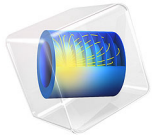


k·p Method for Strained Wurtzite GaN Band Structure

This benchmark model computes the valence band structure of an unstrained and a strained bulk GaN wurtzite crystal, as a tutorial for users who wish to set up multiple wave-function components with the Schrödinger Equation interface. The model follows the formulation given in the reference paper by Chuang and Chang (Ref. 1). The diagonal and off-diagonal elements of the Hamiltonian matrix are entered using built-in features, with detailed instructions in the model documentation. The computed eigenvalues agree well with the analytic solution and Fig. 5 in the paper.

Introduction

For the Schrödinger Equation physics interface, if the wave function has more than one component, then the Hamiltonian becomes a matrix. The number of elements of the matrix grows as the square of the number of wave-function components. Each element can include several terms of zero, one, or two partial derivatives. A number of built-in features have been created to provide flexible and efficient ways to enter these terms into the graphical user interface within limited window size.

Because the main purpose of this model is to illustrate the usage of these built-in features, a particularly simple system of bulk GaN crystal is chosen for clarity. Specifically, the model uses the upper left 3-by-3 matrix of the block-diagonalized 6-by-6 Hamiltonian for the demonstration. Once you have understood the procedure for setting up this simple Hamiltonian matrix, you should be able to build your own models of higher complexity.

An additional benefit of this simple system is that an analytic formula for the matrix elements exists and the result from the solution of the Schrödinger Equation can be compared against the eigenvalues of the 3-by-3 matrix equation with analytic coefficients.

Model Definition

Gallium nitride (GaN) is an important wideband-gap semiconductor material for optoelectronics, high-power, and high-frequency applications. Chuang and Chang published their derivation and computation of the 6-by-6 Hamiltonian matrix for wurtzite crystals including GaN in 1996 (Ref. 1). In Eq. (45) of the paper, the 6-by-6 Hamiltonian matrix is block diagonalized, and the upper left 3-by-3 matrix reads

$$H^U = \begin{bmatrix} F & K_t & -iH_t \\ K_t & G & \Delta - iH_t \\ iH_t & \Delta + iH_t & \lambda \end{bmatrix} \tag{1}$$

The matrix elements are given by Eqs. (34) and (42) in Ref. 1. To compare with Fig. 5 in the paper, set the crystal momentum k_y to zero. For the Schrödinger Equation interface, k_x and k_z are replaced by the partial derivatives $i\partial/\partial x$ and $i\partial/\partial z$, respectively. 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 $\exp(ikx-i\omega t)$.

As an example of entering the matrix elements into the graphical user interface, consider the element F at the (1,1) position of the 3-by-3 Hamiltonian matrix. Eq. (34) in the paper gives

$$F = \Delta_1 + \Delta_2 + \lambda + \theta \tag{2}$$

$$\lambda = \frac{\hbar^2}{2m_e}\left[i\frac{\partial}{\partial z}A_1 i\frac{\partial}{\partial z} + i\frac{\partial}{\partial x}A_2 i\frac{\partial}{\partial x}\right] + \lambda_\varepsilon \tag{3}$$

$$\theta = \frac{\hbar^2}{2m_e}\left[i\frac{\partial}{\partial z}A_3 i\frac{\partial}{\partial z} + i\frac{\partial}{\partial x}A_4 i\frac{\partial}{\partial x}\right] + \theta_\varepsilon \tag{4}$$

$$\lambda_\varepsilon = D_1\varepsilon_{zz} + D_2(\varepsilon_{xx} + \varepsilon_{yy}) \tag{5}$$

$$\theta_\varepsilon = D_3\varepsilon_{zz} + D_4(\varepsilon_{xx} + \varepsilon_{yy}) \tag{6}$$

In Equation 3 and Equation 4, the partial derivative on the left side is understood to operate on both the A_i coefficient and the wave function (not explicitly displayed on the right end). In general, the A_i coefficients and other material parameters can be spatially varying, for example, in heterostructures or quantum dots. Here, for the simple case of a bulk crystal, all of these parameters are constants.

The first terms in Equation 3 and Equation 4 involve second-order derivatives, while the last terms λ_ε and θ_ε are strain-dependent constants given by the formulas Equation 5 and Equation 6. The built-in features **Second Order Hamiltonian** and **Zeroth Order Hamiltonian** (or **Electron Potential Energy** for diagonal elements) will be used to enter each type of terms in the model, respectively, as detailed in the Modeling Instructions section.

Since the model solves for the bulk crystal, it suffices to create a small square domain (smaller than the smallest wavelength of interest), and use the **Floquet-Bloch** periodic boundary conditions. In this case, a small number of mesh elements is enough.

For the analytic solution, a global equation is used to set up the 3-by-3 matrix equation. The **All** option of the **Eigenvalue search method** is used to obtain all 3 eigenvalues.

Results and Discussion

Figure 1 and Figure 2 show the computed unstrained and strained heavy hole (HH), light hole (LH), and crystal-field split-off hole (CH) dispersions along the positive x-axis and negative z-axis directions, agreeing well with analytic solution (circles) and Fig. 5 in Ref. 1.

