Toy Model Calculations: Spin-Orbit Coupling

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sample

1 Introduction

To understand the effect of the spin-orbit interaction (SOI), we explore the relatively simple case of the tight-binding model on a square lattice with periodic boundary conditions. This is not the most general model, as the name suggests the electrons must be tightly bound to their atoms, but it will be easy to see the effect of the SOI. In short, the SOI will split degenerate states in the tight-binding model, so the dispersion in one and two dimensions will have two curves with SOI instead of one.

2 Calculations

The tight-binding Hamiltonian is

$$\hat{H}_{TB} = -t \sum_{\langle i,j \rangle, \sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma}).$$

We can include the SOI in the Hamiltonian as follows

$$\hat{H}_{TB} = -t \sum_{\langle i,j \rangle} c^{\dagger}_{i,\sigma} R^{\sigma,\sigma'}_{i,j} c_{j,\sigma'} + h.c.,$$

where $R^{\sigma,\sigma'}_{i,j}$ is the hopping integral from the particle with spin σ' at site j to the particle with spin σ at site i. This term will incorporate the SOI, and $h.c.$ denotes the hermitian conjugate of the first term.

To analyze the SOI we need to Fourier Transform to momentum space (k-space) with the following transformations

$$c_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{ikx_i} c_{i,k}$$

$$c^{\dagger}_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{-ikx_i} c^{\dagger}_{i,k}.$$

Since we can traverse the reciprocal lattice by adding or subtracting reciprocal vectors we can recast x_j as

$$x_j = x_i + G,$$

where G is a reciprocal lattice vector.
The Hamiltonian then becomes

$$\hat{H}_{TB} = -\frac{t}{N}\sum_{k,k'}\sum_{x_i,\sigma} c^{\dagger}_{k,\sigma} R^{\sigma,\sigma'}_{k} c_{k',\sigma} e^{i(k-k')\cdot x_i} e^{ik'\cdot G} + h.c.,$$

but using the fact that $\sum_{x_i} e^{i(k-k')\cdot x_i} = N\delta_{kk'}$

$$\hat{H}_{TB} = -t\sum_{k,\sigma} c^{\dagger}_{k,\sigma} R^{\sigma,\sigma'}_{k} c_{k,\sigma} e^{ik\cdot G} + h.c.,$$

where $R^{\sigma,\sigma'}_{k}$ is the Fourier Transform of $R^{\sigma,\sigma'}_{i,j}$.

Now, we can write the Hamiltonian in a familiar form

$$\hat{H}_{TB} = -t\sum_{k} \psi^{\dagger}_{k} H(k) \psi_k,$$

where

$$\psi_k = (c_{k,\sigma}, c_{k,\sigma'})^T$$

$$\begin{pmatrix} 0 & R^{\sigma,\sigma'}_{k} e^{ik\cdot G} \\ (R^{\sigma,\sigma'}_{k})^{\dagger} e^{-ik\cdot G} & 0 \end{pmatrix},$$

and the energy spectrum is given by $E_{\pm} = -t\left(\pm|R^{\sigma,\sigma'}_{k}|\right)$. The $-t$ comes from the prefactor in the Hamiltonian and $\pm|R^{\sigma,\sigma'}_{k}|$ are the eigenvalues. As a quick sanity check, it makes sense that the SOI would be on the off-diagonal since it couples different states and breaks degeneracy.

$R_{i,j}$ is given by $\exp[i\vec{A}\cdot(\vec{r}_i - \vec{r}_j)]$ (Cole 2012), where $\vec{A}$ is the non-Abelian gauge $(\alpha\sigma_y, \beta\sigma_x, 0)$. The case where $\beta = -\alpha$ corresponds to Rashba spin-orbit coupling.

