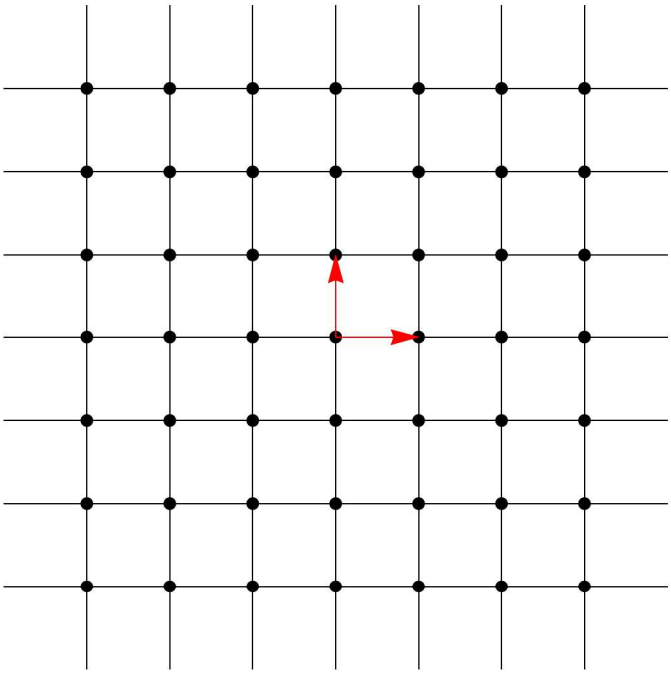
Topological Band Theory (Haldane Model on a Square Lattice)

Topological band theory refers to band theory where one does not ignore the property of the eigenvectors. In the past, band theorists would only care about the dispersion relation of the bands (i.e. the eigenvalues) -- that would give one the band structure. However, it has emerged since the discovery of the quantum hall effect that the eigenvectors need also be computed and can indeed have a remarkable affect on the band structure (especially at the edges of the sample). Here, we will solve a model that will illuminate much of what we now call topological band theory by examining a particular model. The model was first examined by Haldane in a honeycomb lattice, but has been adapted here for a square lattice [1].

Let us consider a square lattice with nearest-neighbor hoppings in a tight-binding model. The lattice can be seen below with the arrows labelling the x- and y- axes:

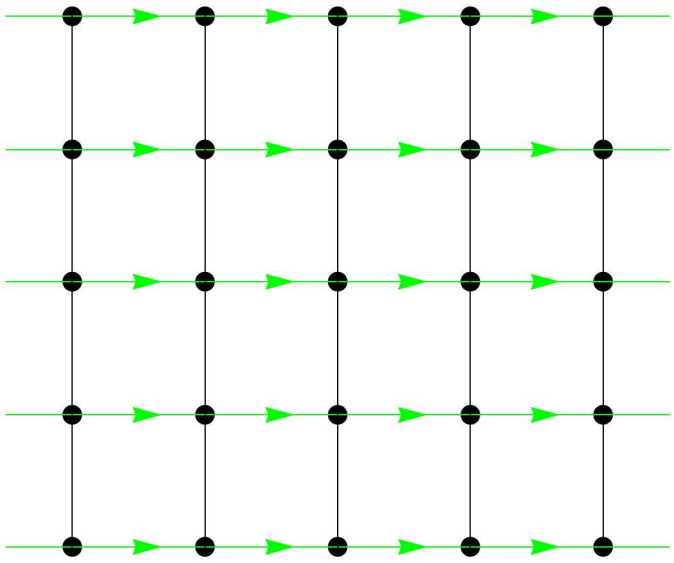


This model is easy to solve (using either first or second quantization):

$$H_{\text{sq}} = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j = \sum_k \epsilon_{\text{sq}}(k)\, a_k^\dagger a_k \tag{1}$$

where $\epsilon_{\text{sq}}(k) = 2\cos(k_x) + 2\cos(k_y)$, and we set the lattice parameter to be a=1.

Now, let us consider the case of complex hoppings as seen in the image below. If in the x-direction one hops in the direction of the arrow, then the hopping amplitude is $t\, e^{i\phi}$ and against the arrow it is $t\, e^{-i\phi}$. A complex hopping can arise from an Aharanov-Bohm type phase arising from a magnetic field or spin-orbit coupling. See reference [2] for instance.



The complex hoppings in this case do not fundamentally alter the dispersion relation. This is because each plaquette (each sqaure) encloses a zero total flux:

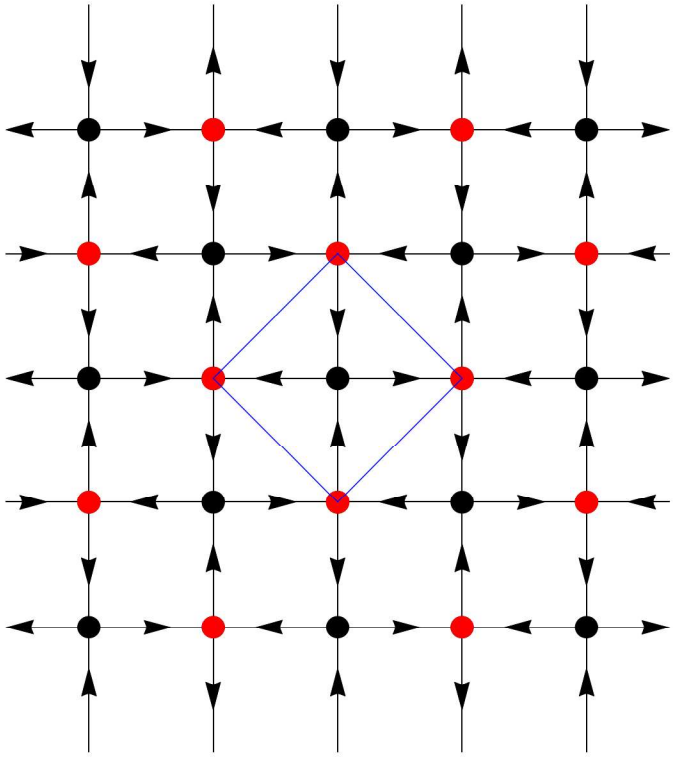
$$\phi_{a\,b} + \phi_{b\,c} + \phi_{c\,d} + \phi_{d\,a} = \phi + 0 + 0 - \phi = 0 \tag{2}$$

The tight-binding model here then yields for the dispersion relation:

$$H_{\text{ch}} = -t\, e^{i\phi} \sum_i a_i^\dagger\, a_{i+x} - t\, e^{-i\phi} \sum_i a_i^\dagger\, a_{i-x} - t \sum_i a_i^\dagger\, a_{i+y} - t \sum_i a_i^\dagger\, a_{i-y} = \sum_k \epsilon_{\text{ch}}(k)\, a_k^\dagger\, a_k \tag{3}$$

where $\epsilon_{\text{ch}}(k) = 2\cos(k_x + \phi) + 2\cos(k_y)$, and we again set the lattice parameter to be a=1. This phase can be removed with a gauge transformation to show that the two models, with and without the complex hopping, are indeed identical.

If we now consider the following scenario, however, things are a little bit different. In the image below, there are now two different atoms per unit cell (the unit cell is drawn in blue). Let us also give a hopping amplitude $-t\, e^{i\pi/4}$ if hopping in the direction of the arrow and $-t\, e^{-i\pi/4}$ if hopping in the direction opposite to the arrow.



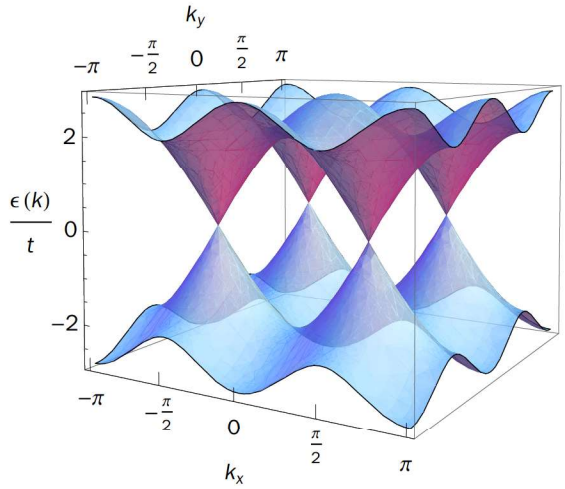
With two atoms per unit cell, our Hamiltonian becomes a 2x2 matrix:

$$H_{nn} = -t \sum_{\langle i,j \rangle} a_i^\dagger b_j = \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} 0 & h_{a\,b}(k_x, k_y) \\ h_{a\,b}^*(k_x, k_y) & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{4}$$

where $h_{a\,b}(k_x, k_y) = -2\,t\left(\cos(k_x)\,e^{-i\pi/4} + \cos(k_y)\,e^{i\pi/4}\right)$. Therefore, the band dispersion can easily be seen to be:

$$\epsilon_{nn\pm}(k) = \pm 2\,t\,\sqrt{\cos^2(k_x) + \cos^2(k_y)} \tag{5}$$

The dispersion, plotted below with $t = 1$, can be seen to have Dirac points at the two points $(k_x, k_y) = \left(\frac{\pi}{2}, \pm\frac{\pi}{2}\right)$.



Since this model yields a semi-metal with Dirac points, we cannot obtain a topological index (as topological indices are only defined for insulators). However, let us examine what the edge of the sample looks like

anyway. This will make for an apt comparison when we examine the topologically non-trivial case. To obtain the edge states, one needs to Fourier transform back the y-component back to real space using the transformation:

$$c^{\dagger}_{k_x,k_y} = \frac{1}{L}\sum_j e^{-i\,k_y\,j}\,c^{\dagger}_{k_x,\,j} \qquad \text{and} \qquad c_{k_x,k_y} = \frac{1}{L}\sum_j e^{i\,k_y\,j}\,c_{k_x,\,j} \tag{6}$$

where we denote $c_{k_x,k_y} \equiv \begin{pmatrix} a_{k_x,k_y} \\ b_{k_x,k_y} \end{pmatrix}$ and $c^{\dagger}_{k_x,k_y} \equiv \begin{pmatrix} a^{\dagger}_{k_x,k_y} & b^{\dagger}_{k_x,k_y} \end{pmatrix}$ for simplicity. Before transforming back to real space, we write the Hamiltonian as so:

$$H_{\text{nn}} = \sum_k c^{\dagger}_k\left(H_x\,\sigma_x + H_y\,\sigma_y\right)c_k = \sum_{k_x,k_y}\frac{1}{L^2}\sum_j e^{-i\,k_y\,j}\,c^{\dagger}_{k_x,\,j}\left(H_x\,\sigma_x + H_y\,\sigma_y\right)\sum_{j'} e^{i\,k_y\,j'}\,c_{k_x,\,j'} \tag{7}$$