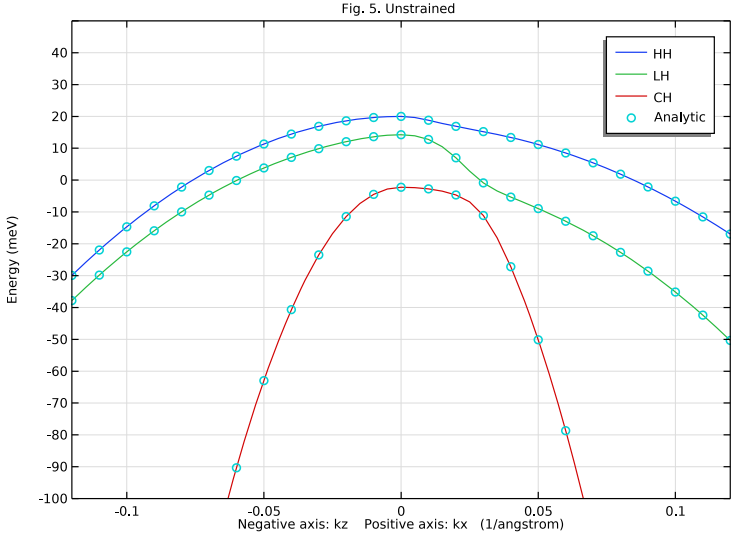


Figure 1: Unstrained valence band structure of bulk GaN wurtzite crystal.

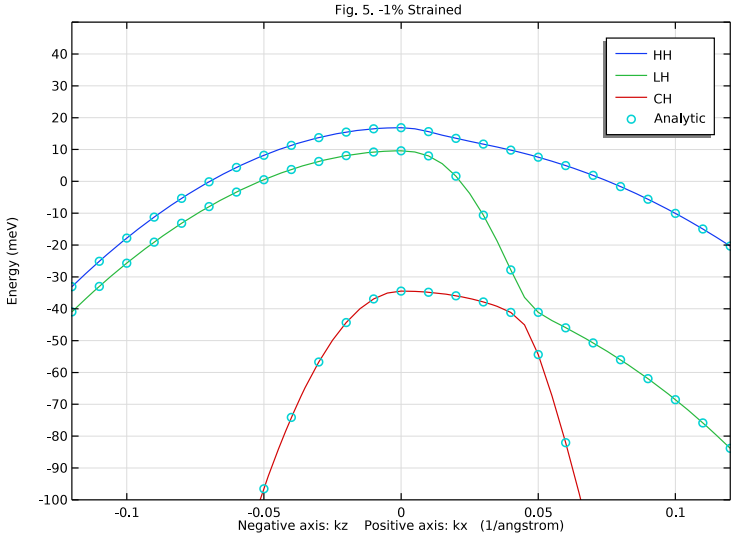


Figure 2: Strained valence band structure of bulk GaN wurtzite crystal.

Figure 3 compares the 2D band energy surfaces along the x and z directions for the 3 valence bands between computed values (color surface) and analytic solution (gray wireframe). The agreement is very good.

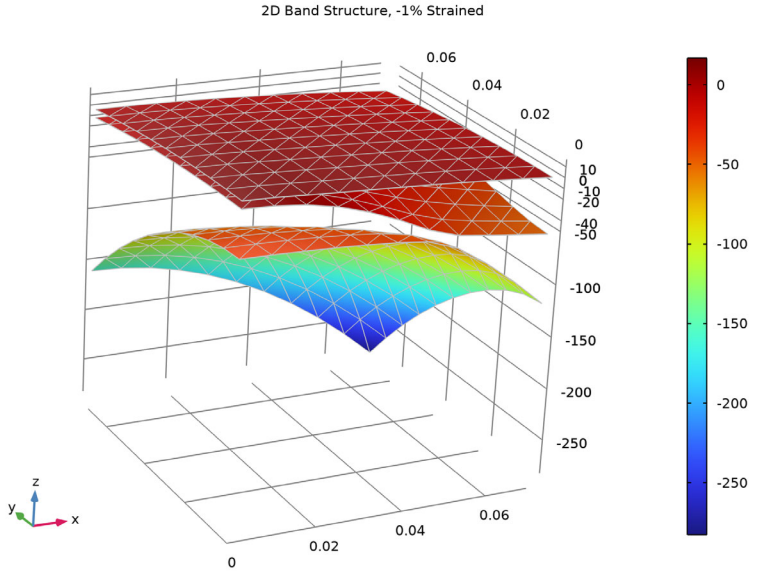


Figure 3: Strained valence band structure of bulk GaN wurtzite crystal.

Reference

1. S.L. Chuang and C.S. Chang, "k·p method for strained wurtzite semiconductors," *Phys. Rev. B*, vol. 54, p. 2491, 1996.

Application Library path: `Semiconductor_Module/Verification_Examples/k_dot_p_method_strained_wurtzite_gan_band_structure`

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**.

Since there are 3 valence bands of interest, set the number of wave function components to 3.

4 In the **Number of wave function components** text field, type 3.

5 Click **Study**.

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

7 Click **Done**.

GEOMETRY 1

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

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

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

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

The geometry can be a simple square for setting up the Floquet-Bloch boundary conditions. The size of the domain should be smaller than the shortest wavelength, to prevent spurious modes (a related mechanical model is thin_film_baw_resonator_dispersion_diagram in the MEMS Module, where a narrow domain is used).

Square 1 (sq1)

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

2 In the **Settings** window for **Square**, click **Build All Objects**.

In this 2D model we will look at the valence band dispersion along the x and z directions. Change the default second axis name from y to z for clarity.

COMPONENT 1 (COMP1)

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

2 In the **Settings** window for **Component**, locate the **Frames** section.

3 Find the **Spatial frame coordinates** subsection. In the table, enter the following settings:

First	Second	Third
x	z	y

4 Find the **Material frame coordinates** subsection. In the table, enter the following settings:

First	Second	Third
X	Z	Y

Enter the GaN material parameters as listed in Table III of Chuang and Chang's paper. Only the valence band parameters are needed for this model. First enter the energy parameters Δ_1, Δ_{so}, Δ_2, Δ_3, and Δ.