2.1 1-D Case

In one dimension $R_{i,j}$ evaluates to

$$R^{\hat{x}}_{i,j} = \exp[\pm i\alpha\sigma_y] = 1 \pm i\alpha\sigma_y - \frac{\alpha^2\cdot I}{2!} \mp i\frac{\alpha^3\cdot\sigma_y}{3!} + ... =$$
$$= I\cdot\left(1 - \frac{\alpha^2}{2!} + \frac{\alpha^4}{4!} + ...\right) \pm i\sigma_y\left(\alpha - \frac{\alpha^3}{3!} + ...\right) =$$
$$= \cos\alpha \pm i\sin\alpha\cdot\sigma_y,$$

where the $\pm$ denotes the positive and negative x-direction. This is the term that contains the SOI physics in our model.

The Hamiltonian can be written in the form

$$\boldsymbol{d}_0 + \boldsymbol{d}(\vec{\boldsymbol{k}}) \cdot \boldsymbol{\sigma},$$

where $\boldsymbol{\sigma}$ is a vector of Pauli-matrices. These give the eigenvalues (Zhang 2014)

$$E_{\pm}(\boldsymbol{k}) = \boldsymbol{d}_0 \pm |\boldsymbol{d}(\vec{\boldsymbol{k}})|.$$

Since we have already factored our Hamiltonian, which contains all of the physics in the middle 2x2 matrix, we can perform with calculation with $R_{i,j}^{\sigma,\sigma'}$.

The Fourier Transform is given by

$$\boldsymbol{d}_0 \xrightarrow{FT} \sum_x \cos\alpha(\cos kx + i\sin kx) = \sum_x \cos\alpha\cos kx + \text{Im}$$

$$\boldsymbol{d}(\vec{\boldsymbol{k}}) \xrightarrow{FT} \sum_x \pm i\sin\alpha(\cos kx + i\sin kx) = \sum_x \mp\sin\alpha\sin kx + \text{Im}.$$

The eigenvalues are then given by

$$\sum_x \cos\alpha\cos kx \pm |\mp\sin\alpha\sin kx| = \sum_x \cos\alpha\cos kx \pm \sin\alpha\sin kx$$

$$\Rightarrow \sum_x \frac{1}{2}\left[cos(kx-\alpha) + cos(kx+\alpha)\right] \pm \frac{1}{2}\left[cos(kx-\alpha) - cos(kx+\alpha)\right]$$

$$\Rightarrow 2\cos(k \pm \alpha),$$

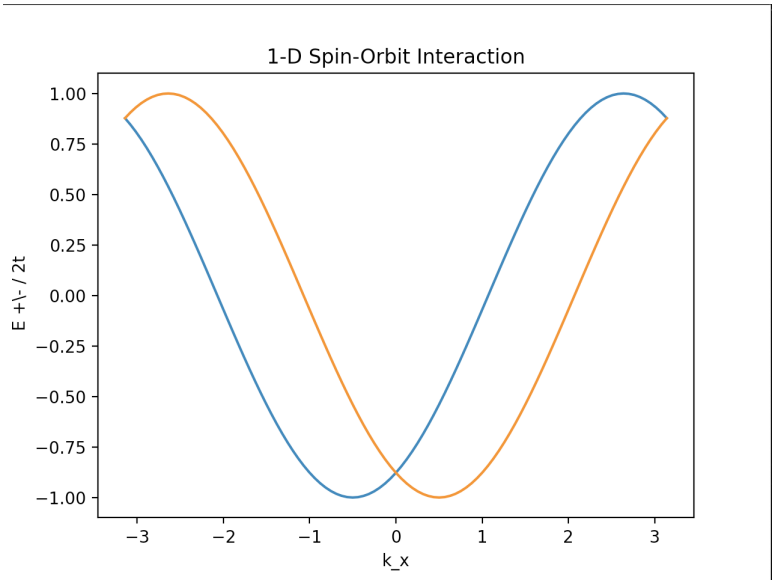
when taking into account hopping in both directions in the First Brillouin Zone (FBZ). The Hamiltonian also contains a $-t$ prefactor, so