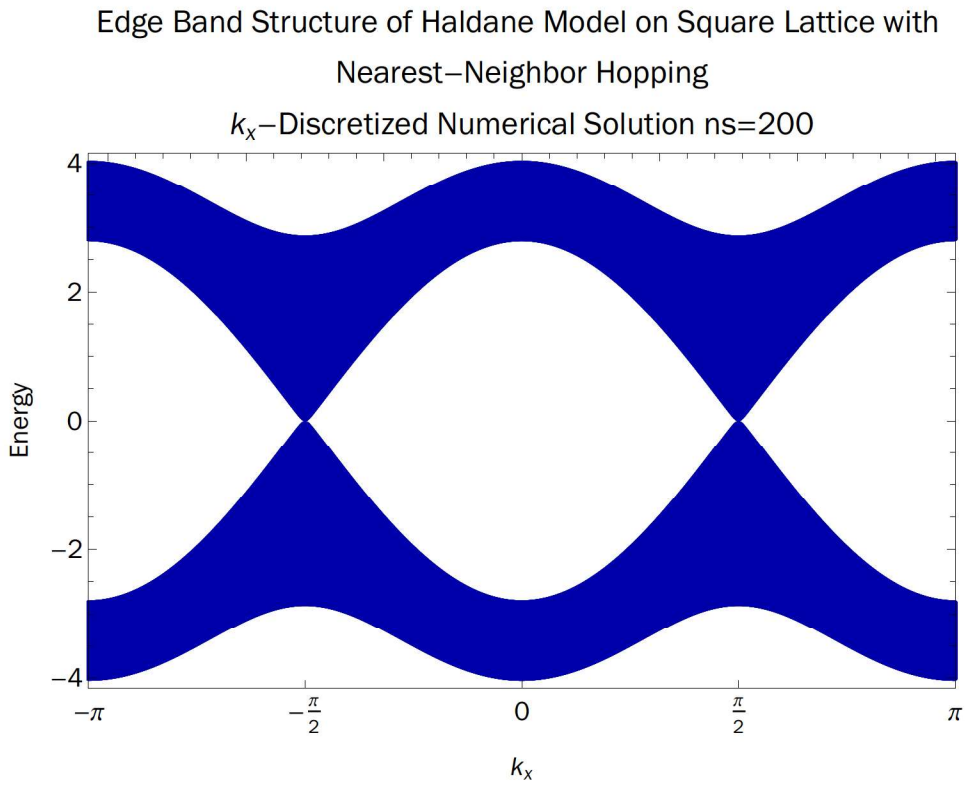
where we have written the Hamiltonian in terms of Pauli matrices with $H_x = 2\,t\,(\cos(\text{kx}) + \cos(\text{ky}))$ and $H_y = 2\,t\left(\cos(k_y) - \cos(k_x)\right)$. Now, we write the k_y-terms as exponentials (i.e. $\cos(k_y) = \frac{1}{2}\left(e^{i k_y} + e^{-i k_y}\right)$) and use the fact that $\sum_{k_y} e^{i k_y (j-j'-1)} = L\,\delta_{j,j'+1}$ and $\sum_{k_y} e^{i k_y (j-j'+1)} = L\,\delta_{j,j'-1}$. These collapse the j' summations so that we can write the Hamiltonian as so:

$$H_{\text{nn}}(k_x,\,j) = \frac{1}{L}\left(2\,t\sum_{k_x,j} c^{\dagger}_{k_x,\,j}\cos(k_x)\left(\sigma_x - \sigma_y\right)c_{k_x,\,j} + t\sum_{k_x,j} c^{\dagger}_{k_x,\,j}\left(\sigma_x + \sigma_y\right)c_{k_x,\,j-1} + t\sum_{k_x,j} c^{\dagger}_{k_x,\,j}\left(\sigma_x + \sigma_y\right)c_{k_x,\,j+1}\right) \tag{8}$$

