**Topological surface state**

In these notes we create a simple tight binding model that shows topological non-trivial system. We then create a slab using this model and discuss the surface states that "have to" rise between a topological trivial (vacuum) and non-trivial (by construction) state.

### Bulk

The model we use is a tight binding model of a square lattice. On each site there is a s and a p orbital. The tight binding Hamiltonian is thus a 4 by 4 matrix and has the parameters: $\epsilon_s, \epsilon_p, ss, sp, pp$. We will later add spin-orbit coupling and thus the spin-orbit coupling constant ($\zeta$) is a parameter as well.

```math
ClearAll[\epsilon_s, \epsilon_p, ss, sp, pp, \zeta]
```

The basis of our Hamiltonian is $px$, $py$, $pz$ and the s orbital. Only nearest neighbor hopping of $s$ type is included

$$
H = \begin{pmatrix}
\epsilon_p + pp & 0 & 0 & sp (e^{i \pi xx} - e^{-i \pi xx}) \\
(e^{i \pi xx} + e^{-i \pi xx}) & 0 & sp (e^{i \pi xy} - e^{-i \pi xy}) & 0 \\
0 & sp (e^{i \pi xy} - e^{-i \pi xy}) & 0 & sp (e^{i \pi xx} - e^{-i \pi xx}) \\
(sp (e^{i \pi xx} + e^{-i \pi xx}) & sp (e^{-i \pi xx} + e^{i \pi xx}) & sp (e^{-i \pi xx} + e^{i \pi xx}) & es + ss (e^{i \pi xx} + e^{-i \pi xx}) + e^{i \pi xy} + e^{-i \pi xy} + e^{i \pi xx} + e^{-i \pi xx})
\end{pmatrix}
$$

In order to get a topological nontrivial state we need the entanglement between orbital and spin. This is realized by the relativistic spin-orbit coupling. Spin-orbit coupling can be included in a tight binding Hamiltonian by simply doubling the basis, i.e. adding a spin up and spin down orbital for each state in the original basis. Then the spin-orbit coupling Hamiltonian is given as:
The CharacterToThicknessSOC and CharacterToColorSOC functions can be defined using a module function. The function can be defined as:

\[ \text{HSOC} = \begin{pmatrix}
  0 & 1/2 & 0 & 0 & 0 & -1/2 & 0 \\
  -1/2 & 0 & 0 & 0 & 0 & -1/2 & 0 \\
  0 & 0 & 0 & 1/2 & 1/2 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 1/2 & 0 & 1/2 & 0 & 0 \\
  0 & 0 & -1/2 & 0 & 1/2 & 0 & 0 \\
  -1/2 & 1/2 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix};
\]

\[ \text{HSOC}[\{1, 4, 1, 4\}] = \text{H}; \]
\[ \text{HSOC}[\{5, 8, 5, 8\}] = \text{H}; \]

To plot a band structure, the path in k-space is given as:

\[ \text{KPathDefine} = \{
  \{"R", \{1, 1, 1\}, 87\},
  \{"Γ", \{0, 0, 0\}, 50\},
  \{"X", \{1, 0, 0\}, 50\},
  \{"M", \{1, 1, 0\}, 71\},
  \{"Γ", \{0, 0, 0\}, 1\},
  \{"Γ", \{0, 0, 0\}, 0\}
\}; \]

Let's define colors for the bands: s band will be blue, the p bands in red. Here, we first do it for NO spin-orbit coupling

\[ \text{CharacterToColor}[\text{Character}_\_] := \text{Module}[[\text{VRed}, \text{VGreen}, \text{VBlue}]],
  \text{VRed} = \text{Character}[[\{1, 2, 3\}]].\text{Character}[[\{1, 2, 3\}]]^*;
  \text{VGreen} = 0;
  \text{VBlue} = \text{Character}[[\{4\}]].\text{Character}[[\{4\}]]^*;
  \text{RGBColor}[[\text{VRed}, \text{VGreen}, \text{VBlue}]] \]

The same needs to be done for the calculation with spin-orbit coupling. In this case a slightly different function is needed as the basis size is different (both spin up and down are in the basis)

\[ \text{CharacterToColorSOC}[\text{Character}_\_] := \text{Module}[[\text{VRed}, \text{VGreen}, \text{VBlue}]],
  \text{VRed} = \text{Character}[[\{1, 2, 3, 5, 6, 7\}]].\text{Character}[[\{1, 2, 3, 5, 6, 7\}]]^*;
  \text{VGreen} = 0;
  \text{VBlue} = \text{Character}[[\{4, 8\}]].\text{Character}[[\{4, 8\}]]^*;
  \text{RGBColor}[[\text{VRed}, \text{VGreen}, \text{VBlue}]] \]