$$\boxed{E_{\pm}(k) = -2tcos(k \pm \alpha)}.$$

This is the dispersion produced by the SOI. Comparing to the dispersion for the tight-binding model without SOI, which was calculated in homework two

$$-2tcos(k),$$

we can see that the effect of the SOI is to split the degeneracy into two distinct bands (recall: in homework 2 we found that the energies of the tight-binding model have spatial symmetry, so there are actually two degenerate energies corresponding to $G = \pm a$).




```python
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm

t = 5
a = 1
alpha = 0.5

x = np.linspace(-1*np.pi/a, np.pi*a, 101)
y = np.linspace(-1*np.pi/a, np.pi*a, 101)

k_x, k_y = np.meshgrid(x, y)
k_x = np.linspace(-1*np.pi/a, np.pi*a, 101)

E = 2*t*(np.cos(k_x + a) + np.cos(k_y + a))

E_1 = -1*np.cos(k_x + alpha)
E_2 = -1*np.cos(k_x - alpha)


plt.xlabel('k_x')
plt.ylabel(' E +\- / 2t')
plt.title('1-D Spin-Orbit Interaction')
plt.plot(k_x, E_1)
plt.plot(k_x, E_2)
plt.show()
```

We notice from the graph that this spatial symmetry is broken, so the energy dispersion is different in the positive direction than in the negative direction. Additionally, adding a Zeeman term would introduce a band gap and make this material an insulator, where the bottom band would be the valence band and the top would be the conduction band. If there is no way to adiabatically transform this material into a normal insulator without first passing through a conduction phase, then it is called a topological insulator.

2.2 2-D Case

Now, we add the SOI in the y direction by adding the analogous hopping matrix to the Hamiltonian

$$R_{i,j}^{\hat{y}} = cos\beta \pm isin\beta\sigma_x.$$

In two dimensions the Hamiltonian $H(k)$ in matrix form with the SOI in both positive directions is

$$H^{+\hat{x},+\hat{y}}(k) = \begin{bmatrix} cos\alpha + cos\beta & sin\alpha + isin\beta \\ -sin\alpha + isin\beta & cos\alpha + cos\beta \end{bmatrix}.$$

To be explicit, the hopping integrals are indeed matrices since each term is multiplied by the identity or a pauli-matrix (i.e. $R_{i,j}^{\sigma,\sigma'} = cos\alpha I \pm isin\alpha \cdot \sigma_y$, where I is the identity matrix). It is also important to note that this matrix is written in the spin basis, so the diagonal terms give spin conserving hopping and the off diagonal terms are spin flips resulting from the SOI. We can decompose this (and any other) Hamiltonian into a sum of pauli-matrices and the identity (which is how we made it), which gives the energy dispersion (Zhang 2014)

$$E_{\pm}(\boldsymbol{k}) = d_0(\boldsymbol{k}) \pm |\boldsymbol{d}(\boldsymbol{k})|,$$

where $\boldsymbol{d}(\boldsymbol{k})$ is the vector of coefficients multiplying pauli-matrices and $d_0(\boldsymbol{k})$ is the coefficient multiplying the identity. Recall that the above hopping matrix was composed of

$$R_{i,j}^{\hat{y}} = cos\alpha \pm isin\alpha\sigma_y$$

$$R^{\hat{y}}_{i,j} = cos\beta \pm isin\beta\sigma_x,$$

which give the decomposition

$$d_0 = cos\alpha + cos\beta$$

$$\boldsymbol{d} = (isin\beta, isin\alpha, 0).$$

Finally, we need to Fourier Transform this vector representation of the Hamiltonian to find the dispersion in k-space. If we recall from the one dimensional case, α was attached to σ_y, which got k_x, therefore, β should get k_y since it is attached to σ_x.

