16 nextnano software: Examples

16.1 Software

Download the zip file of the next**nano** software. No installation is required. Unzip the file and open "nextnanomat.exe".

16.2 Instruction manual

There are two possibilities to open an input file and start the simulation: The obvious one is in the *'Input'* tab. The second option in the *'Template'* tab that has more options to perform the calculation, e.g. by creating a sweep of parameters.

16.2.1 Input

- **Open input file**
  'File' $\Rightarrow$ 'Open input file...' $\Rightarrow$ `nextnano\nextnanomat\nextnano3 sample files\ParabolicQW_infinite_analytic_1D_nn3.in` $\Rightarrow$ 'Open'

- **Calculation and simulation**
  $\Rightarrow$ Click on the icon 'Save input file and run the simulation (F8)'

To visualize the results, switch to the *'Output'* tab, select the relevant simulation folder on the left side and select the relevant output file on the right.

16.2.2 Template

- **Open input file**
  Select 'Template' or 'Input' tab $\Rightarrow$ Click on $\boxed{...}$ $\Rightarrow$ `nextnano\nextnanomat\nextnano3 sample files\QW_infinite_1D_nn3.in`

- **Create sweep**
  Typically, one wants to sweep parameters such as the quantum well width and compare the corresponding results. This can be achieved by opening the input file within the tab *Template*. Now by selecting 'List of values' or 'Range of values' the chosen variable, such as quantum well width, will be swept automatically.

- **Calculation and simulation**
Click $\boxed{\text{Create input files}}$ $\Rightarrow$ Switch to *'Run'* tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'

16.2.3   Run

The files created in the *'Template'* tab are managed here. By using the icons on the top, simulations can be started and existing input files can be added or removed.

16.2.4   Output

- **Visualization**
Select the relevant simulation folder on the left side and select the relevant output file on the right.

- **Comparing sweep files**
If a value is swept automatically, then the results for different values can be easily compared by choosing the result file for output in the bottom right menu. Then by switching between the simulation folders in the bottom left menu the corresponding result file will be automatically displayed. (Switch per mouse or arrow keys.)

- **Overlay**
By using the $\boxed{+}$ icon, the current data will be added to the overlay and turns gray. Now another output file can be plotted at the same time. New feature: The data in the *Overlay* can be exported and plotted with *gnuplot*.

- **Adjusting the view**
On the left side menu there are several options included to personalize the view, e.g. changing the scale of the axes.

- **History**
Use the green arrows in the top menu to skip back and forward in history.

- **Additional features**
Zoom and export options are available if you right-click in the graph

window. Zoom also works if you draw a rectangle by pressing the left mouse button.

16.3 Black Body Spectrum

`BlackBodySpectrum.in`
In this example we calculate the spectrum of a black body. The software calculates the

- spectral energy density $\rho_\lambda(\lambda, T)$, $\rho_\nu(\nu, T)$, $\rho_\omega(\omega, T)$, $\rho_E(E, T)$
  in units of J/m^3/spectral unit

- spectral radiance (which is *emitted* per m^2 and per unit solid angle sr
  (sr = steradian)
  in units of W/m^2/sr/spectral unit

- spectral irradiance (which is *received* per m^2)
  in units of W/m^2/spectral unit

Each of them are calculated with respect to different spectral units, i.e. the spectral energy density is calculated per *wavelength* λ (m), per *frequency* ν (Hz), per *angular frequency* ω (s^{-1}) and per *photon energy* E (eV). The units are different and also the peaks in the spectra differ, e.g. for the sun ($T = 5778$ K) the peak for $\rho_\lambda(\lambda, T)$ is at $\lambda = 510$ nm (green light) while the peak for $\rho_\nu(\nu, T)$ is at $\nu = 1.5$ THz (infrared). To obtain the *spectral energy density* from the *spectral radiance* one has to multiply the radiance by $4\pi/c$. To obtain the *spectral irradiance* from the *spectral radiance* one has to multiply the radiance by π.

16.3.1 Results

This input file should be opened within the tab *Template* of the next**nano**mat software so that the temperature can be swept automatically. Select 'Template' tab $\Rightarrow$ Click on '...' $\Rightarrow$ 'nextnano\nextnanomat\nextnano3 sample files\BlackBodySpectrum.in' $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'Temperature' $\Rightarrow$ Click on the button 'Create input files' $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'
Then the spectra are calculated. It is recommended to plot the spectra of several temperatures simultaneously in order to see how the height and the

position of the peaks change with temperature. Additional information on the peaks can be found in the file `BlackBody_info.txt`.

For comparison, the spectral irradiance of the sun can be found in the folder `nextnano3\Syntax\Solar cell files\solar spectra\`. The maximum of the cosmic microwave background measured by the COBE satellite ($T = 2.7260\,\text{K}$) is around $\lambda = 1\,\text{mm}$. For solar cells it is important to convert as much photons as possible into electron–hole pairs. Therefore the semiconductor structure has to be designed in order to take into account the shape of the black body spectrum of the sun ($T = 5778\,\text{K}$). The sun emits light in the UV, visible and infrared regime, and most of the light is emitted in the visible regime. The visible spectral region is within a frequency range of $430\,\text{THz}$ to $750\,\text{THz}$, within a wavelength range of $\lambda = 400\,\text{nm}$ to $\lambda = 700\,\text{nm}$, and within a photon energy range of $E = 1.75\,\text{eV}$ to $E = 3.1\,\text{eV}$, respectively. The terrestrial spectrum (air mass 1.5, AM1.5) slightly differs from the extraterrestrial spectrum (air mass zero, AM0) due to absorption of photons in the atmosphere leading to dips in the spectrum. The spectrum depends on the solar zenith angle, i.e. the position with respect to the equator. A nuclear explosion is at around $T \approx 10^7\,\text{K}$. Therefore the peak is within the X-ray regime around $\lambda \approx 0.1\,\text{nm}$.

16.5   Infinite Quantum Well

`QW_infinite_1D_nn3.in`
In this example we calculate the wave functions $\psi_n(x)$ and probability densities $\psi_n^2(x)$ of a quantum well with infinite barriers of width L.