GLOBAL DEFINITIONS

Parameters 1 - GaN

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

2 In the **Settings** window for **Parameters**, type `Parameters 1 - GaN` in the **Label** text field.

3 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
Del1	16[meV]	2.5635E-21 J	Energy parameters
Delso	12[meV]	1.9226E-21 J	
Del2	Delso/3	6.4087E-22 J	
Del3	4[meV]	6.4087E-22 J	
Del	sqrt(2)*Del3	9.0633E-22 J	

Next enter the valence band effective-mass parameters $A_1 \sim A_6$.

4 In the table, enter the following settings:

Name	Expression	Value	Description
A1	-6.56	-6.56	Valence band effective mass parameters
A2	-0.91	-0.91	
A3	5.65	5.65	
A4	-2.83	-2.83	
A5	-3.13	-3.13	
A6	-4.86	-4.86	

Next enter the deformation potentials $D_1 \sim D_4$.

5 In the table, enter the following settings:

Name	Expression	Value	Description
D1	0.7[eV]	1.1215E-19 J	Deformation potentials
D2	2.1[eV]	3.3646E-19 J	
D3	1.4[eV]	2.243E-19 J	
D4	-0.7[eV]	-1.1215E-19 J	

Next enter the elastic stiffness constants C_{13} and C_{33}.

6 In the table, enter the following settings:

Name	Expression	Value	Description
C13	15.8e11[dyn/cm^2]	1.58E11 N/m²	Elastic stiffness constants
C33	26.7e11[dyn/cm^2]	2.67E11 N/m²	

Finally to prevent too long a list of parameters when setting up sweeps, exclude these parameters from the selection list.

7 Click to expand the **Visibility** section. Clear the **Show in parameter selections** check box.

Now set up the swept parameters.

Parameters 2 - Sweeps

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type Parameters 2 - Sweeps in the **Label** text field.

3 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
epsxx	-0.01	-0.01	Strain,xx
epsyy	epsxx	-0.01	Strain,yy
epszz	-2*C13/C33*epsxx	0.011835	Strain,zz

To conveniently create a plot to compare with Fig. 5 in the paper, set up a swept parameter kp such that its positive axis represents the kx axis and the negative axis represents the kz axis.

4 In the table, enter the following settings:

Name	Expression	Value	Description
kp	0[rad/nm]	0 rad/m	Positive axis: kx, negative axis: kz
kx	if(kp>0,kp,0[rad/nm])	0 rad/m	
ky	0[rad/nm]	0 rad/m	
kz	if(kp<0,-kp,0[rad/nm])	0 rad/m	

For comparing with analytic solutions, enter the formulas from Eq. (34) and Eq. (42) in the paper. These parameters also are not needed to be in the selection list. In these formulas, the wave vectors kx and kz are numerical parameters. Therefore a 3X3 Hermitian matrix can be constructed and diagonalized to provide the eigenvalues for analytic comparison. Later on when setting up the Schrödinger equation, the wave vectors kx and kz will be replaced by differential operators, not just numbers. This distinction should be kept in mind. First enter the diagonal parameters F, G, λ, λ_ε, θ, and θ_ε in Eq. (34).

Parameters 3 - Analytic formula

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type Parameters 3 - Analytic formula in the **Label** text field.

3 Locate the **Visibility** section. Clear the **Show in parameter selections** check box.

4 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
F	Del1+Del2+lm+th	2.7003E-21 J	Eq. (34)
G	Del1-Del2+lm+th	1.4186E-21 J	
lm	hbar_const^2/2/me_const*(A1*kz^2+A2*(kx^2+ky^2))+lmeps	-5.4018E-21 J	
lmeps	D1*epszz+D2*(epsxx+epsyy)	-5.4018E-21 J	
th	hbar_const^2/2/me_const*(A3*kz^2+A4*(kx^2+ky^2))+theps	4.8977E-21 J	
theps	D3*epszz+D4*(epsxx+epsyy)	4.8977E-21 J	

Then enter the off-diagonal terms K_t and H_t in Eq. (42).

5 In the table, enter the following settings:

Name	Expression	Value	Description
Kt	hbar_const^2/2/me_const*A5*kt^2	0 J	Eq. (42)
Ht	hbar_const^2/2/me_const*A6*kt*kz	0 J	
kt	sqrt(kx^2+ky^2)	0 rad/m	

Set up a global equation to diagonalize the 3X3 Hermitian matrix - the upper-left Hamiltonian in Eq. (45) in the paper. Use the reserved name `lambda` for the eigenvalue in the global equation. Scale the Hamiltonian with the energy scale of 1 meV so that the source term is about order of unity, and the eigenenergy is the eigenvalue in the unit of meV. Add some blank spaces in the expressions to align the columns of the matrix.

ADD PHYSICS

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

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

3 In the tree, select **Mathematics>ODE and DAE Interfaces>Global ODEs and DAEs (ge)**.

4 Click **Add to Component 1** in the window toolbar.

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

GLOBAL ODES AND DAES (GE)

Global Equations 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Global ODEs and DAEs (ge)** click **Global Equations 1**.

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
u1	(F * u1+Kt *u2-i*Ht *u3)/ 1[meV]- lambda* u1	0	0	
u2	(Kt * u1+G *u2+ (Del-i* Ht)*u3)/ 1[meV]- lambda* u2	0	0	
u3	(i*Ht* u1+(Del+ i*Ht)* u2+lm *u3)/ 1[meV]- lambda* u3	0	0	

The text is yellow colored because at this point the eigenvalue variable `lambda` is not defined yet.