$$d_0 \xrightarrow{FT} cos\alpha cosk_x + cos\beta cosk_y$$

$$\boldsymbol{d} \xrightarrow{FT} (isin\beta sink_y, isin\alpha sink_x, 0).$$

Here, we need to be very careful with our algebra. The expression for the dispersion energy involves the modulus of the d-vector. We have so far only done the calculation for $H^{+\hat{x},+\hat{y}}(k)$, but we also need to consider $H(k)$ in the $+\hat{x}/-\hat{y}$, $-\hat{x}/+\hat{y}$ and $-\hat{x}/-\hat{y}$ directions. A little bit of thought shows that the cross terms will cancel and the outer terms will add (and we also have a prefactor of $-t$ in front of the Hamiltonian). Taking all of these into account we finally arrive at the d-vector

$$d_0(\boldsymbol{k}) = -2t(cos\alpha cosk_x + cos\beta cosk_y)$$

$$\boldsymbol{d}(\boldsymbol{k}) = -2t(sin\beta sink_y, sin\alpha sink_x, 0),$$

which gives the energy dispersion in two dimensions by

$$E_{\pm}(\boldsymbol{k}) = d_0(\boldsymbol{k}) \pm |\boldsymbol{d}(\boldsymbol{k})|.$$

We can see that the SOI splits the degenerate energy levels in the normal tight-binding model (from homework 2: $E(\boldsymbol{k}) = -2t(cosk_x + cosk_y)$) into two distinct bands. Check $(k_x, k_y) = (0, 0)$ for width of band gap. Additionally, the eigenvectors of the matrix written above are easy to find with Mathematica:

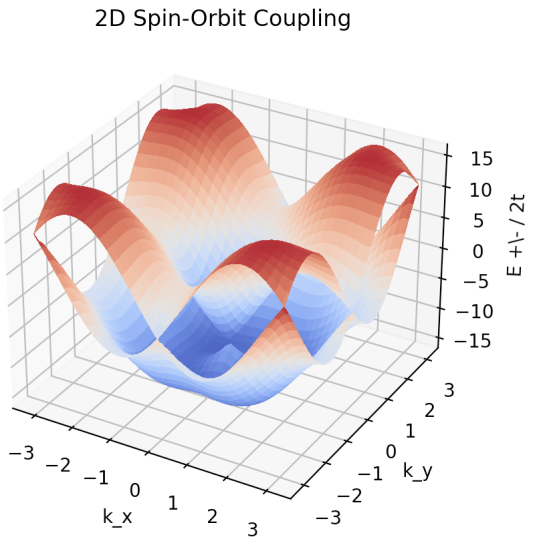
$$\chi_{\pm} = \left(1, \pm\frac{\sin\alpha\sin k_x - \sin\beta\sin k_y}{\sqrt{(\sin\alpha\sin k_x)^2 + (\sin\beta\sin k_y)^2}}\right),$$

which can be recast as

$$\chi_{\pm}(\boldsymbol{k}) = (1, \mp ie^{i\phi_{\boldsymbol{k}}}),$$

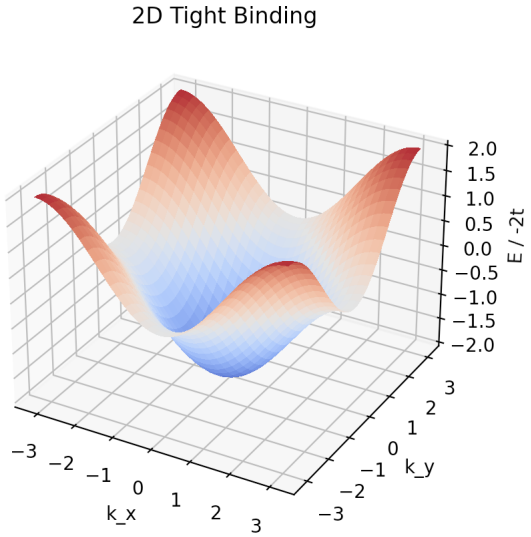
$$\text{where } \phi_{\boldsymbol{k}} = \arctan\left(\frac{\sin\beta\sin k_y}{\sin\alpha\sin k_x}\right) = \arctan\left(d_x/d_y\right).$$

These eigenvectors spin in different directions in k-space if they are in the top or bottom bands.