16.5.1   Results

This input file can be opened within the tab *Template* of the next**nano**mat software so that the quantum well width L can be swept automatically.
Select 'Template' tab $\Rightarrow$ Click on $\boxed{...}$ $\Rightarrow$ `nextnano\nextnanomat\nextnano3 sample files\QW_infinite_1D_nn3.in` $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'QW_width' $\Rightarrow$ Click $\boxed{\text{Create input files}}$ $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'
Then the eigenvalues for different quantum well widths are calculated.

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the wave functions $\psi_n(x)$ which are shifted with respect to their energy eigenvalues E_n so that there confinement energy can be directly seen. They are given by

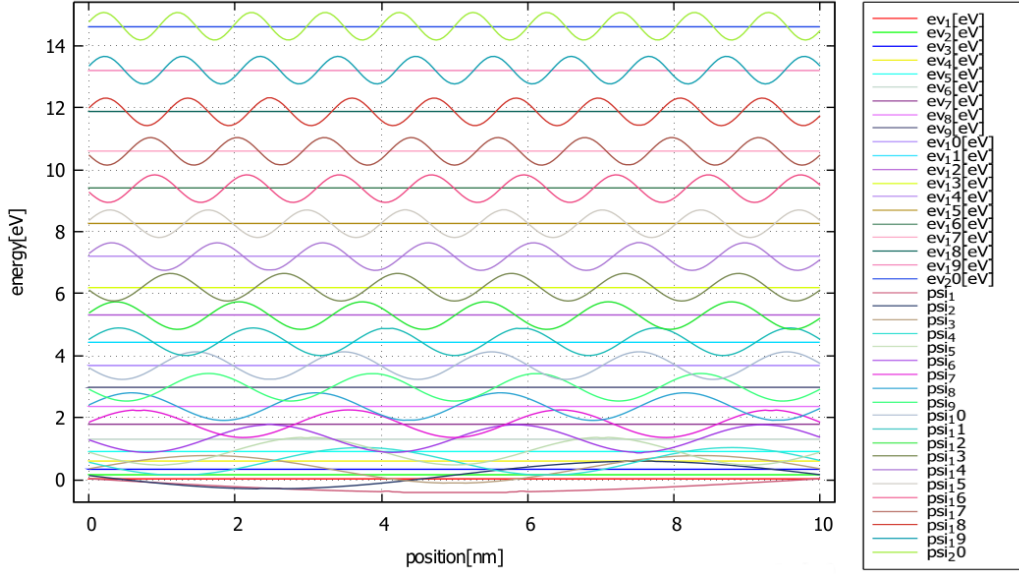$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}. \tag{437}$$

Figure 6: Wave functions of an infinite quantum well: They are alternating *even* or *odd* because the potential energy profile is symmetric with respect to the center of the well.

- The file `cb1_qc1_sg1_deg1_psi_squared_shift.dat` contains the probability densities $\psi_n^2(x)$ which are shifted with respect to their energy eigenvalues E_n for better visibility.

- The file `ev_cb1_qc1_sg1_deg1.dat` contains the energy levels $E_n = \frac{h^2}{8mL^2}n^2$ where $n = 1, 2, 3, \ldots$.

The results for different quantum well widths can be easily compared by choosing the result file for simulation in the bottom right menu. Then, by switching between the output folders in the bottom left menu, the correspondingly result file will be automatically displayed (switch per mouse or arrow keys). With growing quantum width L is the energy E_n and the amplitude of the wave functions $\psi_n(x)$ decreasing.

- The intraband matrix elements $\langle \psi_f \, | \, \psi_i \rangle$ (spatial overlap), $\langle \psi_f \, | \, \hat{x} \, | \, \psi_i \rangle$ and $\langle \psi_f \, | \, \hat{p}_x \, | \, \psi_i \rangle$ (dipole moment), and oscillator strengths,

$$O_{fi} = \frac{2}{mE_{fi}} \, |\langle f|\hat{p}_x|i\rangle|^2 = \frac{2mE_{fi}}{\hbar^2} \, |\langle f|x|i\rangle|^2, \qquad (438)$$

112

can also be found in this folder (filenames: `intraband_*`). Some transitions are forbidden due to the symmetry of the wave functions (*selection rules*). The oscillator strength for the transition $1 \rightarrow 2$ is very strong ($O_{21} \approx 0.96$). The user can define customized matrix elements (e.g. $\langle \psi_f \,|\, x^2 \,|\, \psi_i \rangle$) in the input file using `intraband-matrix-elements-operator = "x^2"`. The expectation value $\langle x^2 \rangle$ for the ground state of the $10\,\text{nm}$ quantum well is $\approx 28\,\text{nm}^2$. This quantity is needed to calculate the *standard deviation*.

A similar example is described on this website: http://www.nextnano.com/nextnano3/tutorial/1Dtutorial_IntrabandTransitions.htm

16.5.2   Results: Infinite quantum well subject to a perturbation

`QW_infinite_perturbation_1D_nn3.in`
`QW_infinite_perturbation_electric_field_1D_nn3.in`
In this example we calculate the energy levels E_n, wave functions $\psi_n(x)$ and probability densities $\psi_n^2(x)$ of a quantum well with infinite barriers of width L that is subject to a parabolic symmetric perturbation $V(x) = V_0 x(x - L)$ (see Exercise 8.3), a symmetric perturbation $V(x) = V_0 \cos^2(\pi x/L)$ (see Exercise 8.4), and a perturbation due to an electric field $V(x) = eF_x x$ (see Exercise 8.5). This input file can be opened within the tab *Template* of the next**nano**mat software so that the strength of the perturbation V_0 can be swept automatically.
Select 'Template' tab $\Rightarrow$ Click on $\boxed{...}$ $\Rightarrow$ `nextnano\nextnanomat\nextnano3 sample files\QW_infinite_perturbation_1D_nn3.in` $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'PERTURBATION' $\Rightarrow$ Click on $\boxed{\text{Create input files}}$ $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'
Then the lowest four eigenvalues for different strengths of the perturbation are calculated.
The file `cb_Gamma.dat` contains the potential energy function $V(x)$ which includes the perturbation. The shift in the energy levels can be compared with Exercise 8.3 and Exercise 8.4. It is also instructive to compare the change in the wave functions`cb1_qc1_sg1_deg1_psi.dat`.