We can define a function for the line thickness

\[ \text{CharacterToThickness}[\text{Character}_\_] := \text{Module}[[]],
  \text{Thickness}[0.005 + 0.01 \text{Character}[[\{4\}]].\text{Character}[[\{4\}]]^*] \]

And again a slightly different function for the case with spin-orbit coupling

\[ \text{CharacterToThicknessSOC}[\text{Character}_\_] := \text{Module}[[]],
  \text{Thickness}[0.005 + 0.01 \text{Character}[[\{4, 8\}]].\text{Character}[[\{4, 8\}]]^*] \]

The list of k-points is generated
KPoints = Flatten[
  Table[
    Table[ KPathDefine[[i, 2]] (KPathDefine[[i, 3]] - j + 1) / KPathDefine[[i, 3]] +
      j - 1, KPathDefine[[i + 1, 2]] KPathDefine[[i, 3]]],
    {j, 1, KPathDefine[[i, 3]]}], {i, 1, Length[KPathDefine] - 1}], 1];

and a list of names belonging to some k points

Knames = Table[{KPathDefine[[i, 1]], 1 + Sum[KPathDefine[[ii, 3]], {ii, 1, i - 1}]},
  {i, 1, Length[KPathDefine] - 1}];

As a first start, we set the parameters such that the Hamiltonian does not include p and s mixing terms.

ep = 4.1;
es = 9;
ssc = -3;
ppc = 2;
spc = 0;
ξ = 2.5;
HNointeractionfun[xx_, xy_, xz_] := Evaluate[N[H]]; We can calculate the eigen-states at the k-points defined above

{TBEnergyNointeraction, TBCharacterNointeraction} = Chop[CalculateBands[HNointeractionfun, KPoints]]; and plot the bands.
As a next step we include mixing between the s and p band

\[ e_p = 4.1; \]
\[ e_s = 9; \]
\[ s\sigma_0 = -3; \]
\[ p\sigma_0 = 2; \]
\[ s\sigma = 2; \]
\[ \xi = 2.5; \]
\[ \text{Hfun}[\times, \times_-, \times_+]:= \text{Evaluate}[\text{N[H]}]; \]
\[ \text{HfunSOC}[\times, \times_-, \times_+]:= \text{Evaluate}[\text{N[HSOC]}]; \]

and calculate the eigenstates. We do it once with and once without spin-orbit coupling

\{\text{TB Energy}, \text{TB Character}\} = \text{Chop}[\text{CalculateBands}[\text{Hfun}, \text{KPoints}]]; \\
\{\text{TB Energy SOC}, \text{TB Character SOC}\} = \text{Chop}[\text{CalculateBands}[\text{HfunSOC}, \text{KPoints}]];
And plot the band structure without (left) and with spin-orbit coupling (right).

\[
\text{PltTB} = \text{CharacterPlotBandStructure}[\text{TBEnergy}, \text{TBCharacter}, \\
\quad \text{Knames}, \text{CharacterToColor}, \text{CharacterToThickness}, -10, 30]; \\
\text{PltTBSOC} = \text{CharacterPlotBandStructure}[\text{TBEnergySOC}, \text{TBCharacterSOC}, \\
\quad \text{Knames}, \text{CharacterToColorSOC}, \text{CharacterToThicknessSOC}, -10, 30]; \\
\text{Show}[\text{GraphicsGrid}[\{\{\text{PltTB}, \text{PltTBSOC}\}\}]]
\]

One can see on the left: the s-p mixing creates hybridization gaps between the s and p band. However, at high symmetry points (R={(1,1,1)}, M=\{(1,1,0)}, X=\{(1,0,0)} and \Gamma=\{(0,0,0)} the s and p band do not mix by symmetry. The system without spin-orbit coupling therefore is metallic. On the right we included spin-orbit coupling and this splits the p-bands into a j=1/2 and j=3/2 state. Now a single band splits off and if there is a filling of 2 electrons per site this band is fully occupied and the system is an insulator.

The gap, which is of indirect type (maximum of the valance band is at X, minimum of the conduction band at M or/and R) is between states of p character.

