Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 8: Topological Insulator Properties

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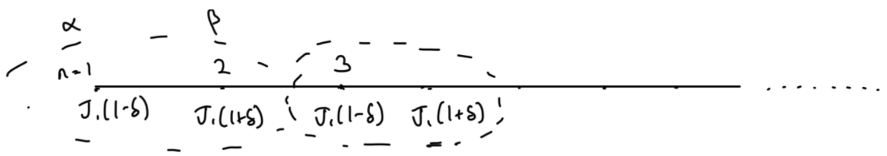
In this lecture, some special cases in the SSH model was discussed. After that, some properties of topological insulators were introduced.

1 Some Variations in the SSH Model



Considering the SSH model with the bond strengths given by :

$$\delta_1 = J(1-\delta)$$
$$\delta_2 = J(1+\delta)$$

for $\delta > 0$ (i.e., the last bond is weaker), there is a $E = 0$ state, which is exponentially localised at the end.

At around the $E = 0$, we can expand the state as:

$$\psi = \psi_R e^{i\frac{\pi x}{2d}} + \psi_L e^{-i\frac{\pi x}{2d}} \tag{1}$$

And, writing the state is in the form:

$$\psi = \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{2}$$

We can write:

$$i\frac{\partial \psi}{\partial t} = \begin{pmatrix} -iv\frac{\partial}{\partial x} & 0 \\ 0 & iv\frac{\partial}{\partial x} \end{pmatrix} \psi + \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix} \psi \tag{3}$$

Here,

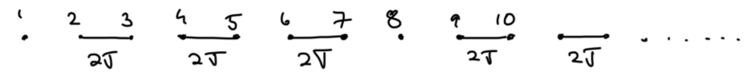
$$E = vk \to \psi_R$$
$$= -vk \to \psi_L$$

$$\implies i\frac{\partial \psi}{\partial t} = \left[-iv\frac{\partial}{\partial x}\sigma^z + \delta\sigma^x \right] \psi \tag{4}$$

For $\psi = e^{i(kx-Et)}$,

$$E\psi = [vk\sigma^z + \delta\sigma^x]\psi \tag{5}$$
$$= \pm\sqrt{v^2k^2+\delta^2}\psi \tag{6}$$

1.1 Explanations for End Mode: $\delta \to 1$



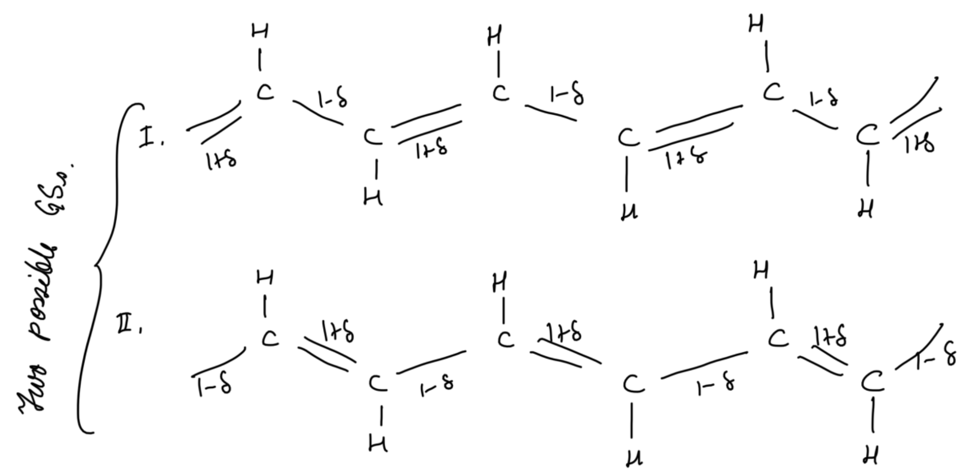
In the case that $\delta \to 1$, the hopping amplitude between site 1 and 2 in the 1-d lattice tends to 0. Hence, the Hamiltonian will start wth the terms:

$$H = 2J(c_2^\dagger c_3 + c_3^\dagger c_2)$$

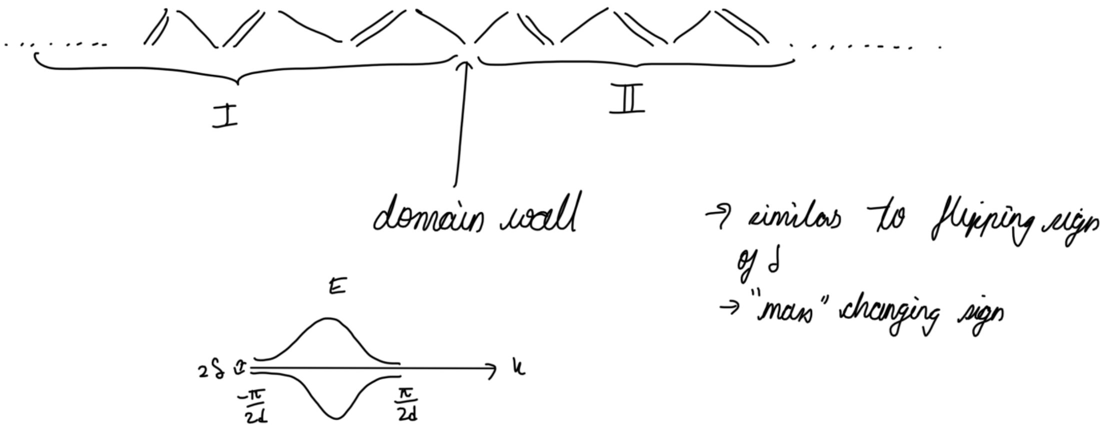
This means that the energy $E \to \pm 2J$. Also note that there is no term with $c_1, c_1^\dagger$, thus no energy is needed to add an electron to site 1.

1.2 Flipping the Sign of δ

Recall that for an end mode, we required: $|1-\delta| < |1+\delta|$
$\to$The question is, what happens if the δ changes sign somewhere? The two possible configurations (ground states) are given below:



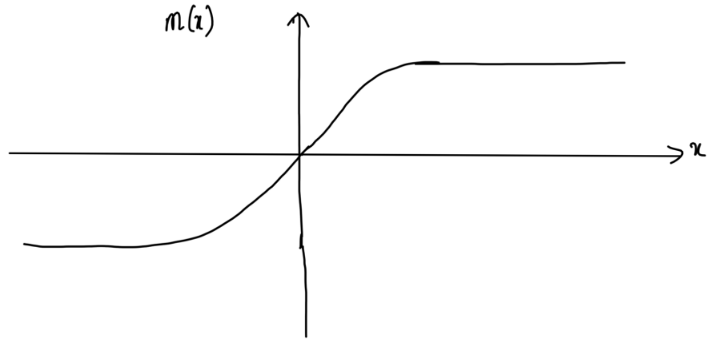
Then we can have a case where both of these configurations are there together.



This is equivalent to the "mass" of the electron changing sign as we go along the lattice because the δ term is effectively the mass term of the Dirac Hamiltonian we are considering. Recall equation (4) but now with δ replaced by $m(x)$.

$$i\frac{\partial \psi}{\partial t} = \left[-iv\frac{\partial}{\partial x}\sigma^z + m(x)\sigma^x\right]\psi \tag{7}$$

The above shown configuration means that $m(x)$ varies as shown below:



Let us try the ansatz: $\psi = f(x)e^{-iEt}$ and suppose there is a state with $E = 0$. Then we can write:

$$\left[-iv\sigma^z\frac{\partial}{\partial x} + m(x)\sigma^x\right]\psi = 0$$
$$\left[-iv\frac{\partial}{\partial x} + im(x)\sigma^y\right]\psi = 0$$
$$\implies \left[-v\frac{\partial}{\partial x} + m(x)\sigma^y\right]\psi = 0$$

Let ψ satisfy $\sigma^y\psi = c\psi$, where c is some constant.