The electric field example does not have to be opened within the Template tab. If it is run, it automatically calculates two sweeps, one with electric field switched off, and another one where it is switched on. The files are labeled with `*E000*` (electric field off, sweep step #0) and `*E001*` (electric field on,

sweep step #1).

- The intraband matrix elements $\langle \psi_f \,|\, \psi_i \rangle$ (spatial overlap), $\langle \psi_f \,|\, \hat{x} \,|\, \psi_i \rangle$ and $\langle \psi_f \,|\, \hat{p}_x \,|\, \psi_i \rangle$ (dipole moment) can also be found in this folder (file-names: `intraband_*`). Some transitions are forbidden due to the symmetry of the wave functions (*selection rules*). The user can define customized matrix elements (e.g. $\langle \psi_f \,|\, V_0 x(x - L) \,|\, \psi_i \rangle$) in the input file using `intraband-matrix-elements-operator = "V_0*x*(x-L)"`. Here, we use this flag in order to specify the perturbation potential operator $\hat{\mathbf{H}}'$.

- The expectation value $\langle \psi_n | \hat{\mathbf{H}}' | \psi_n \rangle = \langle \psi_n | V_0 x(x - L) | \psi_n \rangle$ for the energy level E_n can be found in the file `intraband_ExpectationValue_cb1_qc1_sg1_deg1.dat`. If the operator is the *perturbation potential* operator, then the units of this file are eV, and the expectation values are equivalent to the 1$^{\text{st}}$-order corrections to the energies $E_n^{(1)}$ using nondegenerate perturbation theory.

- If the operator is the *perturbation potential* operator, then the file `intraband_2ndOrder_cb1_qc1_sg1_deg1.dat` contains the 2$^{\text{nd}}$-order corrections $E_n^{(2)}$ to the energy eigenvalues using nondegenerate perturbation theory.

- The file `intraband_MatrixElement_cb1_qc1_sg1_deg1.dat` contains the matrix elements $\langle \psi_f | \hat{\mathbf{H}}' | \psi_i \rangle$ and the transition energy $E_{fi} = E_f - E_i$. The file `intraband_MatrixElement_cb1_qc1_sg1_deg1_2Dplot.dat` contains the matrix elements $\langle \psi_f | \hat{\mathbf{H}}' | \psi_i \rangle$ as a 2D plot.

- The file `intraband_Coefficient_cb1_qc1_sg1_deg1.dat` contains the matrix elements

$$\frac{\langle \psi_f | \hat{\mathbf{H}}' | \psi_i \rangle}{E_f - E_i}, \tag{439}$$

and the file `intraband_Coefficient_cb1_qc1_sg1_deg1_2Dplot.dat` visualizes these matrix elements as a 2D plot. These coefficients are needed for the 1$^{\text{st}}$-order correction to the wave functions and the 2$^{\text{nd}}$-order correction to the energies in nondegenerate perturbation theory.

16.6 Quantum Harmonic Oscillator

ParabolicQW_infinite_analytic_1D_nn3.in
In this example we calculate the wave functions $\psi_n(x)$ and probability densities $\psi_n^2(x)$ of the harmonic oscillator. The potential energy is given by $V(x) = \frac{1}{2}m\omega^2 x^2$. The Hamiltonian reads

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x) = E\psi(x). \tag{440}$$

The input file ParabolicQW_infinite_analytic_1D_nn3.in contains a line
potential-from-function = " - 1/2 * %m_omega_squared_eVnm * x^2 "
where you can define the potential function and another line where you can define the energy $\hbar\omega$ in units of eV,
%hbar_omega_in_eV_units = 1.000.
Note that you need an additional '−' sign for the potential function because the software interprets this is as an electrostatic potential ϕ rather than a potential energy, $V = -e\phi$. The position x has to be specified in units of nm.

16.6.1 Results

- The file cb_Gamma.dat contains the potential energy function $V(x)$ which is the parabolic harmonic oscillator profile.

- The file cb1_qc1_sg1_deg1_psi_shift.dat contains the wave functions $\psi_n(x)$ which are shifted with respect to their energy eigenvalues E_n so that they can be nicely plotted together with the potential energy profile $V(x)$.

In order to plot the data of several output files together, i.e. $V(x)$ and $\psi_n(x)$, you have to use the 'Overlay' feature of next**nano**mat.
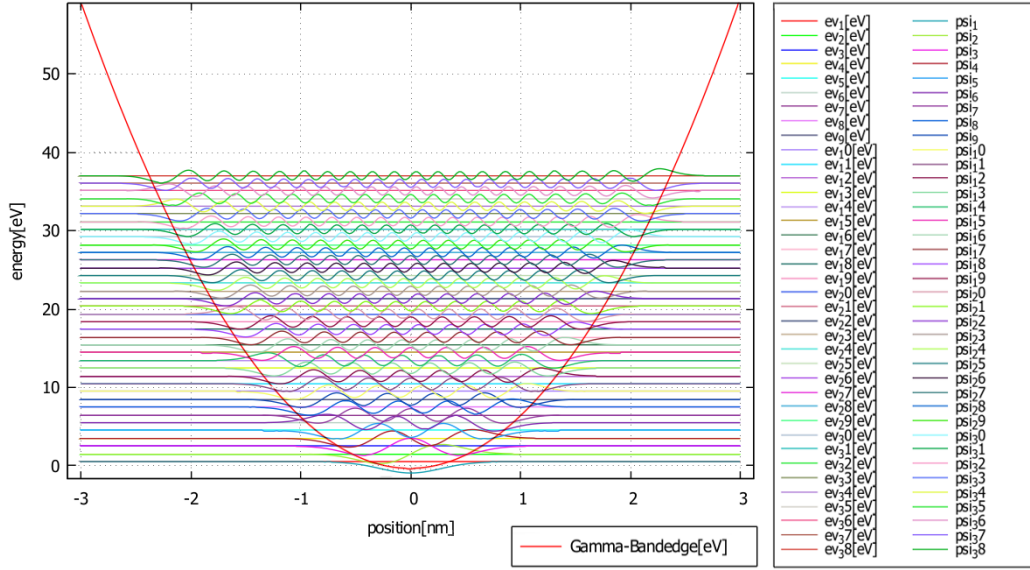
Figure 7: The potential energy profile $V(x)$ and shifted wave functions $\psi_n(x)$ of a parabolic quantum well plotted together.