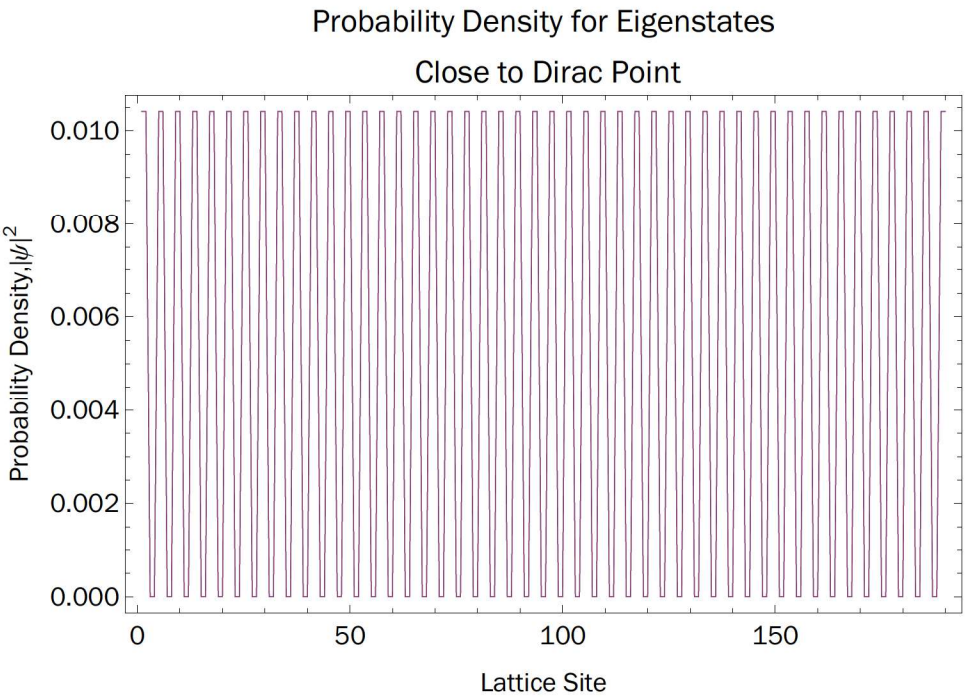
Now that we have a model with a momentum space representation in the x-direction and a real space in the y-direction, we can build a finite lattice in the y-direction and look if the edges yield any effects. An example of the Hamiltonian matrix (or kernel) that we need to diagonalize therefore looks like so (for a y-direction chain length of 2):

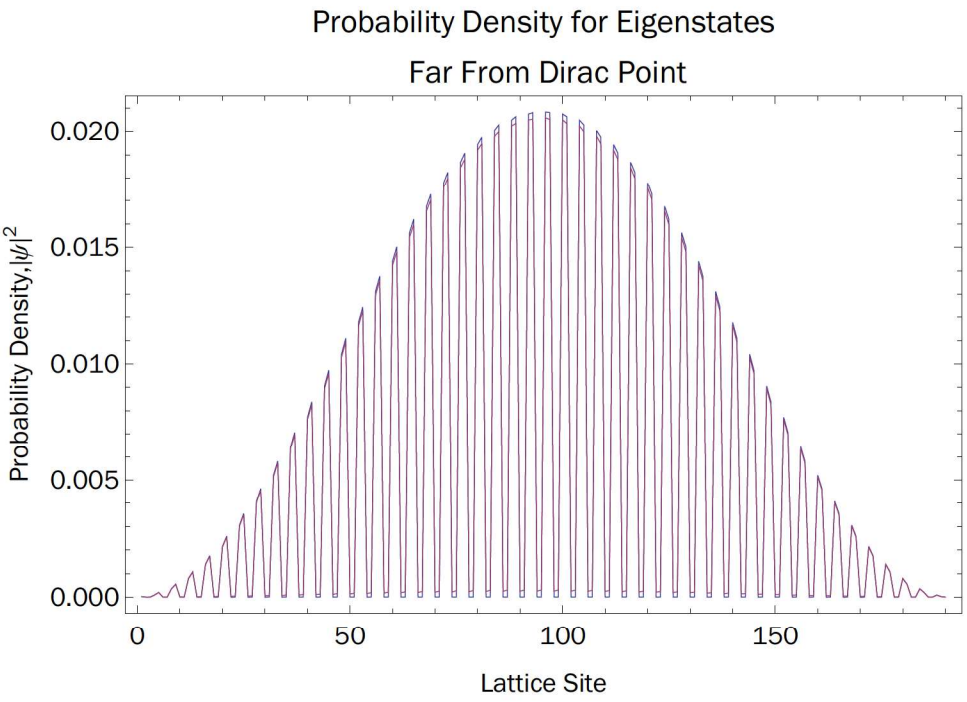
$$h_{\text{nn}}(k_x,\,j) = -t\begin{pmatrix} 0 & 2\cos(\text{kx})\,(1+i) & 0 & (1-i) \\ 2\cos(k_x)\,(1-i) & 0 & (1+i) & 0 \\ 0 & (1-i) & 0 & 2\cos(\text{kx})\,(1+i) \\ (1+i) & 0 & 2\cos(k_x)\,(1-i) & 0 \end{pmatrix} \tag{9}$$

The eigenvalues and eigenvectors of this matrix give the band structure and wavefunctions respectively. The band structure for the 100-chain matrix can be seen below. It is reminiscent of a projection of the full band structure onto the k_x-axis.