**Topology**

We now can test if the state with two electrons per site is a topological insulator or not. For cubic systems the number that distinguishes topological trivial case from a topological nontrivial case is calculated as the product of the parity of the occupied wave functions at \Gamma, X, M, and R. If +1, then the system is trivial and if -1, the system is topological.

We can make the following parity table

<table>
<thead>
<tr>
<th></th>
<th>s</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>\Gamma</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>X</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>M</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>R</td>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>
Since we now consider an electron filling of 2, we only need to consider the parities of the single filled band. At Γ, the band is blue (s-orbital). Therefore the parity is +1. At X, p-character (red), therefore parity is -1. At M, p-character (red), parity is -1. At R, again p-character, parity is -1. So, we now need to take the product of these parities (+1 * -1 * -1 * -1). This gives a total of -1. Therefore, the system above is thus topological - non-trivial.

Real Space

So far it is beautiful math that has very nice realization in the real world. But there is more.

The vacuum is topologically trivial (as most other insulators). If I have a surface of a topological nontrivial system with that of vacuum, there is a boundary between an entangled and non-entangled state. These have to be matched in some way. The way to do this is to create a surface state that crosses the Fermi energy. I.e. a topological insulator has a metallic surface state. This surface state is independent to surface roughness, impurity level etc. If one destroys the surface over a large range one might find that somewhere buried there is a metallic layer and the junk on top is topological trivial, but there will be somewhere a metallic state

This is of course nice for practical applications, as it creates a two dimensional electron gas on the surface, which is used in modern day electronics.

ClearAll[es, ep, ssσ, spσ, ppσ, ξ, Δbottom];

In order to capture the surface state we will create a slab and calculate the x and y dispersion of the bands.

A finite slab always has two surfaces. In order to separate them we put in a tiny potential gradient. It should be much smaller that the smallest energy scale of interest.

\[
H_{\text{shift}} = \begin{pmatrix}
\Delta_{\text{bottom}} & 0 & 0 & 0 \\
0 & \Delta_{\text{bottom}} & 0 & 0 \\
0 & 0 & \Delta_{\text{bottom}} & 0 \\
0 & 0 & 0 & \Delta_{\text{bottom}}
\end{pmatrix};
\]

\[
H_{\text{shiftSOC}} = \begin{pmatrix}
\Delta_{\text{bottom}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \Delta_{\text{bottom}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \Delta_{\text{bottom}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \Delta_{\text{bottom}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \Delta_{\text{bottom}} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \Delta_{\text{bottom}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \Delta_{\text{bottom}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta_{\text{bottom}}
\end{pmatrix};
\]

The spin-orbit coupling Hamiltonian
I want to be able to calculate the spin expectation value of the surface state, so I need the spin operators. Here I define $S_x$, $S_y$ and $S_z$. 

\[
\text{HSOC} = \begin{pmatrix}
0 & \frac{1}{2} & 0 & 0 & 0 & -\frac{1}{2} & 0 \\
-\frac{1}{2} & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0 & 0 \\
0 & 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
-\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]
Next, let's create a slab in the z direction. I first define the Hamiltonian of a single layer

\[
\begin{align*}
SxLayer &= \begin{pmatrix}
0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\
0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}
\end{pmatrix}; \\
SyLayer &= \begin{pmatrix}
0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\
0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2}
\end{pmatrix}; \\
SzLayer &= \begin{pmatrix}
-\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2}
\end{pmatrix};
\end{align*}
\]

Next, let's create a slab in the z direction. I first define the Hamiltonian of a single layer

\[
HLayer = \begin{pmatrix}
\epsilon p + pp\sigma (e^{\frac{i}{2}xx} + e^{-\frac{i}{2}xx}) & 0 & 0 & sp\sigma (e^{\frac{i}{2}xx} - e^{-\frac{i}{2}xx}) \\
0 & \epsilon p + pp\sigma (e^{\frac{i}{2}xy} + e^{-\frac{i}{2}xy}) & 0 & sp\sigma (e^{\frac{i}{2}xy} - e^{-\frac{i}{2}xy}) \\
0 & 0 & \epsilon p & 0 \\
sp\sigma (-e^{\frac{i}{2}xx} + e^{-\frac{i}{2}xx}) & sp\sigma (-e^{\frac{i}{2}xy} + e^{-\frac{i}{2}xy}) & 0 & \epsilon s + ss\sigma (e^{\frac{i}{2}xx} + e^{-\frac{i}{2}xx} + e^{\frac{i}{2}xy} + e^{-\frac{i}{2}xy})
\end{pmatrix};
\]