- The file `cb1_qc1_sg1_deg1_psi_squared_shift.dat` contains the probability densities $\psi_n^2(x)$ which are shifted with respect to their energy eigenvalues E_n for better visibility.

- The file `ev1D_cb1_qc1_sg1_deg1.dat` contains the energy levels $E_n = \left(n - \frac{1}{2}\right)\hbar\omega$ where $n = 1, 2, 3, ...$

- The intraband matrix elements $\langle \psi_i | \psi_j \rangle$ (spatial overlap), $\langle \psi_i | \hat{x} | \psi_j \rangle$ and $\langle \psi_i | \hat{p}_x | \psi_j \rangle$ (dipole moment) can also be found in this folder.

116

`ParabolicQW_infinite_analytic_half_1D_nn3.in`

This file contains only the right half of the parabola.
The eigenvalues of the "half-harmonic oscillator" are

$$E_n = \left(2n - \frac{1}{2}\right)\hbar\omega \qquad (n = 1, 2, 3, ...). \qquad (441)$$

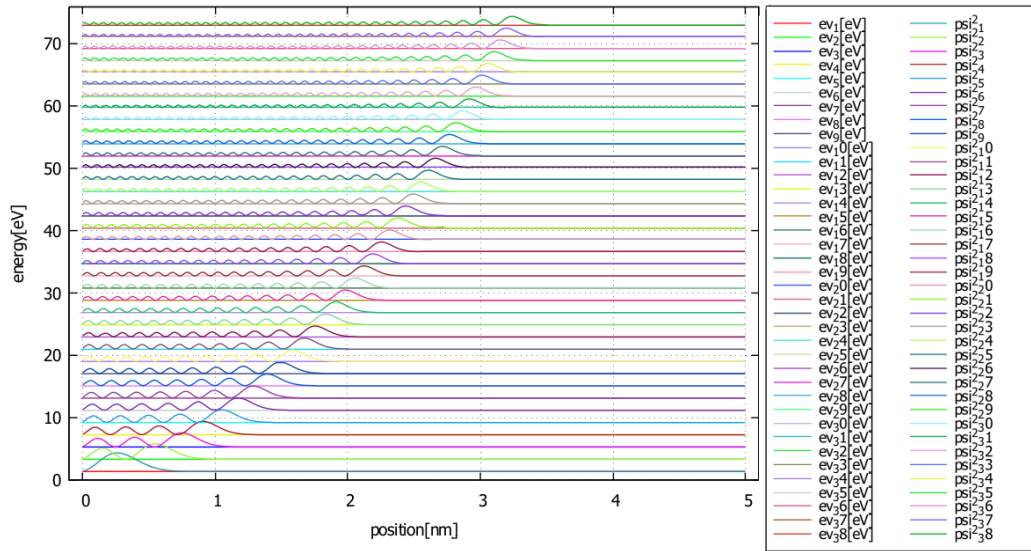These are the *odd* energies of the full harmonic oscillator.

Figure 8: Probability densities $\psi_n^2(x)$ of a potential energy profile containing only the right half of a parabolic quantum well.

`ParabolicQW_infinite_analytic_anharmonic_1D_nn3.in`

This file contains an *anharmonic* oscillator potential.
In the 'Input' tab of next**nano**mat any energy potential can be defined.

A similar example is described on this website: http://www.nextnano.com/nextnano3/tutorial/1Dtutorial_ParabolicQW.htm
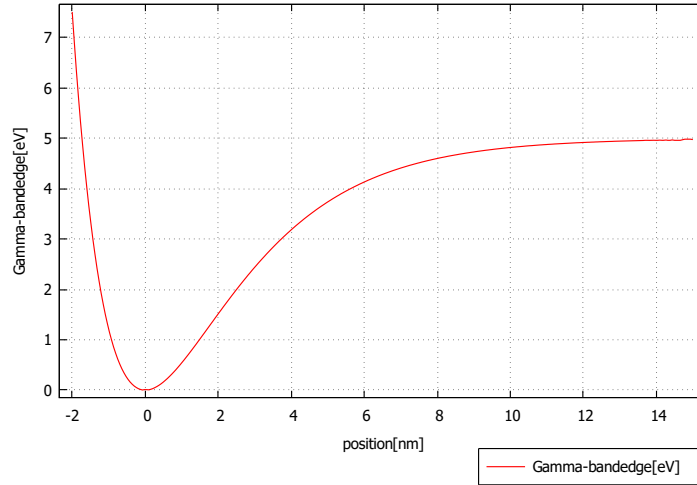
Figure 9: Anharmonic potential energy function $V(x)$

16.7 Triangular Quantum Well

QW_triangular_1D_nn3.in
In this example we calculate the wave functions $\psi_n(x)$ and probability densities $\psi_n^2(x)$ of a triangular quantum well. The potential energy is given by $V(x) = eFx$ where F is the electric field along the x direction given in units of V/m. The Hamiltonian reads

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + eFx \right)\psi(x) = E\psi(x). \tag{442}$$

16.7.1 Results

This input file can be opened within the tab 'Template' of the next**nano**mat software so that the electric field F can be swept automatically. Select 'Template' tab $\Rightarrow$ Click on $\boxed{...}$ $\Rightarrow$
nextnano\nextnanomat\nextnano3 sample files\QW_triangular_1D_nn3.in
$\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'Electric_Field' $\Rightarrow$ Click $\boxed{\text{Create input files}}$
$\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'
Then the eigenvalues for different triangular potential shapes are calculated.

