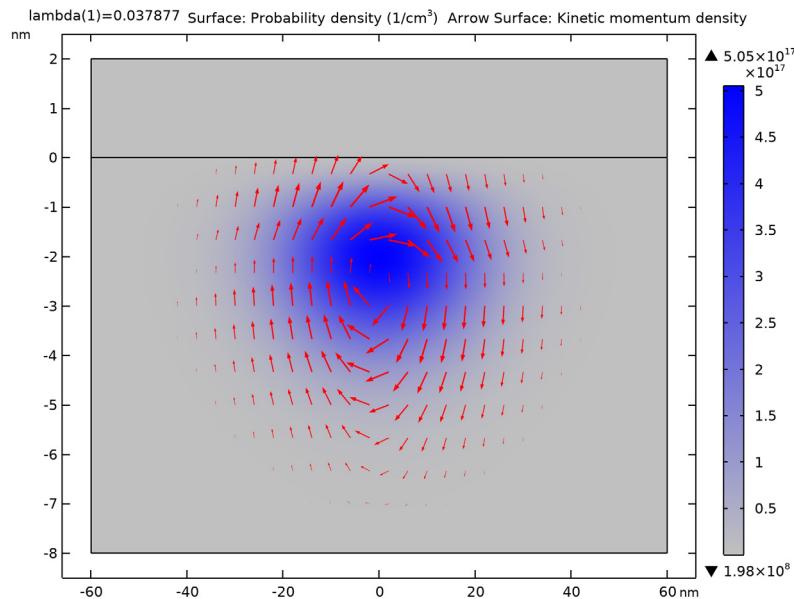
#### *Axis*

- 1** In the **Model Builder** window, expand the **Results>Views>View 2D 2** node, then click **Axis**.
- 2** In the **Settings** window for **Axis**, locate the **Axis** section.
- 3** From the **View scale** list, choose **Automatic**.
- 4** Click  **Update**.

#### *Supplementary Figure 1*

- 1** Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 2** In the **Model Builder** window, under **Results** click **Supplementary Figure 1**.

- 3 In the **Supplementary Figure 1** toolbar, click **Plot**.



Finally create a 3D plot of the eighth excited state for the model thumbnail. Use an isosurface plot to show the probability density with a filter subnode to cut out a quadrant to show the surfaces clearer and a transparent subnode for additional visual effects. Use an arrow plot to show the kinetic momentum density.

#### *Eighth excited state*

- 1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type **Eighth excited state** in the **Label** text field.
- 3 Click .
- 4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.
- 5 Click the **Show Grid** button in the **Graphics** toolbar.
- 6 Click the **Show Legends** button in the **Graphics** toolbar.

#### *Isosurface 1*

- 1 Right-click **Eighth excited state** and choose **Isosurface**.
- 2 In the **Settings** window for **Isosurface**, locate the **Expression** section.
- 3 In the **Expression** text field, type **schr.Pr.**

- 4 In the **Unit** field, type  $1/\text{cm}^3$ .
- 5 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.
- 6 Click  **Range**.
- 7 In the **Range** dialog box, choose **Number of values** from the **Entry method** list.
- 8 In the **Start** text field, type  $0.2\text{e}17$ .
- 9 In the **Stop** text field, type  $3.2\text{e}17$ .
- 10 In the **Number of values** text field, type 5.
- II Click **Replace**.

#### *Filter* /

- 1 Right-click **Isosurface 1** and choose **Filter**.
- 2 In the **Settings** window for **Filter**, locate the **Element Selection** section.
- 3 In the **Logical expression for inclusion** text field, type  $x>0.1[\text{nm}] \ || \ z<-2[\text{nm}]$ .

#### *Transparency* /

- 1 In the **Model Builder** window, right-click **Isosurface 1** and choose **Transparency**.
- 2 In the **Settings** window for **Transparency**, locate the **Transparency** section.
- 3 In the **Transparency** text field, type 0.4.

#### *Arrow Volume* /

- 1 In the **Model Builder** window, right-click **Eighth excited state** and choose **Arrow Volume**.
- 2 In the **Settings** window for **Arrow Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (compl)> Schrödinger Equation>schr.PiX,...,schr.PiZ - Kinetic momentum density**.
- 3 Locate the **Arrow Positioning** section. Find the **X grid points** subsection. In the **Points** text field, type 26.
- 4 Find the **Y grid points** subsection. From the **Entry method** list, choose **Coordinates**.
- 5 In the **Coordinates** text field, type -30 30.
- 6 Find the **Z grid points** subsection. In the **Points** text field, type 15.
- 7 Locate the **Coloring and Style** section.
- 8 Select the **Scale factor** check box. In the associated text field, type  $1\text{e}7$ .
- 9 From the **Color** list, choose **Magenta**.

10 In the **Eighth excited state** toolbar, click  **Plot**.