1. $\sigma^y\psi = \psi$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \implies \psi = \begin{pmatrix} 1 \\ i \end{pmatrix} f(x)$$

2. $\sigma^y\psi = -\psi$

$$\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \implies \psi = \begin{pmatrix} 1 \\ -i \end{pmatrix} g(x)$$

Then with the other term in the Hamiltonian, we can write:

1. $\left[-v\frac{\partial}{\partial x} + m(x)\right]\psi = 0$
   $\implies \psi = \begin{pmatrix} 1 \\ i \end{pmatrix} exp\left(\int_0^x dx' \frac{m(x')}{v}\right)$
2. $\left[-v\frac{\partial}{\partial x} - m(x)\right]\psi = 0$
   $\implies \psi = \begin{pmatrix} 1 \\ -i \end{pmatrix} exp\left(-\int_0^x dx' \frac{m(x')}{v}\right)$

The solution in (2) $\to 0$ at both $x \to \infty$ and $x \to -\infty$.
Thus, we have a solution and it is a localised state.
Note: With the Dirac equation, when mass changes sign, we get a localised $E = 0$ state.

2 Topological Insulator Properties

- Insulating in the bulk
- Conducting states at the boundaries
- Bulk-boundary correspondence: Wavefunctions of thr bulk states are characterised by a topological invariant $\to$ number of boundary states

3 3-D Topological Insulators

Examples: Bi_2Se_3, Bi_2Te_3.
In 3-D topological insulators, spin-orbit coupling plays an important role.
The H-atom spin-orbit coupling is due to the effective magnetic field experienced by a revolving electron around the nucleus,

$$\vec{B} = \frac{\vec{v}}{c} \times \vec{E}$$

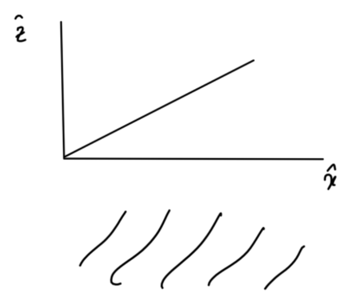
Then the Zeeman coupling term is:$-\frac{gq}{2mc}\vec{S} \cdot \vec{B}$
Spin-orbit coupling is given by:

$$\begin{aligned} H_{S-O} &= A\vec{S} \cdot (\vec{v} \times \vec{E}) \\ &= \frac{A}{m}\vec{S} \cdot (\vec{p} \times \vec{E}) \end{aligned}$$

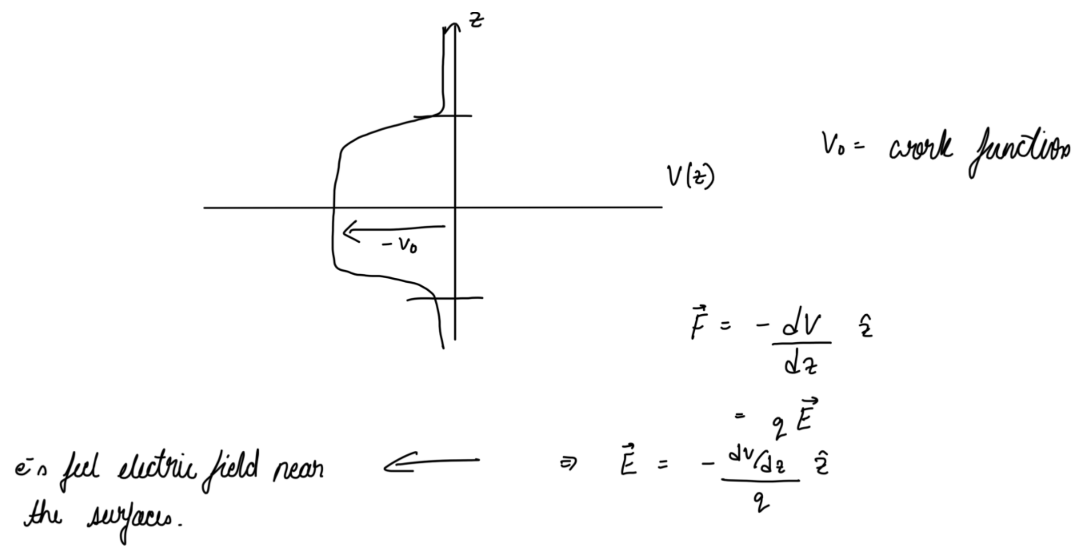
In materials like Bi_2Se_3, Bi_2Te_3, the H_{S-O} term is of the order of magnitude of the other terms in the Hamiltonian - can also be the dominant term.