- The file cb_Gamma.dat contains the potential energy function $V(x)$ which is the triangular quantum well profile.

118

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the wave functions $\psi_n(x)$ which are shifted with respect to their energy eigenvalues E_n so that they can be nicely plotted together with the potential energy profile $V(x)$. The wave functions of the triangular potential profile are called *Airy functions*. In order to plot the data of several output files together, i.e. $V(x)$ and $\psi_n(x)$, you have to use the 'Overlay' feature of next**nano**mat.
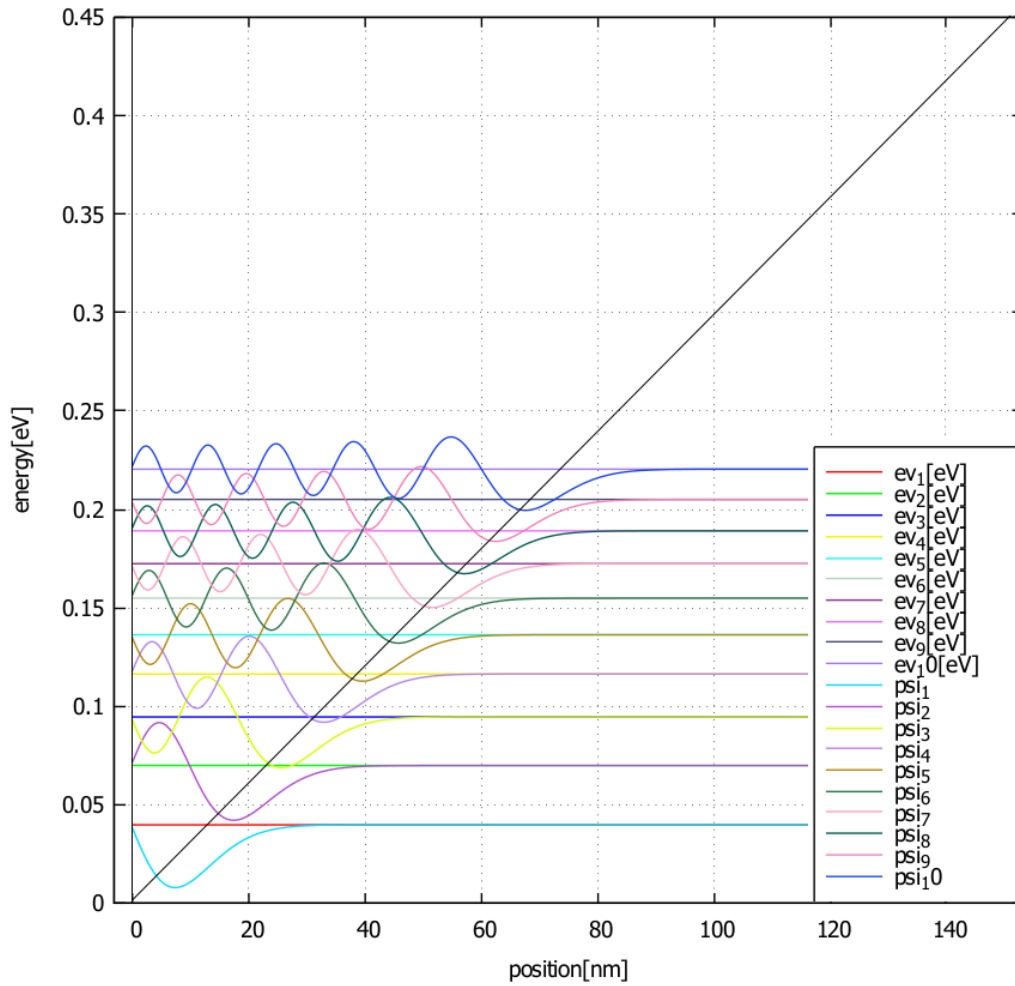

Figure 10: Wave functions of a triangular potential energy profile $V(x)$

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the probability den-

119

sities $\psi_n^2(x)$ which are shifted with respect to their energy eigenvalues E_n for better visibility.

- The file `ev1D_cb1_qc1_sg1_deg1.dat` contains the energy levels E_n where $n = 1, 2, 3, ...$ One can see that the distance between the energy levels decreases with increasing n because the quantum well width gets larger for higher energies. The triangular potential is not symmetric in x, thus the wave functions lack the even or odd symmetry that one obtains for the square quantum well.

- The intraband matrix elements $\langle \psi_i \,|\, \psi_j \rangle$ (spatial overlap), $\langle \psi_i \,|\, \hat{x} \,|\, \psi_j \rangle$ and $\langle \psi_i \,|\, \hat{p}_x \,|\, \psi_j \rangle$ (dipole moment) can also be found in this folder.

A similar example is described on this website: http://www.nextnano.com/ nextnano3/tutorial/1Dtutorial_GaAs_triangular_well.htm

16.8 Finite Quantum Well

`QW_finite_1D_nn3.in`
In this example we calculate the wave functions $\psi_n(x)$ and probability densities $\psi_n^2(x)$ of a quantum well with finite barriers of width L to study the penetration of the wave functions into the barriers.

16.8.1 Results

This input file can be opened within the tab 'Template' of the next**nano**mat software so that the quantum well width L or barrier height V_0 can be swept automatically.
Select 'Template' tab $\Rightarrow$ Click $\boxed{\texttt{\_\_\_}}$ $\Rightarrow$ `nextnano\nextnanomat\nextnano3 sample files\QW_finite_1D_nn3.in` $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'QW_width' or 'Barrier_Height' $\Rightarrow$ Click $\boxed{\text{Create input files}}$ $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'
Then the eigenvalues for different quantum well widths are calculated.

- The file `cb_Gamma.dat` contains the potential energy function $V(x)$ which is the square well profile.

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the wave functions $\psi_n(x)$ which are shifted with respect to their energy eigenvalues E_n so

that there confinement energy can be directly seen. They are alternating *even* or *odd* because the potential profile is symmetric with respect to the center of the well.