Set up the physics. Unlike the analytic formulas where everything is a number, here in the Schrödinger equation the wave vectors `kx` and `kz` will be replaced by differential operators. Thus some terms contain just numbers while others contain operators, and they will be entered in different physics features. Some patience and attention to details will help a lot to avoid mistakes. (To compare with Fig. 5 in the paper and for simplicity, let `ky` stay at zero.)

For example, consider the (1,1) element of the matrix $F = \Delta_1 + \Delta_2 + \lambda + \theta$. It contains terms that are just numbers: $\Delta_1 + \Delta_2 + \lambda_\varepsilon + \theta_\varepsilon$. It also has terms containing the wave vectors `kx` and `kz`, which will be replaced by the differential operators id/dx and id/dz, respectively (the differentiations here and next are partial derivatives). 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 $exp(ikx - i\omega t)$. Thus the terms for F that contains differential operators are $(hbar^2/2m_e)(id/dz)(A_1 + A_3)(id/dz)$ and $(hbar^2/2m_e)(id/dx)(A_2 + A_4)(id/dx)$.

Since these two terms have second order differentiations, they are entered using the **Second Order Hamiltonian** feature. Each term occupies one row in the **Hamiltonian input table**. The position (1,1) in the matrix and the two differentiation operators are specified by drop-down menus. The A parameters are entered in the input field. A factor of $(hbar^2/2m_e)$ is already included in the feature.

SCHRÖDINGER EQUATION (SCHR)

To conveniently create a plot to compare with Fig. 5 in the paper, set the eigenvalue scale to the same energy unit as the vertical axis (meV), so that the eigenvalue takes on the numerical value of the eigenenergy in the same unit (meV).

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Schrödinger Equation (schr)**.
2. In the **Settings** window for **Schrödinger Equation**, locate the **Model Properties** section.
3. Find the **Eigenvalue study** subsection. In the λ_{scale} text field, type `1[meV]`.

Second Order Hamiltonian 1: Diagonal F, G, lambda

1. In the **Physics** toolbar, click **Domains** and choose **Second-Order Hamiltonian**.
2. In the **Settings** window for **Second-Order Hamiltonian**, type `Second Order Hamiltonian 1: Diagonal F, G, lambda` 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)	Left differential operator (i)	A parameter (l)	Right differential operator (j)	Description
1	1	i ?/?z	A1+A3	i ?/?z	F: lambda+ theta

Note in the table how one differential operator is located on the left side of the A parameter and the other one is on the right. In general, such as in heterostructures or quantum dots, the A parameter can be spatially varying. In those cases, the differential operator on the left side acts on both the A parameter and the wave function. This is shown in the Equation section as well. Here for bulk material the A parameter is just a constant. Now add a row for the other term $(hbar^2/2m_e)(id/dx)(A_2 + A_4)(id/dx)$.

5 Click + **Add**.

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

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (l)	Right differential operator (j)	Description
1	1	i ?/?x	A2+A4	i ?/?x	F: lambda+ theta

This finishes the two terms with differential operators for the (1,1) element of the matrix F. Before entering the terms that are just numbers for F, while we are still in this feature, enter the terms with differential operators for the (2,2) and (3,3) elements G and λ.

The following instructions add the contributions from G and λ one row at a time. Alternatively, it is possible to save some time by copying and pasting. For example, since the contribution to the second order Hamiltonian from F is the same as the one from G, except the position in the matrix is different - F is at (1,1) and G is at (2,2), we can select the two rows for F in the table by mouse drag, right-click to copy, click on the **Add** button to add a new row, and then right click the first cell of the new row to paste the two rows that have been copied. After that, change the position of the two pasted rows from (1,1) to (2,2) and update the description from F to G, leaving the differential operators and the A parameters the same as the ones for F.

7 Click + **Add**.

8 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
2	2	i ?/?z	A1+A3	i ?/?z	G: lambda+ theta

9 Click + **Add**.

10 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
2	2	i ?/?x	A2+A4	i ?/?x	G: lambda+ theta

11 Click + **Add**.

12 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
3	3	i ?/?z	A1	i ?/?z	lambda

13 Click + **Add**.

14 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
3	3	i ?/?x	A2	i ?/?x	lambda

The **Second Order Hamiltonian** feature that we just finished entering for the diagonal elements corresponds to the kinetic energy terms normally added by the default **Effective Mass** feature. So we should disable it to remove the unwanted default contribution to the Hamiltonian.

Effective Mass 1

In the **Model Builder** window, right-click **Effective Mass 1** and choose **Disable**.

Now enter the terms that are just numbers for the 3 diagonal elements F, G and λ. They are $\Delta_1 + \Delta_2 + \lambda_{\varepsilon} + \theta_{\varepsilon}$ for F, $\Delta_1 - \Delta_2 + \lambda_{\varepsilon} + \theta_{\varepsilon}$ for G, and simply λ_{ε} for λ. For the diagonal elements, it is easiest to use the default **Electron Potential Energy** feature.

Electron Potential Energy 1: Diagonal F, G, lambda

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: Diagonal F, G, lambda` in the **Label** text field.