3.1 Spin-Orbit Locking

A 3-D topological insulator can be considered as below:

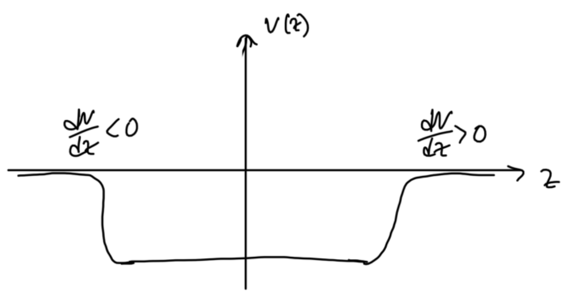


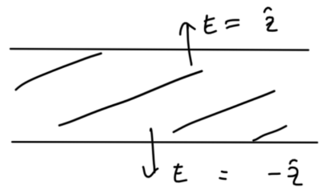
The potential felt by an electron in this sytem can be plotted as below:



Now, for spin-orbit coupling, we need an electric field. At the surface of these materials, we can have an effective electric field even without applying an external electric field because there is a high potential gradient at the surface.
We can write the force on the electron as: $\vec{F} = -\frac{dV}{dz}\hat{z} = q\vec{E}$
$\implies \vec{E} = -\frac{\frac{dV}{dz}}{q}\hat{z}$

Thus, the potential profile and the direction of electric field can be seen below:



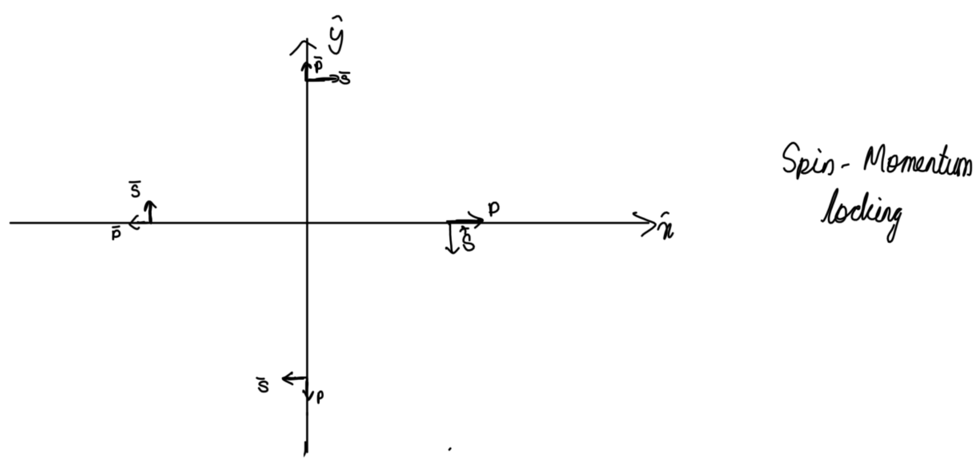


Now, the spin-orbit coupling part of the Hamiltonian can be written as:

$$
\begin{aligned}
H_{S-O} &= \vec{S} \cdot (\vec{p} \times \vec{E}) \\
H_{top} &= \vec{\sigma} \cdot (\vec{p} \times \hat{z}) \\
&= v(\sigma_x p_y - \sigma_y p_x) \rightarrow E = \pm v\sqrt{p_x^2 + p_y^2} \rightarrow \text{relativistic type of dispersion but } m = 0 \\
H_{bot} &= -v(\sigma_x p_y - \sigma_y p_x)
\end{aligned}
$$

Consider graphene. The two Dirac points at k and k' will have:

$$
i\hbar \frac{\partial \psi}{\partial t} = \hbar v \left(\sigma^x \left(-i \frac{\partial}{\partial x} \right) + \sigma^y \left(-i \frac{\partial}{\partial y} \right) \right) \tag{8}
$$