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the probability densities $\psi_n^2(x)$ which are shifted with respect to their energy eigenvalues E_n for better visibility.
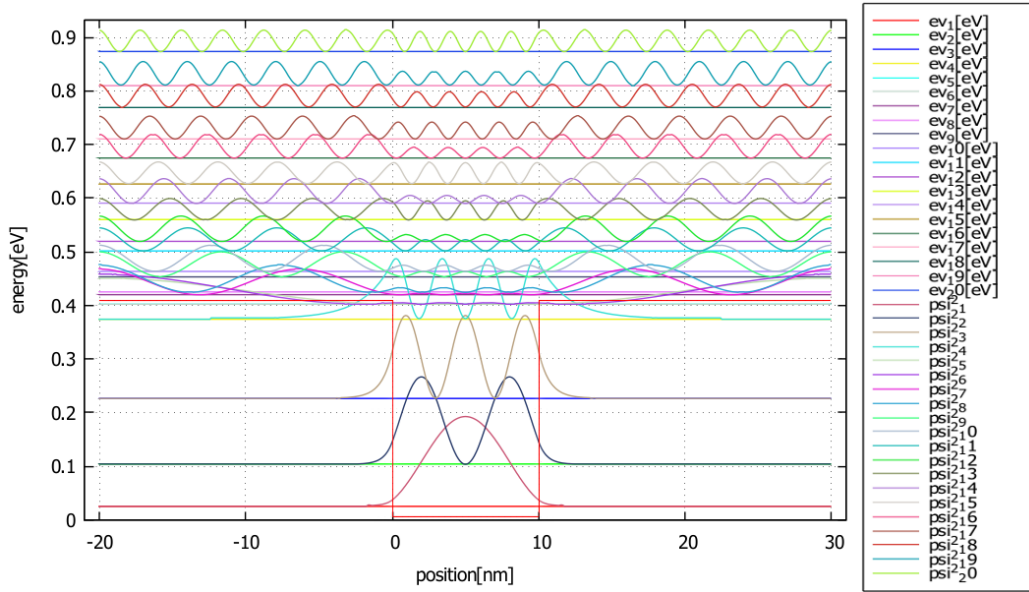

Figure 11: The probability densities of a finite quantum well. There are four states confined in the quantum well.

- The file `ev1D_cb1_qc1_sg1_deg1.dat` contains the energy levels E_n where $n = 1, 2, 3, ...$

- The intraband matrix elements $\langle \psi_i | \psi_j \rangle$ (spatial overlap), $\langle \psi_i | \hat{x} | \psi_j \rangle$ and $\langle \psi_i | \hat{p}_x | \psi_j \rangle$ (dipole moment) can also be found in this folder.

16.9 Transmission

In this example we calculate the transmission function $T(E)$ for an electron for the following potential profiles:

- Potential step
  `Transmission_Step_1D_nn3.in`

- Potential barrier
  `Transmission_Barrier_1D_nn3.in`

- Quantum well
  `Transmission_Quantum_Well_1D_nn3.in`

- Double barrier
  `Transmission_Double_Barrier_1D_nn3.in`

16.9.1   Results

These input files can be opened within the tab *Template* of the next**nano**mat software so that the quantum well and barrier widths, or barrier heights can be swept automatically.

- The file `cb_Gamma.dat` contains the potential energy function $V(x)$ for the potential step, potential barrier, quantum well or double barrier, respectively.

- The file `transmission1D_cb_sg1_CBR.dat` contains the transmission function $T(E)$.

- The file `DOS1D_sg1.dat` contains the density of states $DOS(E)$.

- The file `LocalDOS_at_boundaries1D_sg1.dat` contains the local density of states
  $LDOS(E, x_i)$ at the left ($x_i = x_1$) and right boundary ($x_i = x_N$) of the structure.

- The file `LocalDOS1D_sg1.fld` contains the local density of states $LDOS(E, x)$. The data of this file is the sum of the local density of the left lead (`LocalDOS1D_sg1_Lead1.fld`) and the right lead (`LocalDOS1D_sg1_Lead2.fld`).

Similar examples are described on these websites:

- http://www.nextnano.com/
  nextnano3/tutorial/1Dtutorial_Transmission_NEGF.htm

- http://www.nextnano.com/nextnano3/nextnano.MSB/Tutorials/
  tutorial_Transmission_DoubleBarrier.htm
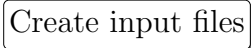
16.10 Double Quantum Well

`DoubleQuantumWell_nn3.in`

In this example we calculate the energy levels and wave functions of a double quantum well. The quantum wells are separated by a barrier. We vary the width of this barrier. Then we can study the formation of bonding and anti-bonding states and their energy separation as a function of barrier width. This example is described in full detail on this website:

http://www.nextnano.com/nextnano3/tutorial/1Dtutorial_DoubleQW.htm

16.10.1 Results

This input file can be opened within the tab 'Template' of the next**nano**mat software so that the width of the barrier (i.e. quantum well separation `%QW_SEPARATION`) can be swept automatically.

Select 'Template' tab $\Rightarrow$ Click $\boxed{\text{---}}$ $\Rightarrow$ `nextnano\nextnanomat\nextnano3 sample files\DoubleQuantumWell_nn3.in` $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'QW_SEPARATION' $\Rightarrow$ Click $\boxed{\text{Create input files}}$ $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'

Then the eigenvalues for different quantum well separations are calculated.

- The file `cb_Gamma.dat` contains the potential energy function $V(x)$ which is the double square well profile.

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the wave functions $\psi_n(x)$ which are shifted with respect to their energy eigenvalues E_n so that there confinement energy can be directly seen. If the quantum well separation is small, the two lowest states show a bonding and an antibonding wave function.

- The file `cb1_qc1_sg1_deg1_psi_shift.dat` contains the probability densities $\psi_n^2(x)$ which are shifted with respect to their energy eigenvalues E_n for better visibility. If the quantum well separation is small, the second state (antibonding) has zero probability density in the middle of the structure.