3 Locate the **Electron Potential Energy** section. In the $V_{e,11}$ text field, type `Del1+Del2+lmeps+theps`.

4 In the $V_{e,22}$ text field, type `Del1-Del2+lmeps+theps`.

5 In the $V_{e,33}$ text field, type `lmeps`.

We have finished entering the 3 diagonal elements F, G and λ. Now enter the off-diagonal elements. Again some are just numbers (Δ), and others have partial derivatives (K_t and H_t). They will be entered into different features. First the ones with partial derivatives.

Second Order Hamiltonian 2: Off-diagonal Kt, Ht

1 In the **Physics** toolbar, click **Domains** and choose **Second-Order Hamiltonian**.

2 In the **Settings** window for **Second-Order Hamiltonian**, type `Second Order Hamiltonian 2: Off-diagonal Kt, Ht` 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)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
1	2	i ?/?x	A5	i ?/?x	Kt

5 Click **Add**.

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

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
2	1	i ?/?x	A5	i ?/?x	Kt

7 Click **Add**.

8 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
1	3	i ?/?x	-i*A6	i ?/?z	Ht

9 Click + **Add**.

10 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
3	1	i ?/?x	i*A6	i ?/?z	Ht

11 Click + **Add**.

12 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
2	3	i ?/?x	-i*A6	i ?/?z	Ht

13 Click + **Add**.

14 In the **Hamiltonian input table** table, enter the following settings:

Hamiltonian row index (m)	Hamiltonian column index (n)	Left differential operator (i)	A parameter (1)	Right differential operator (j)	Description
3	2	i ?/?x	i*A6	i ?/?z	Ht

Finally enter the off-diagonal elements that are just numbers (Δ), using the **Zeroth Order Hamiltonian** feature. 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 1: Off-diagonal Delta

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: Off-diagonal Delta` 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 (1/m^2)	Description
2	3	`Del*2*me_const/hbar_const^2`	`Delta`

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 (1/m^2)	Description
3	2	`Del*2*me_const/hbar_const^2`	`Delta`

Next set up the Floquet-Bloch periodic boundary conditions. Use the parameters `kx` and `kz` for the wave vector. Select opposing boundary pairs.

Periodic Condition 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

2 Select Boundaries 1 and 4 only.

3 In the **Settings** window for **Periodic Condition**, locate the **Periodicity Settings** section.

4 From the **Type of periodicity** list, choose **Floquet-Bloch periodicity**.

5 Specify the $\mathbf{k}_F$ vector as

kx	X
kz	Z

Periodic Condition 2

1 Right-click **Periodic Condition 1** and choose **Duplicate**.

2 In the **Settings** window for **Periodic Condition**, locate the **Boundary Selection** section.

3 Click **Clear Selection**.

4 Select Boundaries 2 and 3 only.

Now set up the mesh. Since we have created a domain that is much smaller than the wavelength, there is no need for many mesh elements. In addition, the periodic boundary

conditions require the meshes on the pair of source and destination boundaries to match. In this case, a simple Mapped Mesh works well.

MESH 1

Mapped 1

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

Distribution 1

1. Right-click **Mapped 1** and choose **Distribution**.
2. In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
3. From the **Selection** list, choose **All boundaries**.
4. Locate the **Distribution** section. In the **Number of elements** text field, type `2`.
5. In the **Mesh** toolbar, click **Build Mesh**.

Set up studies to compute the valence band structure for an unstrained and a 1% compressively strained GaN wurtzite crystal, to be compared to Fig. 5 in the paper. Sweep the parameter `epsxx` for the strain. Sweep the parameter `kp` prepared earlier such that on its negative axis, `kx=0` and `kz=-kp`, while on its positive axis, `kz=0` and `kx=kp`. Use one study for the Schrödinger equation and a second study for the global equation (analytic formula).

STUDY 1: FIG. 5. SCHRÖDINGER EQ.

1. In the **Model Builder** window, click **Study 1**.
2. In the **Settings** window for **Study**, type `Study 1: Fig. 5. Schrödinger Eq.` 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: Fig. 5. Schrödinger Eq.** click **Step 1: Eigenvalue**.
2. In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.
3. In the **Search for eigenvalues around** text field, type `10`.
4. Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Global ODEs and DAEs (ge)**.
5. Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
6. From the **Sweep type** list, choose **All combinations**.
7. Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
epsxx (Strain,xx)	`0 -0.01`	

9 Click + **Add**.

10 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
kp (Positive axis: kx, negative axis: kz)	`range(-0.12,0.005,0.12)`	`1/angstrom`

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

Create plots to compare to Fig. 5 in the paper. First the unstrained case. Make one global plot for each band by selecting the appropriate eigenvalue from the drop-down menu for the dataset.

RESULTS

Fig. 5. Unstrained

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

2 In the **Settings** window for **1D Plot Group**, type `Fig. 5. Unstrained` 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 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `Negative axis: kz  Positive axis: kx  (1/angstrom)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `Energy (meV)`.

9 Locate the **Axis** section. Select the **Manual axis limits** check box.

10 In the **x minimum** text field, type `-0.12`.

11 In the **x maximum** text field, type `0.12`.

12 In the **y minimum** text field, type `-100`.

13 In the **y maximum** text field, type `50`.

Global 1 - Schrödinger Eq. HH

1 Right-click **Fig. 5. Unstrained** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global 1 - Schrödinger Eq. HH` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1: Fig. 5. Schrödinger Eq./ Solution 1 (sol1)**.

4 From the **Parameter selection (epsxx)** list, choose **First**.

5 From the **Eigenvalue selection** list, choose **Last**.

6 Locate the **y-Axis Data** section. Click **Clear Table**.

7 In the table, enter the following settings:

Expression	Unit	Description
`lambda`		HH

8 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **All solutions**.