And the Hamiltonian of a single layer with spin orbit coupling (double the basis)


\[
H_{\text{LayerSOC}} = H_{\text{SOC}};
\]

\[
H_{\text{LayerSOC}}[[1 ;; 4, 1 ;; 4]] = H_{\text{Layer}};
\]

\[
H_{\text{LayerSOC}}[[5 ;; 8, 5 ;; 8]] = H_{\text{Layer}};
\]

Then the interaction between layers

\[
H_{\text{Hop}} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & p_{sp} & s_{sp} & 0 \\
0 & -s_{sp} & s_{sp} & 0
\end{pmatrix}.
\]

And the interaction between two layers with spin-orbit coupling

\[
H_{\text{HopSOC}} = \text{IdentityMatrix}[8];
\]

\[
H_{\text{HopSOC}}[[1 ;; 4, 1 ;; 4]] = H_{\text{Hop}};
\]

\[
H_{\text{HopSOC}}[[5 ;; 8, 5 ;; 8]] = H_{\text{Hop}};
\]

Now create a slab of 50 layers. The total basis becomes 50 times larger than that of a single layer. The layers are repeated and between two neighboring layers the interaction between layers is added

\[
N_{\text{Layer}} = 50;
\]

\[
H_{\text{tot}} = \text{SparseArray}[], \{4 N_{\text{Layer}}, 4 N_{\text{Layer}}\};
\]

\[
H_{\text{totSOC}} = \text{SparseArray}[], \{8 N_{\text{Layer}}, 8 N_{\text{Layer}}\};
\]

\[
S_{z} = \text{SparseArray}[], \{8 N_{\text{Layer}}, 8 N_{\text{Layer}}\};
\]

\[
S_{y} = \text{SparseArray}[], \{8 N_{\text{Layer}}, 8 N_{\text{Layer}}\};
\]

\[
S_{x} = \text{SparseArray}[], \{8 N_{\text{Layer}}, 8 N_{\text{Layer}}\};
\]

\[
\text{For} [i = 0, i < N_{\text{Layer}}, i++]
\]

\[
H_{\text{tot}}[[4 i + 1 ;; 4 i + 4, 4 i + 1 ;; 4 i + 4]] = H_{\text{Layer}} + N[i / N_{\text{Layer}}] H_{\text{Shift}};
\]

\[
H_{\text{totSOC}}[[8 i + 1 ;; 8 i + 8, 8 i + 1 ;; 8 i + 8]] = H_{\text{LayerSOC}} + N[i / N_{\text{Layer}}] H_{\text{ShiftSOC}};
\]

\[
S_{z}[[8 i + 1 ;; 8 i + 8, 8 i + 1 ;; 8 i + 8]] = S_{z_{\text{Layer}}};
\]

\[
S_{y}[[8 i + 1 ;; 8 i + 8, 8 i + 1 ;; 8 i + 8]] = S_{y_{\text{Layer}}};
\]

\[
S_{x}[[8 i + 1 ;; 8 i + 8, 8 i + 1 ;; 8 i + 8]] = S_{x_{\text{Layer}}};
\]

\[
\text{For} [i = 1, i < N_{\text{Layer}}, i++]
\]

\[
H_{\text{tot}}[[4 (i - 1) + 1 ;; 4 (i - 1) + 4, 4 i + 1 ;; 4 i + 4]] = H_{\text{Hop}};
\]

\[
H_{\text{totSOC}}[[8 (i - 1) + 1 ;; 8 (i - 1) + 8, 8 i + 1 ;; 8 i + 8]] = H_{\text{HopSOC}};
\]

\[
H_{\text{totSOC}}[[8 (i) + 1 ;; 8 i + 8, 8 (i - 1) + 1 ;; 8 (i - 1) + 8]] = H_{\text{HopSOC}}';
\]

In order to do the calculations we need to set the parameters

\[
\begin{align*}
\epsilon & = 4.1; \\
\epsilon_{s} & = 9; \\
\epsilon_{ss} & = -3; \\
p_{sp} & = 2; \\
sp & = 2; \\
\zeta & = 2.5; \\
\Delta_{\text{bottom}} & = 0.000001;
\end{align*}
\]

\[
H_{\text{funtot}}[x_{x}, x_{y}, x_{z} :] = \text{Evaluate}[N[H_{\text{tot}}]];
\]

\[
H_{\text{funtotSOC}}[x_{x}, x_{y}, x_{z} :] = \text{Evaluate}[N[H_{\text{totSOC}}]];
\]