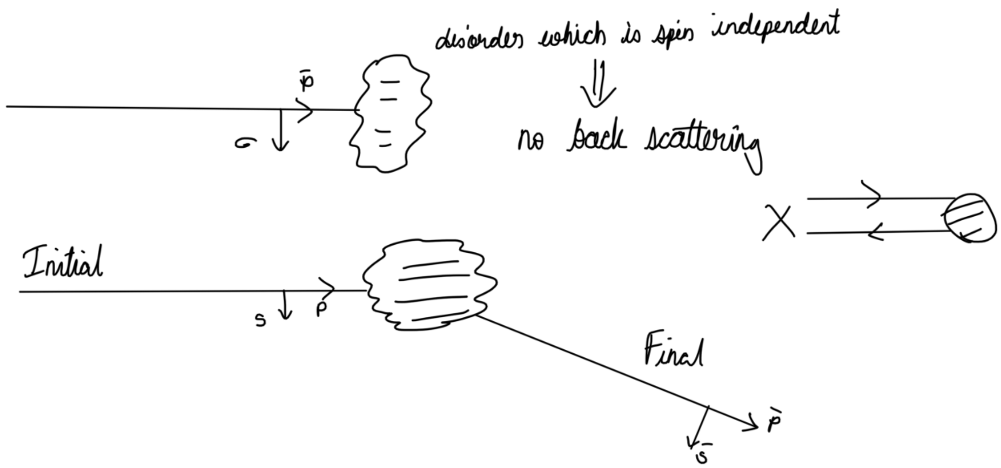
So now, the spin $\vec{\sigma}$ will always be at right angles to the momentum $\vec{p}$. This is called spin-orbit locking.

3.2 Disorders

Disorders in a condensed matter system can be:

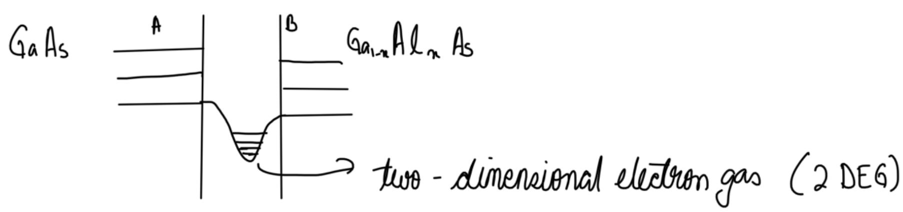
- potential (spin-independent) disorder)
- spin-dependent disorder

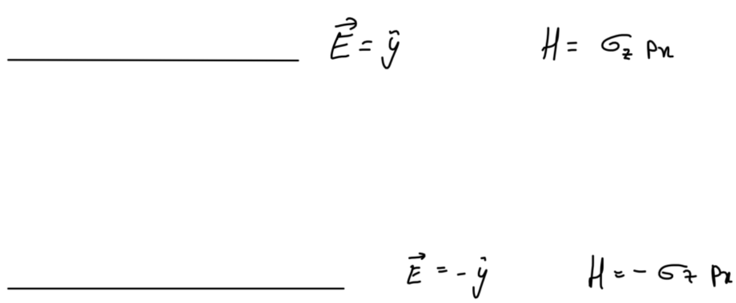
For spin-independent disorders, the spin-orbit locking will prevent any sort of back scattering from these because for back-scattering, the spin will have to be completely flipped, which is not possible for spin-independent disorders.



3.3 Semiconductor Heterostructures

Heterostructures are systems in which different materials are made to form an interface. An example would be that of $GaAs$ and $Ga_{1-x}Al_xAs$, where at the interface, there is a layer formed, which is studied as a two-dimensional electron gas.

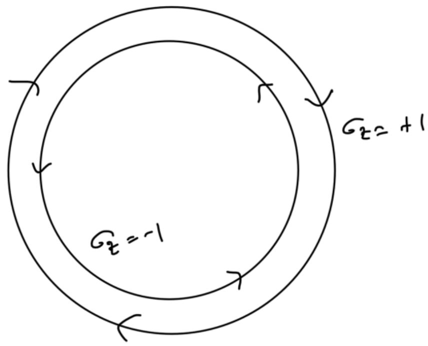




Upper edge: $H = \sigma_z p_x$
$E = \pm p_x$

$\longrightarrow p_x, \ \sigma_z = +1$

$\longleftarrow p_x, \ \sigma_z = -1$



Spin - momentum locking

The edge states in 2-D topological insulators are completely robust i.e., there is no chance of back scattering. There is ballistic conductance.

$$\sigma = \frac{e^2}{h}$$