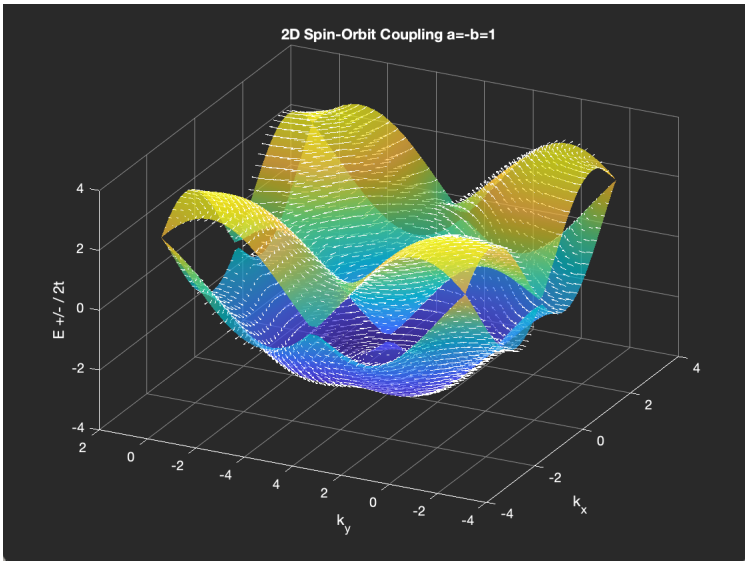



```python
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm

t = 5
a = 1
b = 1
eta = 0

x = np.linspace(-1*np.pi/a, np.pi*a, 101)
y = np.linspace(-1*np.pi/a, np.pi*a, 101)

k_x, k_y = np.meshgrid(x, y)

d0 = -2*t*(np.cos(a)*np.cos(k_x) + np.cos(b)*np.cos(k_y))
dx = -2*t*np.sin(b)*np.sin(k_y)
dy = -2*t*np.sin(a)*np.sin(k_x)

magd = np.sqrt( dx**2 + dy**2 )

E_1 = d0 + magd
E_2 = d0 - magd

fig, ax = plt.subplots(subplot_kw={"projection": "3d"}, nrows=1, ncols=1)


ax.plot_surface(k_x, k_y, E_1, cmap=cm.coolwarm,
                       linewidth=0, antialiased=False)
ax.plot_surface(k_x, k_y, E_2, cmap=cm.coolwarm,
                       linewidth=0, antialiased=False)
ax.set_xlabel('k_x')
ax.set_ylabel('k_y')
ax.set_zlabel(' E +\- / 2t')
plt.title('2D Spin-Orbit Coupling')

plt.show()
```

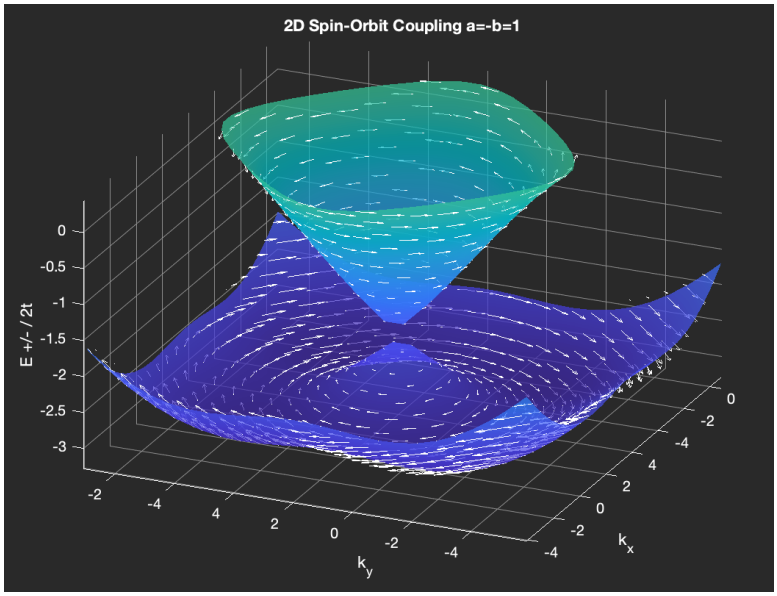
Comparing this to the band structure obtained through tight-binding model without SOI, we can clearly see that the SOI breaks the degeneracy and creates a topologically different band structure.