9 From the **Parameter** list, choose **Expression**.

10 In the **Expression** text field, type `kp/1[angstrom^-1]`.

Global 1 - Schrödinger Eq. LH

1 Right-click **Global 1 - Schrödinger Eq. HH** and choose **Duplicate**.

2 In the **Settings** window for **Global**, type `Global 1 - Schrödinger Eq. LH` in the **Label** text field.

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

4 In the **Eigenvalue indices (1-3)** text field, type 2.

5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`lambda`		LH

Global 1 - Schrödinger Eq. CH

1 Right-click **Global 1 - Schrödinger Eq. LH** and choose **Duplicate**.

2 In the **Settings** window for **Global**, type `Global 1 - Schrödinger Eq. CH` in the **Label** text field.

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

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`lambda`		`CH`

Duplicate the plot for the strained case. Change the plot label and the selection of the strain parameter `epsxx`.

Fig. 5. -1% Strained

1 In the **Model Builder** window, right-click **Fig. 5. Unstrained** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Fig. 5. -1% Strained` in the **Label** text field.

Global 1 - Schrödinger Eq. HH

1 In the **Model Builder** window, expand the **Fig. 5. -1% Strained** node, then click **Global 1 - Schrödinger Eq. HH**.

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

3 From the **Parameter selection (epsxx)** list, choose **Last**.

Global 1 - Schrödinger Eq. LH

1 In the **Model Builder** window, click **Global 1 - Schrödinger Eq. LH**.

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

3 From the **Parameter selection (epsxx)** list, choose **Last**.

Global 1 - Schrödinger Eq. CH

1 In the **Model Builder** window, click **Global 1 - Schrödinger Eq. CH**.

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

3 From the **Parameter selection (epsxx)** list, choose **Last**.

Now set up a study to solve the analytic 3X3 matrix equation configured with the global equation. Use the `All` eigenvalue option to obtain all 3 eigenvalues of the 3X3 matrix equation.

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 **Empty Study**.

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

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

STUDY 1: FIG. 5. SCHRÖDINGER EQ.

Step 1: Eigenvalue

In the **Model Builder** window, under **Study 1: Fig. 5. Schrödinger Eq.** right-click **Step 1: Eigenvalue** and choose **Copy**.

STUDY 2: FIG. 5. ANALYTIC

1. In the **Model Builder** window, click **Study 2**.
2. In the **Settings** window for **Study**, type `Study 2: Fig. 5. Analytic` in the **Label** text field.
3. Locate the **Study Settings** section. Clear the **Generate default plots** check box.
4. Right-click **Study 2: Fig. 5. Analytic** and choose **Paste Eigenvalue**.

Step 1: Eigenvalue

1. In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.
2. From the **Eigenvalue search method** list, choose **All (filled matrix)**.
3. Locate the **Physics and Variables Selection** section. In the table, enter the following settings:

Physics interface	Solve for	Equation form
Schrödinger Equation (schr)		Automatic (Eigenvalue)
Global ODEs and DAEs (ge)	√	Not applicable

4. Locate the **Study Extensions** section. In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
kp (Positive axis: kx, negative axis: kz)	`range(-0.12,0.01,0.12)`	`1/angstrom`

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

Add the analytic solution to the 2 plots to compare with the numerical solution.

RESULTS

Global 1 - Analytic

1. In the **Model Builder** window, right-click **Global 1 - Schrödinger Eq. CH** and choose **Duplicate**.
2. In the **Settings** window for **Global**, type `Global 1 - Analytic` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Fig. 5. Analytic/ Solution 2 (sol2)**.

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

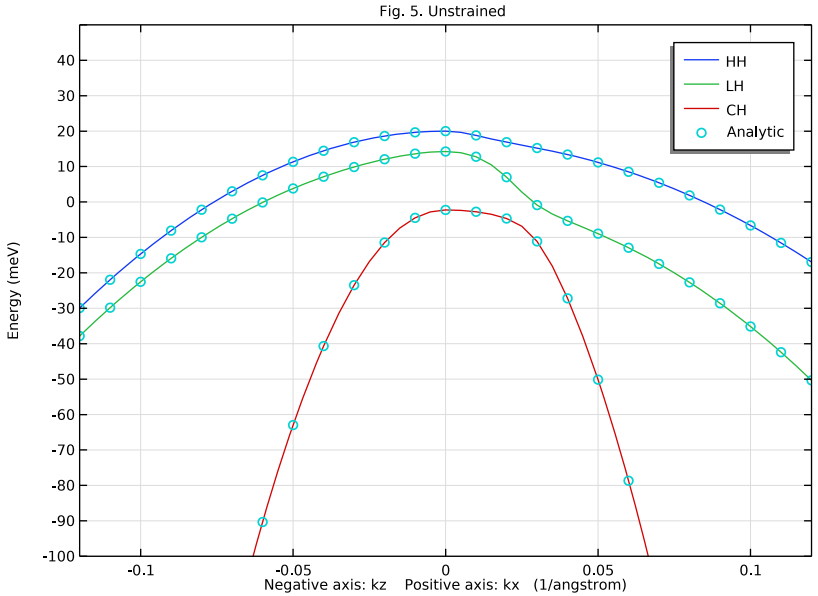
5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`lambda`		`Analytic`