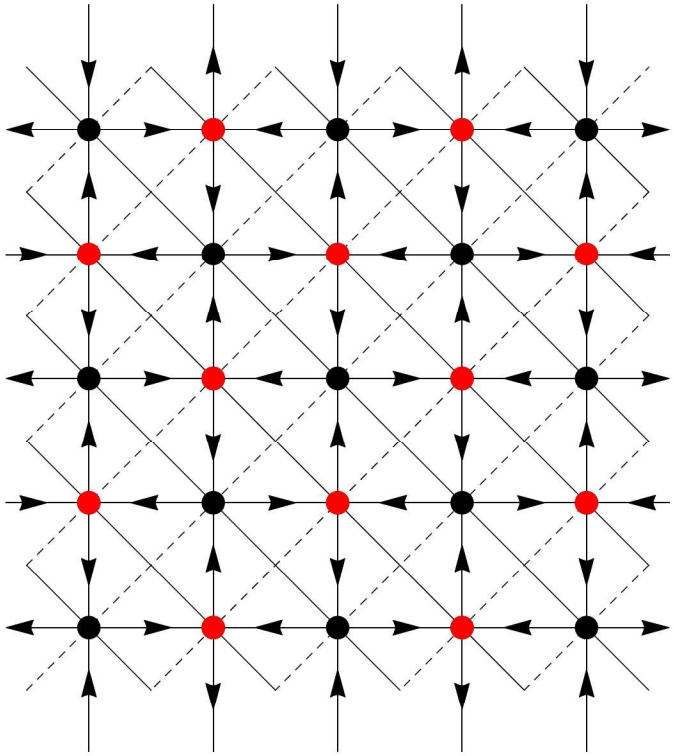


The probability densities for this model all exhibit fairly delocalized behavior and there is are no edge states for this model. For the purpose of illustation, we can plot the probability density of the eigenstates both close to and far away from the Dirac point.





Let us now include a next-nearest neighbor hopping in the Hamiltonian. This means that a red-site atom can hop to its nearest red-site atoms, and simliar for the black atoms. In reference to the image below, the dashed diagonal lines have hopping matrix element t' and the solid diagonal lines have hopping matrix element $-t'$.



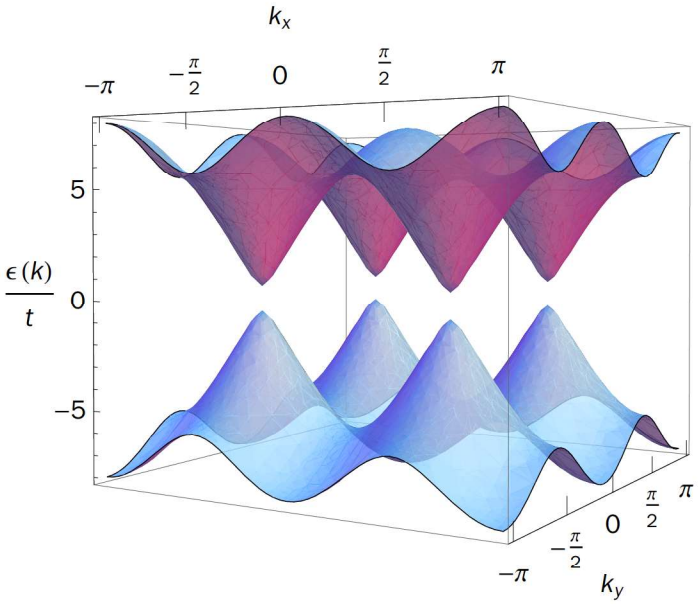
Therefore we have for the next-nearest-neighbor term:

$$H_{\text{nnn}} = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j = \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} h_{\text{aa}}(k_x, k_y) & 0 \\ 0 & h_{\text{bb}}(k_x, k_y) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{10}$$

where

$h_{\text{aa}} = -h_{\text{bb}} = -t \left(e^{i(k_x+k_y)} + e^{-i(k_x+k_y)} - e^{i(k_x-k_y)} - e^{-i(k_x+k_y)} \right) = -2t\left(\cos(k_x+k_y) - \cos(k_x-k_y)\right) = 4t \sin(k_x)\sin(k_y)$.

We can add this term to H_{nn} to obtain the full band structure as before, so that $H = H_{\text{nn}} + H_{\text{nnn}}$. Once we do this, we can obtain the full band structure. It is plotted below with $t' = 0.15$:



The most glaring difference between this band structure and the one obtained with only nearest-neighbor hopping is the opening up of a gap at the Dirac points. Let us now obtain the eigenvalues and eigenvectors symbolically to examine is behavior for any topologcial structure. We can write the Hamiltonian matrix (or kernel) as:

$$H = H_{\text{nn}} + H_{\text{nnn}} = \boldsymbol{\sigma} \cdot H = \left(H_x \sigma_x + H_y \sigma_y + H_z \sigma_z \right) \tag{11}$$

The eigenvalues are, from elementary considerations, $\epsilon(k) = \pm |H|$. Let us obtain the lowest eigenvector by solving for a and b:

$$\begin{pmatrix} H_z + |H| & H_x - i H_y \\ H_x + i H_y & H_z + |H| \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \Longrightarrow \quad u_-^{(\text{I})}(k) = \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{N^{(\text{I})}} \begin{pmatrix} H_z - |H| \\ H_x + i H_y \end{pmatrix} \tag{12}$$

We could have also written the eigenvector as:

$$\begin{pmatrix} H_z + |H| & H_x - i H_y \\ H_x + i H_y & H_z + |H| \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \Longrightarrow \quad u_-^{(\text{II})}(k) = \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{N^{(\text{II})}} \begin{pmatrix} -H_x + i H_y \\ H_z + |H| \end{pmatrix} \tag{13}$$