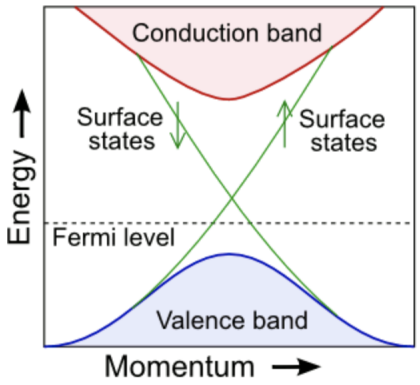
Finally, the spin textures are shown below for Rashba Spin-Orbit coupling ($\alpha = -\beta$) for the parameters $\alpha = 1$ and $\alpha = \pi/2$, respectively.



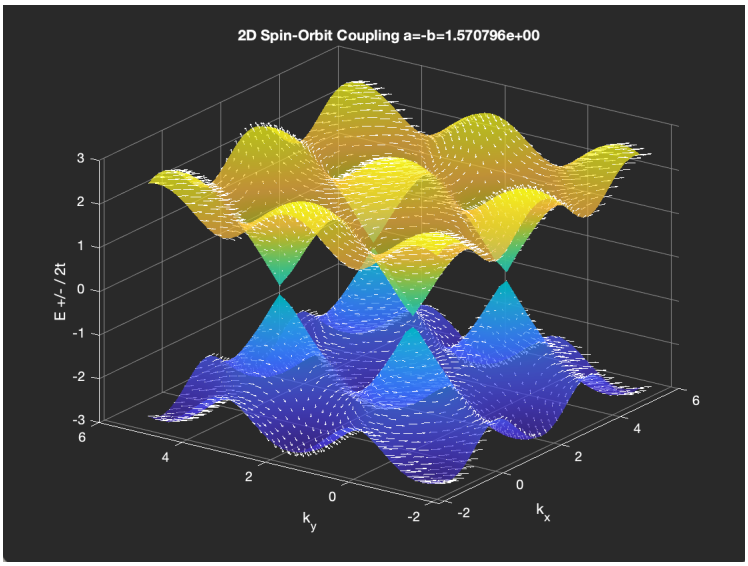
If we zoom into the middle we can see the band gap where the Dirac cone lives with the spins locked in a circle around the cone.



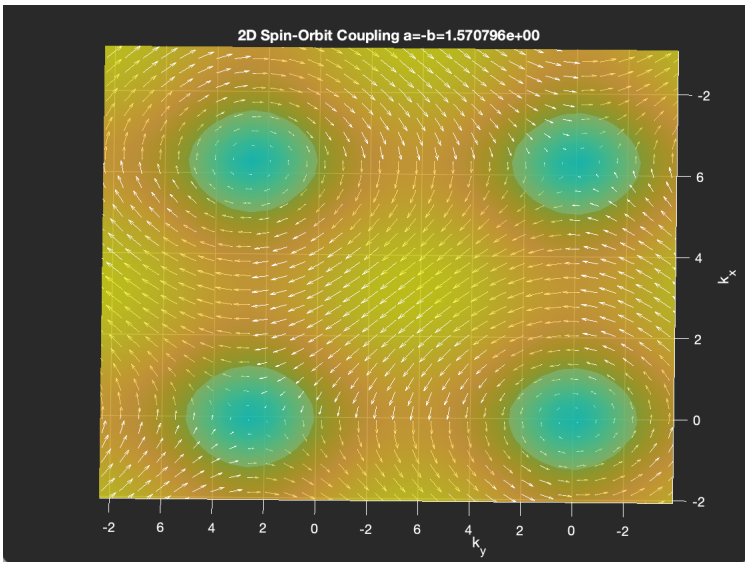
The conduction and valence bands are gapped and topologically distinct, so they are protected and they are twisted. Notice that the spins are locked in momentum space clockwise in the bottom band and counter clockwise in the upper band. This suggests the band structure of a topological insulator.