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

7 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

8 In the **Fig. 5. Unstrained** toolbar, click **Plot**.



9 Right-click **Global 1 - Analytic** and choose **Copy**.

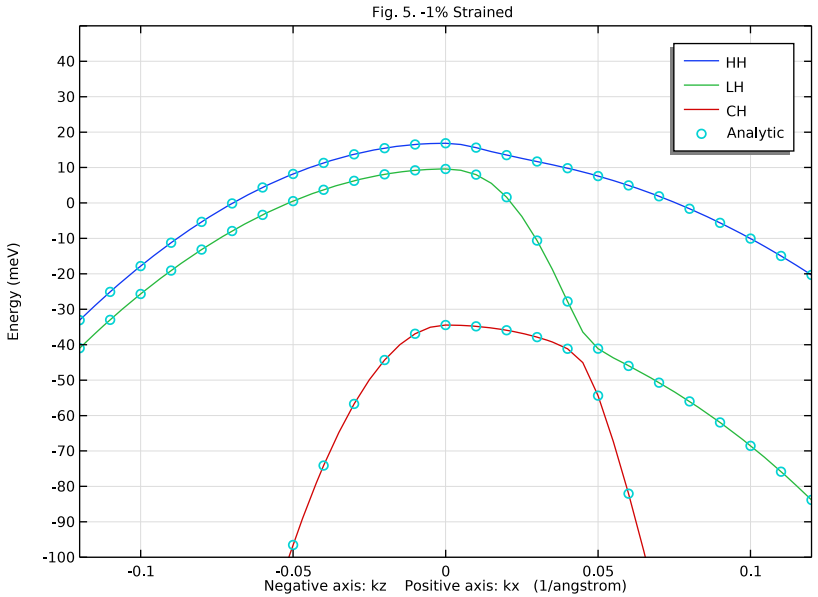
Global 1 - Analytic

1 In the **Model Builder** window, right-click **Fig. 5. -1% Strained** and choose **Paste Global**.

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

3 From the **Parameter selection (epsxx)** list, choose **Last**.

4 In the **Fig. 5. -1% Strained** toolbar, click **Plot**.



Add a new study to compute the 2D band structure in the kx-kz plane, first using the Schrödinger equation.

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 **Empty Study**.

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

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

STUDY 3: 2D DISPERSION SCHRÖDINGER EQ.

1 In the **Settings** window for **Study**, type `Study 3: 2D Dispersion Schrödinger Eq.` in the **Label** text field.

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

STUDY 1: FIG. 5. SCHRÖDINGER EQ.

Step 1: Eigenvalue

In the **Model Builder** window, under **Study 1: Fig. 5. Schrödinger Eq.** right-click **Step 1: Eigenvalue** and choose **Copy**.

STUDY 3: 2D DISPERSION SCHRÖDINGER EQ.

In the **Model Builder** window, right-click **Study 3: 2D Dispersion Schrödinger Eq.** and choose **Paste Eigenvalue**.

Step 1: Eigenvalue

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

2 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
kx	`range(0,0.1,1)*0.07`	`1/angstrom`
kz	`range(0,0.1,1)*0.07`	`1/angstrom`

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

Create one table for each band to plot the 2D band structure using the **Table Surface** plot type for the 3 hole bands. First the heavy hole band (HH).

RESULTS

Evaluation Group 1: HH

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

2 In the **Settings** window for **Evaluation Group**, type `Evaluation Group 1: HH` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: 2D Dispersion Schrödinger Eq./Solution 3 (sol3)**.

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

Global Evaluation 1: Schrödinger eq.

1 Right-click **Evaluation Group 1: HH** and choose **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Global Evaluation 1: Schrödinger eq.` in the **Label** text field.

3 Locate the **Expressions** section. Click **Clear Table**.

4 In the table, enter the following settings:

Expression	Unit	Description
lambda		HH (Schr)

5 In the **Evaluation Group 1: HH** toolbar, click **Evaluate**.

TABLE

1 Go to the **Table** window.

2 Click **Table Surface** in the window toolbar.

RESULTS

Table Surface 1: HH (Schr)

1 In the **Model Builder** window, under **Results>2D Plot Group 3** click **Table Surface 1**.

2 In the **Settings** window for **Table Surface**, type `Table Surface 1: HH (Schr)` in the **Label** text field.

3 Locate the **Data** section. From the **Data column** list, choose **HH (Schr)**.

Height Expression 1

Right-click **Table Surface 1: HH (Schr)** and choose **Height Expression**.

2D Band Structure, -1% Strained

1 In the **Settings** window for **2D Plot Group**, type `2D Band Structure, -1% Strained` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

Then the light hole band (LH).

Evaluation Group 2: LH

1 In the **Model Builder** window, right-click **Evaluation Group 1: HH** and choose **Duplicate**.

2 In the **Settings** window for **Evaluation Group**, type `Evaluation Group 2: LH` in the **Label** text field.

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

4 In the **Eigenvalue indices (1-3)** text field, type `2`.

Global Evaluation 1: Schrödinger eq.

1 In the **Model Builder** window, expand the **Evaluation Group 2: LH** node, then click **Global Evaluation 1: Schrödinger eq.**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
lambda		LH (Schr)

4 In the **Evaluation Group 2: LH** toolbar, click **Evaluate**.

Table Surface 2: LH (Schr)

1 In the **Model Builder** window, right-click **Table Surface 1: HH (Schr)** and choose **Duplicate**.

2 In the **Settings** window for **Table Surface**, type `Table Surface 2: LH (Schr)` in the **Label** text field.

3 Locate the **Data** section. From the **Evaluation group** list, choose **Evaluation Group 2: LH**.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Table Surface 1: HH (Schr)**.

Then the crystal-field split-off hole band (CH).