These two eigenvectors are the same eigenvector up to an arbitrary phase:

$$e^{i\chi(k)} u_-^{(\text{I})}(k) = \frac{\frac{H_z+|H|}{H_x+i H_y}}{\left| \frac{H_z+|H|}{H_x+i H_y} \right|} u_-^{(\text{I})}(k) = \frac{1}{N^{(\text{I})}} \begin{pmatrix} H_z - |H| \\ H_x + i H_y \end{pmatrix} \frac{\frac{H_z+|H|}{H_x+i H_y}}{\left| \frac{H_z+|H|}{H_x+i H_y} \right|} = \frac{1}{N^{(\text{II})}} \begin{pmatrix} \frac{-H_x^2 - H_y^2}{H_x+i H_y} \\ H_z + |H| \end{pmatrix} = \frac{1}{N^{(\text{II})}} \begin{pmatrix} -H_x + i H_y \\ H_z + |H| \end{pmatrix} = u_-^{(\text{II})}(k) \tag{14}$$

This is important because these two eigenvectors are singular at different points in the Brillouin Zone. Noting

that:

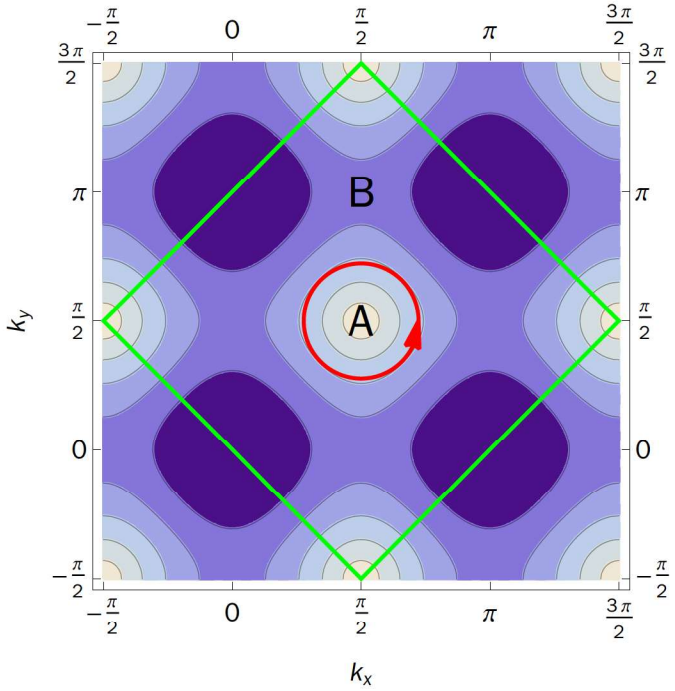
$$\begin{aligned} H_x &= -2\,t\left(\cos(k_x)+\cos(k_y)\right) \\ H_y &= -2\,t\left(\cos(k_y)-\cos(k_x)\right) \\ H_z &= 4\,t\sin(k_x)\sin(k_y) \end{aligned} \tag{15}$$

We can see that $H_x = H_y = 0$ at $\left(\frac{\pi}{2}, \pm\frac{\pi}{2}\right)$. Now, it can easily be seen that $u_-^{(\mathrm{I})}\left(\frac{\pi}{2}, \frac{\pi}{2}\right) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $u_-^{(\mathrm{II})}\left(\frac{\pi}{2}, -\frac{\pi}{2}\right) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. Also, it should be noted that $u_-^{(\mathrm{II})}\left(\frac{\pi}{2}, \frac{\pi}{2}\right) \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $u_-^{(\mathrm{I})}\left(\frac{\pi}{2}, -\frac{\pi}{2}\right) \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. This means that we can partition the Brillouin Zone into two parts and calculate the topological index. We do this by calculating the integral of the Berry connection around the Brillouin Zone in the following way:

$$\int_{\partial(\mathrm{BZ})} A(k)\cdot dk = \tag{16}$$

$$\int_{\partial(A)} A_{\mathrm{I}}(k)\cdot dk + \int_{\partial(B)} A_{\mathrm{II}}(k)\cdot dk = -\int_{\partial(B)} A_{\mathrm{I}}(k)\cdot dk + \int_{\partial(B)} A_{\mathrm{II}}(k)\cdot dk = -\int_{\partial(B)} \nabla\chi(k)\cdot dk = \int_{\partial(A)} \nabla\chi(k)\cdot dk$$

where the Berry connection is defined in the usual way, $A(k) = -i\,\langle u(k)\,|\nabla|\,u(k)\rangle$. Now, we must parameterize k in terms of θ so that we can integrate the red circle below from 0 to $2\,\pi$.



In the region of the red circle, $H_z > 0$ so that we can write:

$$e^{-i\chi(q)} = \frac{\left|\frac{H_z+|H|}{H_x+i\,H_y}\right|}{\frac{H_z+|H|}{H_x+i\,H_y}} = \frac{H_x+i\,H_y}{\left|H_x+i\,H_y\right|} = \tag{17}$$

$$\frac{q_x+q_y+i\left(q_y-q_x\right)}{\left|q_x+q_y+i\left(q_y-q_x\right)\right|} \quad\Longrightarrow\quad -\chi(q) = \mathrm{Arctan}\left(\frac{q_y-q_x}{q_x+q_y}\right) = \mathrm{Arctan}\left(\frac{\sin(\theta)-\cos(\theta)}{\sin(\theta)+\cos(\theta)}\right)$$

where $q_{x,y} = \pi/2 - k_{x,y}$ and where we have written $q_{x,y}$ in terms of the polar angle. This can be re-written using various trigonometric identities to yield:

$$-\chi(\theta) = \text{Arctan}\left(\frac{\sin(\theta)-\cos(\theta)}{\sin(\theta)+\cos(\theta)}\right) = \text{Arctan}\left(\frac{\tan(\theta)-1}{\tan(\theta)+1}\right) = \text{Arctan}\left(\tan\left(-\frac{\pi}{4}+\theta\right)\right) = -\frac{\pi}{4}+\theta \tag{18}$$

where we have used the identity $\tan(u \pm v) = (\tan(u) \pm \tan(v))/(1 + \tan(u)\tan(v))$. Now we can easily show that

$$C = \frac{1}{2\pi}\int_{\partial(A)} \nabla\chi(k)\cdot dk = \frac{1}{2\pi}\int_0^{2\pi} \frac{d}{d\theta}\chi(\theta)\,d\theta = -1 \tag{19}$$