- The file `ev1D_cb1_qc1_sg1_deg1.dat` contains the energy levels E_n where $n = 1, 2$. If the quantum well separation is large, both quantum wells have (nearly) the same ground state energy because the wells are essentially decoupled.
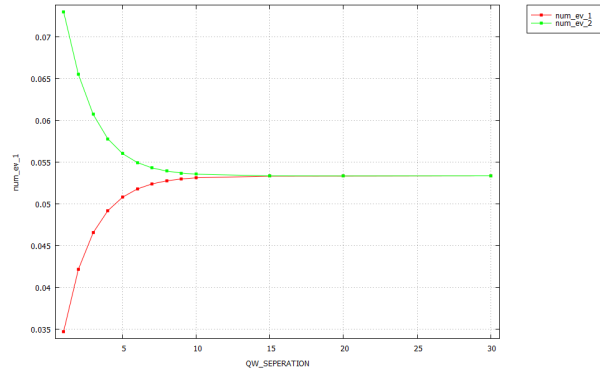
Figure 12: Energies of the bonding (E_1) and antibonding (E_2) states of a double quantum well as a function of quantum well separation. The figure has been generated from next**nano**mat using the *Postprocessing* feature.

16.11   Superlattice

In this example we calculate the energy levels of a periodic structure (superlattice). We want to study the energy levels in order to understand how they form bands.

- *Dirichlet* vs. *periodic* boundary conditions: First, we calculate the eigenvalues of a large structure with Dirichlet ($\psi(0) = \psi(L) = 0$, '*particle in a box*') and periodic boundary conditions ($\psi(0) = \psi(L)$).
  The file `QW_large_1D_nn3.dat` contains a large 'quantum well'.
  Select 'Template' tab $\Rightarrow$ Click on '...' $\Rightarrow$
  'nextnano\nextnanomat\nextnano3 sample files\QW_large_1D_nn3.in'
  $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'BoundaryCondition' $\Rightarrow$ Click on the button 'Create input files' $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'
  Then the eigenvalues for two different boundary conditions are calculated. The eigenvalues for option 'periodic' (Eq. (271)) are twice as far apart compared with 'Dirichlet' (infinite quantum well, Eq. (263)) but they are twofold degenerate ($+k$ and $-k$).

- *Superlattice*: The file `Superlattice_1D_nn3.dat` contains a quantum well superlattice. The length of the structure is $12\,\text{nm}$, and the quantum well width is $6\,\text{nm}$. We vary the barrier height from $0\,\text{eV}$ ('bulk') to $1\,\text{eV}$.

124

Select 'Template' tab $\Rightarrow$ Click on '...' $\Rightarrow$ 'nextnano\nextnanomat\nextnano3 sample files\ Superlattice_1D_nn3.in' $\Rightarrow$ Select 'List of values' $\Rightarrow$ Select variable 'Barrier_Height' $\Rightarrow$ Click on the button 'Create input files' $\Rightarrow$ Switch to 'Run' tab $\Rightarrow$ Click on the icon 'Run simulations (F9)'

Then the eigenvalues for different barrier heights are calculated. The file `sg_dispSL_el_qc1_sg1_deg1_piL_evmin001_evmax004.dat` contains the calculated eigenvalues for each superlattice vector k_{SL}, i.e. the 'miniband dispersion' $E(k_{\mathrm{SL}})$ from $k_{\mathrm{SL}} = -\pi/L$ to $k_{\mathrm{SL}} = +\pi/L$ (1st Brillouin zone). The results for a barrier height of $0\,\mathrm{eV}$ correspond to the energy dispersion of a bulk semiconductor. This is discussed in Section 16.11.1. If the barrier height is nonzero, a quantum well superlattice is formed. The file `cb_Gamma.dat` contains the superlattice band edge profile. The calculated miniband dispersion now contains band gaps. If the barrier height increases, then also the band gaps increase. This input file is a simple example of a one-dimensional artificial crystal. It shows the essential features of a real crystal such as energy bands and band gaps.

The length L of the superlattice period and the number of superlattice vectors is specified in the input file. These two quantities determine the actual crystal size, i.e. the number of identical primitive superlattice unit cells. For instance, if one specifies $N = 20$ superlattice vectors for the interval $[-\pi/L, \pi/L]$ (ignoring counting the Γ point at $k = 0$), the total crystal contains 20 superlattice unit cells along the direction x, and has a total length of $NL = 20L$. It is important to remember that the number of superlattice vectors is not only a property that reflects the 'grid resolution' of the miniband dispersion in k space, but that it actually corresponds to the number of repeated unit cells. k is a quantum number of the system. It characterizes the wave functions corresponding to different states of the same miniband.

16.11.1 Results: Miniband dispersion in a bulk 1D sample

We consider a simple, trivial example where we take a bulk GaAs sample of length $L = 12\,\mathrm{nm}$ which corresponds to our superlattice unit cell. We apply periodic boundary conditions and solve the single-band effective-mass Schrödinger equation for the electrons for each of the 20 superlattice vectors in the interval between $[-\pi/L, +\pi/L]$. Our choice of discreteness of the allowed values of k determines the sample size ($NL = 20L = 240\,\mathrm{nm}$). We
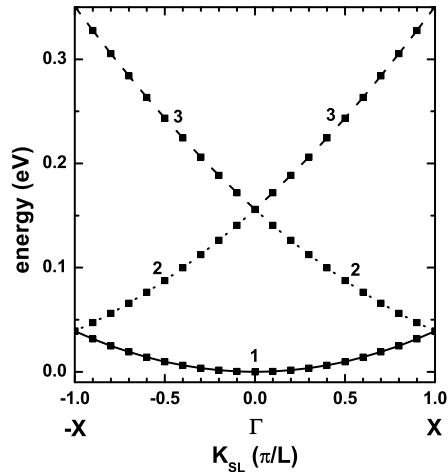
Figure 13: Electron energy dispersion of the three lowest minibands ($n = 1, 2, 3$) of a simple bulk GaAs sample of periodic length $L = 12$ nm. The conduction band edge is set to 0 eV. The lines are a guide to the eye.

plot the energy dispersion for the lowest three minibands ($n = 1, 2, 3$). They arise from the first, second and third eigenstate of the 12 nm wide superlattice unit cell. The energies of the second and third eigenstate are degenerate at $k = 0$, whereas at $k = -\pi/L$ and $k = +\pi/L$, the first and second eigenstate are degenerate. It follows, that there are no band gaps within this miniband spectrum. As we simulated only plain GaAs, the dispersion of these three minibands must follow the parabolic energy dispersion of bulk GaAs, i.e. $E(k) = \frac{\hbar^2}{2m}k^2$, where $m = 0.067m_0$ is the conduction band effective mass of GaAs. For a very large number of superlattice vectors, i.e. for a very large bulk sample, the minibands form an almost continuous spectrum, starting from the conduction band edge.