Diagonalize the Hamiltonian as a function of k (note that kz is not important anymore)

\[
\{\text{TBEnergyTot}, \text{TBCharacterTot}\} = \text{Chop}[\text{CalculateBands}[H_{\text{funtot}}, \text{KPoints}]];
\]

\[
\{\text{TBEnergyTotSOC}, \text{TBCharacterTotSOC}\} = \text{Chop}[\text{CalculateBands}[H_{\text{funtotSOC}}, \text{KPoints}]];
\]

And plot the band structure

\[
\text{PltTBTot} = \text{PlotBandStructure}[\text{TBEnergyTot}, \text{Knames}, -10, 30];
\]

\[
\text{PltTBTotSOC} = \text{PlotBandStructure}[\text{TBEnergyTotSOC}, \text{Knames}, -10, 30];
\]

\[
\text{Show}[\text{GraphicsGrid}[\{\{\text{PltTBTotSOC}\}\}]]
\]
We can zoom into the Fermi energy region. There is a surface state. Remember the slab is topological nontrivial, the vacuum is topological trivial, the interface thus must be metallic. It is.
We can make a three dimensional plot of the surface state. In the x and y direction the dispersion, in the z direction the energy of the state

\[
dk = 0.005;
\]
\[
\text{Encone} = \text{Table}[^{\text{Sort}[\text{Eigenvalues}[H\text{fun}t\text{otSOC}[\text{x}, \text{y}, 0]]][[[99, 101]]],}
\{\text{x}, -0.225, 0.225, dk\}, \{\text{y}, -0.225, 0.225, dk\};
\]

Here a plot of the cone:
In the bulk, each state is doubly degenerate, i.e. spin up and spin down have the same energy. As long as the system has an inversion center, the same is true when spin-orbit coupling is included. The surface state however is only singly degenerate. This also means it is spin polarized. Let's have a look at the spin of this state. First for the lower cone.

\[ \text{SpinVectorFieldlow} = \text{Flatten[} \]
\[ \text{Table[} \{\text{val}, \text{fun}\} = \text{CIEigensystem[HfuntotSOC}[\text{xx, xy, 0}]]\{\text{All, } \{99, 101}\}]; \]
\[ \text{Chop[} \{\text{xx, xy}\}, \{\text{fun}[\text{1}]\}^* \cdot \text{Sx.fun[1]}, \text{fun}[\text{1}]\}^* \cdot \text{Sy.fun[1]}\}\}; \]
\[ \{\text{xx, -0.225, 0.225, 0.05}, \{\text{xy, -0.225, 0.225, 0.05}\}\}]; \]
\[ \}\]; \]

And calculating the spin for the upper cone

\[ \text{SpinVectorFieldhigh} = \text{Flatten[} \]
\[ \text{Table[} \{\text{val}, \text{fun}\} = \text{CIEigensystem[HfuntotSOC}[\text{xx, xy, 0}]]\{\text{All, } \{99, 101}\}]; \]
\[ \text{Chop[} \{\text{xx, xy}\}, \{\text{fun}[\text{2}]\}^* \cdot \text{Sx.fun[2]}, \text{fun}[\text{2}]\}^* \cdot \text{Sy.fun[2]}\}\}; \]
\[ \{\text{xx, -0.225, 0.225, 0.05}, \{\text{xy, -0.225, 0.225, 0.05}\}\}]; \]
\[ \}\]; \]

And plot of the spin polarization.
A surface state is bound to the surface, but that does not mean it only sits on the top most layer. We can see how the surface state decays into the bulk by looking at the eigenstate, at a particular kx and ky point. (close to Γ, but not exactly at Γ in this case)

{valG, funG} = CEigensystem[HfuntotSOC[0, 0.01, 0]];

Now we can plot the layer dependent intensity. As it is a bound state at the surface this should decay exponentially with the distance from the surface:

ListLogPlot[Sum[Chop[funG[[99]] * funG[[99]]] [[i ;; 8 NLayer ;; 8]], {i, 1, 8}], PlotRange -> All, Frame -> True]