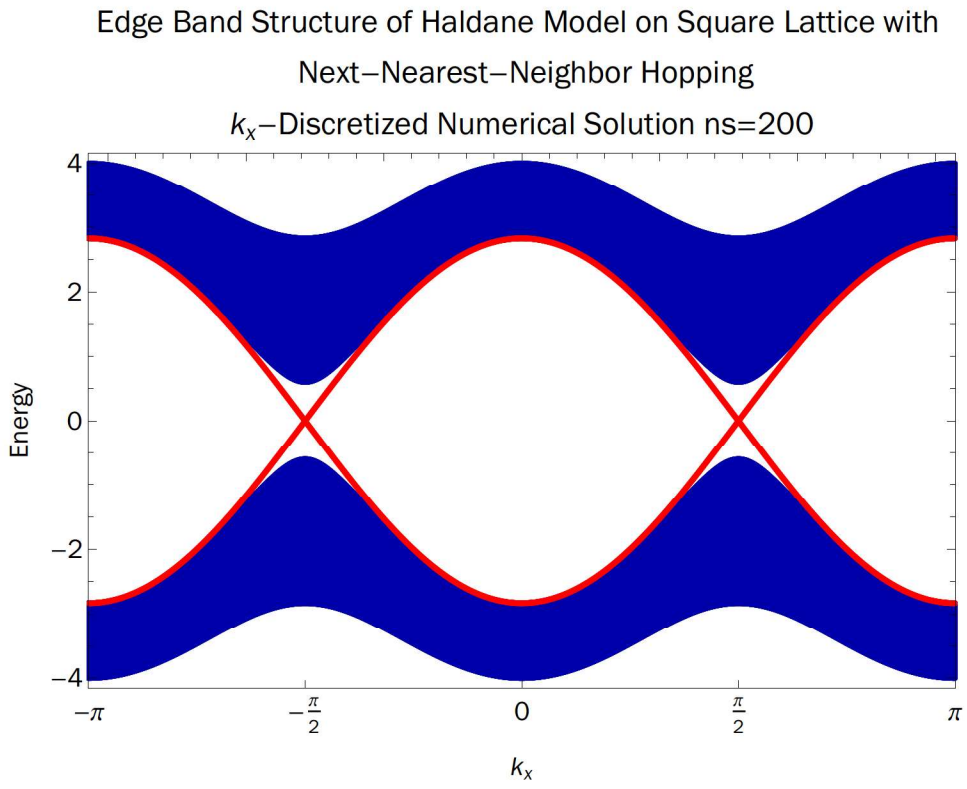
where C denotes the Chern number. We can therefore see that the calculated Chern number from this band theory is -1. Therefore this band theory is a non-trivial topology and should give rise to edge states. Let us repeat the calculation above where we obtain the Hamiltonian in a combination of reciprocal space and real space. This can easily be done using the Fourier transform convention given above. The next-nearest-neighbor Hamiltonian then becomes:

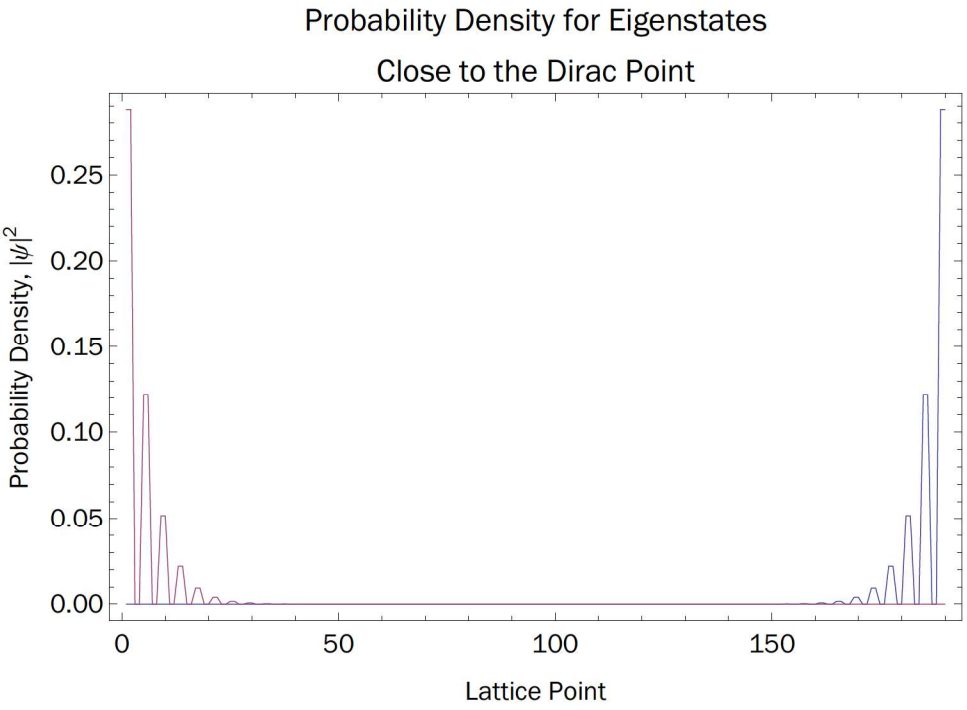
$$H_{\text{nnn}}(k_x, j) = \frac{1}{L}\left(i\,t'\sum_{k_x,j} c^\dagger_{k_x,j}\sin(k_x)\,\sigma_z\,c_{k_x,j-1} - i\,t'\sum_{k_x,j} c^\dagger_{k_x,j}\sin(k_x)\,\sigma_z\,c_{k_x,j+1}\right) \tag{20}$$