Figure 14 shows the energy levels of the three lowest eigenstates E_i and their corresponding probability density (ψ_i^2) (shifted by their eigenenergies E_i) for the superlattice vector $k = 0$ (stationary Bloch states). The square of the ground state wave function ψ_1^2 is constant with its energy $E_1 = 0$ eV equal to the conduction band edge energy. The energies of the second (E_2) and third (E_3) eigenstate are degenerate at $k = 0$. Their wave functions have a cosine and sine shape, respectively.
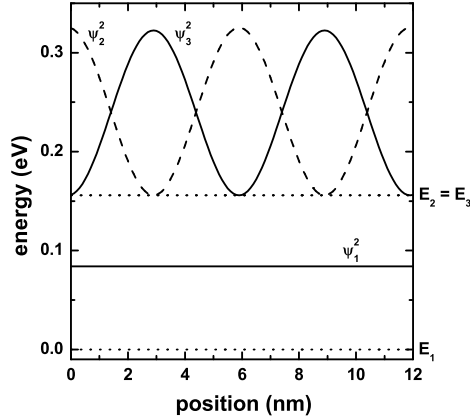
126

Figure 14: Stationary Bloch states of a 12 nm bulk GaAs sample with periodic boundary conditions. Shown are the three lowest energy levels E_1, E_2 and E_3, as well as their associated probability densities (ψ_1^2, ψ_2^2, ψ_3^2). The conduction band edge is set to $0\,\text{eV}$.

16.12   Band structure - Tight-binding method

In this example we calculate the band structure $E_n(\mathbf{k})$ for a few semiconductors using the $sp^3 s^*$ tight-binding model of P. Vogl et al.

- Tight-binding band structure of silicon and germanium
  TightBinding_Si.in (Vogl, $T = 0\,\text{K}$)
  TightBinding_Ge.in (Vogl, $T = 0\,\text{K}$)

- Tight-binding band structure of gallium arsenide (using Klimeck material parameters at $T = 300\,\text{K}$ including spin-orbit splitting and Vogl material parameters ($T = 0\,\text{K}$) without spin-orbit splitting)
  TightBinding_GaAs.in
  TightBinding_GaAs_Vogl.in

- Further input files include the band structure for C, AlAs, AlSb, GaP, InAs, InSb.

These input files are described in full detail on this website:
http://www.nextnano.com/nextnano3/tutorial/
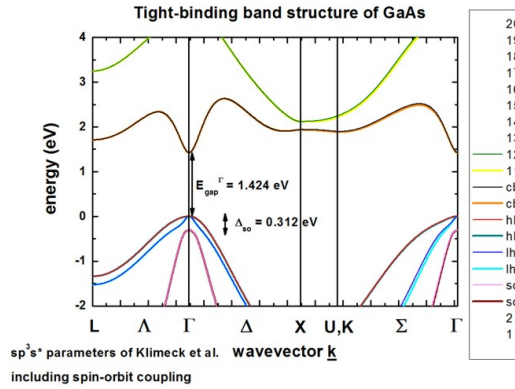1Dtutorial_TightBinding_bulk_GaAs_GaP.htm

Figure 15: Band structure of GaAs calculated with the sp^3s^* tight-binding method using empirical tight-binding parameters of G. Klimeck et al. for $T = 300\,\text{K}$.

16.12.1 Results: Band structure

The band structure is contained in the folder `TightBinding/`.

- The file `BandStructure_shifted.dat` contains the 20 energy levels $E_n(\mathbf{k}) = E_n(k_x, k_y, k_z)$ of the 20×20 Hamiltonian. "`_shifted`" means that all energies E_n are shifted so that the valence band edge maximum at the Γ point $((k_x, k_y, kz) = 0)$ equals $0\,\text{eV}$. Then the band gap can be directly obtained from the minimum of the conduction band energies. Each point $E_n(k_x, k_y, k_z)$ in the output file corresponds to a state vector $|n\mathbf{k}\rangle$. The index n labels the bands. The lowest eight bands (taking into account spin) correspond to the filled valence band states. All other bands correspond to the unoccupied conduction band states. In our examples, the maximum energy of the valence band is always located at the Γ point. The conduction band edge minimum is usually located at the Γ point (GaAs, InAs, ...). For some semiconductors the minimum is located at the L point (Ge), X point (AlAs) or along the line Δ from the Γ point to the X point (Si). The difference between the conduction band edge minimum and the valence band edge maximum is the *band gap*. Within the band gap, no states $|n\mathbf{k}\rangle$ exist.

- The energy levels are split due to spin-orbit coupling if the corresponding tight-binding parameter is nonzero (`%Delta_so_a_GaAs`, `%Delta_so_c_GaAs`).

The file `BandStructure_without_so_shifted.dat` contains the 20 energy levels $E_n(\mathbf{k})$ without taking spin-orbit ("`so`") splitting into account. Each energy level is therefore two-fold degenerate.

- The file `Hamiltonian_Gamma_real.mtx` contains the real part of the matrix elements of the Hamiltonian at the Γ point, i.e. for wave vector $\mathbf{k} = 0$. It is a 20×20 matrix containing two identical 10×10 blocks and two 10×10 blocks that are zero. The imaginary part of the matrix elements is contained in the file `Hamiltonian_Gamma_imag.mtx`. They are due to spin-orbit coupling. If spin-orbit splitting is switched off, then the matrix reduces to a 10×10 matrix and all matrix elements are real at the Γ point. The tight-binding Hamiltonian is hermitian and thus only the upper triangle is shown.