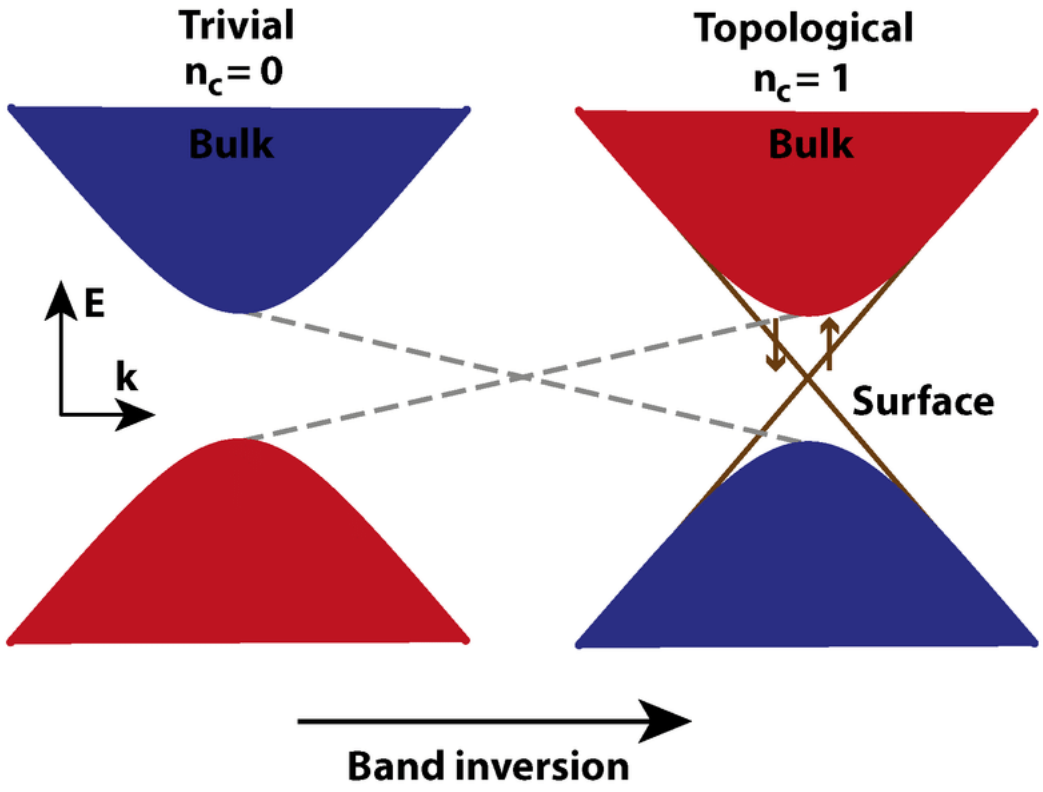


The next graphs pertain to the same system but for the choice of $\alpha = \pi/2$.



A bird's eye view of this band structure and spin texture also show that this is the band structure of a topological insulator.





References

Cole, William S. (2012). "Bose-Hubbard Models with Synthetic Spin-Orbit Coupling: Mott Insulators, Spin Textures, and Superfluidity". In: *Physical Review Letters*. DOI: 10.1103/PhysRevLett.109.085302.

Zhang, Shizhong. (2014). "Spin-orbit Coupling in Optical lattices". In: *Arxiv*. DOI: https://arxiv.org/pdf/1411.2297.pdf.