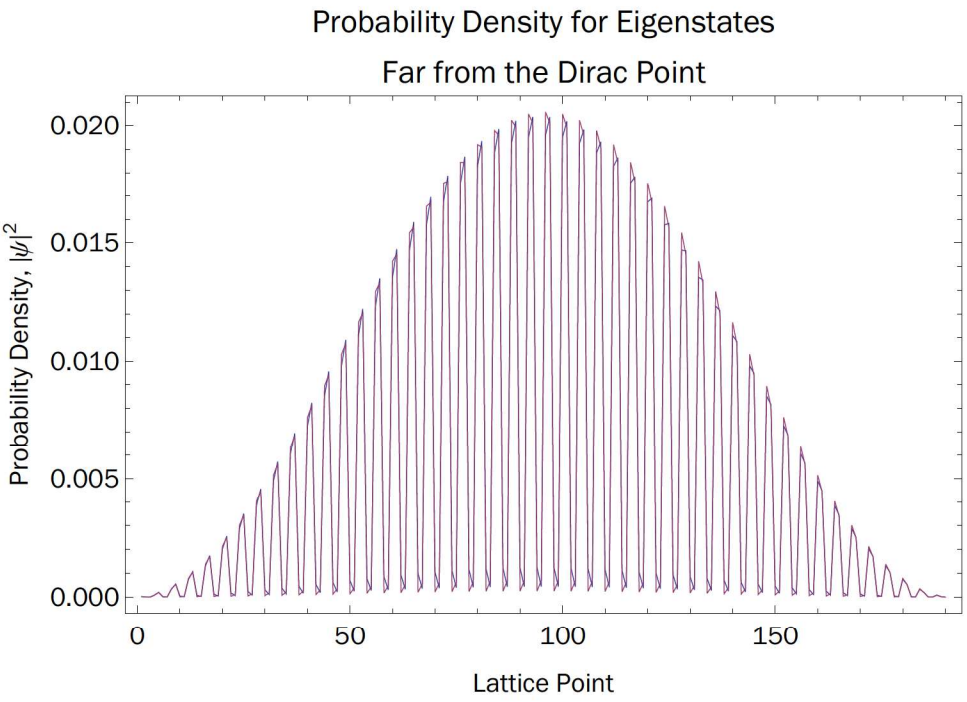
With this term included in the Hamiltonian, an example of the Hamiltonian matrix (or kernel) that we need to diagonalize therefore looks like so (for a y-direction chain length of 2):

$$h(k_x, j) = -\begin{pmatrix} 0 & 2\,t\cos(\text{kx})\,(1+i) & i\,t'\sin(k_x) & t(1-i) \\ 2\,t\cos(k_x)\,(1-i) & 0 & t(1+i) & -i\,t'\sin(k_x) \\ -i\,t'\sin(k_x) & t(1-i) & 0 & 2\,t\cos(\text{kx})\,(1+i) \\ t(1+i) & i\,t'\sin(k_x) & 2\,t\cos(k_x)\,(1-i) & 0 \end{pmatrix} \tag{21}$$

The eigenvalues and eigenvectors of this matrix, which give the band structure and wavefunctions respectively, can be seen plotted below. The band structure is again for a 100-chain matrix. It is now clear that there exist in-gap states characteristic of a topologically non-trivial structure. The plot of the edge-localized wavefunctions demonstrate that the two couterpropagating edge modes are on opposite sides of the sample. Also, it should be noted that far away from the Dirac point, the wavefunctions look the same as in the nearest-neighbor model. The plots below again take $t' = 0.15$ and $t = 1$.


Edge Band Structure of Haldane Model on Square Lattice with
Next−Nearest−Neighbor Hopping
k_x−Discretized Numerical Solution ns=200
Energy
4
2
0
−2
−4
$-\pi$
$-\frac{\pi}{2}$
0
$\frac{\pi}{2}$
π
k_x


Probability Density for Eigenstates
Close to the Dirac Point
Probability Density, $|\psi|^2$
0.25
0.20
0.15
0.10
0.05
0.00
0
50
100
150
Lattice Point



References

1. Haldane, F. D. M., *Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the Parity Anomaly*. Phys. Rev. Lett., 1988.

2. M. Kohmoto, *Topological Invariant and the Quantization of the Hall Conductance*. Annals of Physics, 1985.