Evaluation Group 3: CH

1 In the **Model Builder** window, right-click **Evaluation Group 2: LH** and choose **Duplicate**.

2 In the **Settings** window for **Evaluation Group**, type `Evaluation Group 3: CH` in the **Label** text field.

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

Global Evaluation 1: Schrödinger eq.

1 In the **Model Builder** window, expand the **Evaluation Group 3: CH** node, then click **Global Evaluation 1: Schrödinger eq.**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
lambda		CH (Schr)

4 In the **Evaluation Group 3: CH** toolbar, click **Evaluate**.

Table Surface 3: CH (Schr)

1 In the **Model Builder** window, right-click **Table Surface 2: LH (Schr)** and choose **Duplicate**.

2 In the **Settings** window for **Table Surface**, type `Table Surface 3: CH (Schr)` in the **Label** text field.

3 Locate the **Data** section. From the **Evaluation group** list, choose **Evaluation Group 3: CH**.

4 In the **2D Band Structure, -1% Strained** toolbar, click **Plot**.

Finally set up a study to compute the 2D band structure in the kx-kz plane using the global equation of the analytic formula.

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 **Empty Study**.

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

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

STUDY 4: 2D DISPERSION ANALYTIC

1 In the **Settings** window for **Study**, type `Study 4: 2D Dispersion Analytic` in the **Label** text field.

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

STUDY 3: 2D DISPERSION SCHRÖDINGER EQ.

Step 1: Eigenvalue

In the **Model Builder** window, under **Study 3: 2D Dispersion Schrödinger Eq.** right-click **Step 1: Eigenvalue** and choose **Copy**.

STUDY 4: 2D DISPERSION ANALYTIC

In the **Model Builder** window, right-click **Study 4: 2D Dispersion Analytic** and choose **Paste Eigenvalue**.

Step 1: Eigenvalue

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

2 From the **Eigenvalue search method** list, choose **All (filled matrix)**.

3 Locate the **Physics and Variables Selection** section. In the table, enter the following settings:

Physics interface	Solve for	Equation form
Schrödinger Equation (schr)		Automatic (Eigenvalue)
Global ODEs and DAEs (ge)	√	Not applicable

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

Similarly create one table for each band to plot the analytic 2D band structure using the **Table Surface** plot type for the 3 hole bands. Use the **Wireframe** option for the analytic result

to compare to the numerical result by overlaying the plotted surfaces. First the heavy hole band (HH).

RESULTS

Global Evaluation 2: Analytic

1 In the **Model Builder** window, right-click **Global Evaluation 1: Schrödinger eq.** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: 2D Dispersion Analytic/ Solution 4 (sol4)**.

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

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

Expression	Unit	Description
`lambda`		`HH (Anal)`

6 In the **Evaluation Group 1: HH** toolbar, click = **Evaluate**.

Table Surface 4: HH (Anal)

1 In the **Model Builder** window, right-click **Table Surface 1: HH (Schr)** and choose **Duplicate**.

2 In the **Settings** window for **Table Surface**, type `Table Surface 4: HH (Anal)` in the **Label** text field.

3 Locate the **Data** section. From the **Data column** list, choose **HH (Anal)**.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

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

6 Select the **Wireframe** check box.

7 Locate the **Inherit Style** section. From the **Plot** list, choose **Table Surface 1: HH (Schr)**.

8 Clear the **Color** check box.

Then the light hole band (LH).

Global Evaluation 2: Analytic

1 In the **Model Builder** window, right-click **Global Evaluation 1: Schrödinger eq.** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: 2D Dispersion Analytic/ Solution 4 (sol4)**.

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

5 In the **Eigenvalue indices (1-3)** text field, type `2`.

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

Expression	Unit	Description
`lambda`		`LH (Anal)`

7 In the **Evaluation Group 2: LH** toolbar, click = **Evaluate**.

Table Surface 5: LH (Anal)

1 In the **Model Builder** window, right-click **Table Surface 4: HH (Anal)** and choose **Duplicate**.

2 In the **Settings** window for **Table Surface**, type `Table Surface 5: LH (Anal)` in the **Label** text field.

3 Locate the **Data** section. From the **Evaluation group** list, choose **Evaluation Group 2: LH**.

Then the crystal-field split-off hole band (CH).

Global Evaluation 2: Analytic

1 In the **Model Builder** window, right-click **Global Evaluation 1: Schrödinger eq.** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: 2D Dispersion Analytic/ Solution 4 (sol4)**.

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

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

Expression	Unit	Description
`lambda`		`CH (Anal)`

6 In the **Evaluation Group 3: CH** toolbar, click = **Evaluate**.

Table Surface 6: CH (Anal)

1 In the **Model Builder** window, right-click **Table Surface 5: LH (Anal)** and choose **Duplicate**.

2 In the **Settings** window for **Table Surface**, type `Table Surface 6: CH (Anal)` in the **Label** text field.

3 Locate the **Data** section. From the **Evaluation group** list, choose **Evaluation Group 3: CH**.

4 In the **2D Band Structure, -1% Strained** toolbar, click **Plot**.

Use mouse drag to rotate the energy surfaces around to take a look. Ignore the following instructions on setting camera views.

5 In the **Model Builder** window, expand the **Results>Views** node.

Camera

1 In the **Model Builder** window, expand the **Results>Views>View 3D 3** node, then click **Camera**.

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

3 In the **x** text field, type `-0.2`.

4 In the **y** text field, type `-0.4`.

5 In the **z** text field, type `0.2`.

6 Locate the **Up Vector** section. In the **x** text field, type `0.1`.

7 In the **y** text field, type `0.3`.

8 In the **z** text field, type `0.95`.

9 Click **Update**.