What is a topological insulator ?

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1 Foreword and references

Tpological insulator is a huge domain, and today I only aim to give a short introduction using SSH model. I am not a specialist, and the idea is just to focus on physical consequences of topological insulators. This presentation mostly follows standard condensed matter theory books, and this paper for the topological insulator part: https://arxiv.org/pdf/1906.08435. I also used this paper for symmetries: https://arxiv.org/pdf/1509.02295. I also enjoyed this talk from R. Fleury: https://www.youtube.com/watch?v=oycc2vdRH8c and this one from B. Doucot :

2 What is topology ?

Generically, topology is a branch of mathematics that aims to study spaces regardless of their peculiar local geometry/shape. It is very usefull to define the notion of limit in a very general way. Geometry focuses more on local properties such as local curvature, angles, geodesics. In topology questions of interests are rather: is my set connected ? Is it open or closed ? Can I deform any path to another ? Can I deform one set to another ?

Importantly, all topological properties are left invariant by continuous deformation, which makes them very useful ! If you have two sets and one of their topological invariant differs, then you know for sure they cannot be deformed one into another (the reciprocal is much more difficult). For instance, consider $\mathbb{R}^2$ and $\mathbb{R}^2 \setminus \{0\}$. Can they be continuously deformed one into another, i.e. can one find a bijective continuous map $\phi : \mathbb{R}^2 \to \mathbb{R}^2 \setminus \{0\}$? The answer is no. In $\mathbb{R}^2$, any path can be contracted to a point, the fundamental group of homotopy is said to be trivial. On the other hand, two path in $\mathbb{R}^2 \setminus \{0\}$ can be deformed one into another only if they perform the same number of turns around the origin (fundamental group $\mathbb{Z}$). Hence, no function can continuously send one set on the other.

There exists many connections between geometry and topology. For instance, the Gauss-Bonnet formula relates the number of holes (genus) and the integral of its local curvature (the product of curvature of two orthogonal geodesics passing by a point). For a compact, edge-free, orientable manifold, it reads

$$1 - g = \frac{1}{4\pi} \int K dS \tag{1}$$

Clearly, K is a local quantity that is not invariant by continuous deformation. However, the integral over the total surface is invariant. It is a general rule in topology: continuously moving something somewhere moves something elsewhere, and the two deformations compensate. You have the same thing on the hairy sphere: whatever you do, you cannot define a continuous set of vectors on the sphere (of even dimension) without creating a zero-vector somewhere.

The notion of continuous deformation is central and must be carefully defined. For instance, take a triangle: the sum of its angles is π. If you define a continuous deformation of the triangle as moving its summits, then the sum of the angles is always π and may be called a topological invariant. But you can also consider a triangle as a closed line, and continuously deform it into a square or a circle, for which no angle is defined.

In physics, many processes continuously deform a system i.e. parameters are continuously varied and the system responds accordingly. Topology is then useful to find invariant quantities with respect to these deformations. If these invariants are connected to physical behaviors, then we know that these physical properties will be preserved during the deformation. Note that the deformation does not have to be effective. If you can continuously deform "by thought" (or mathematically) one system

into another, then they share all their topological properties. This can be used to simplify the study of complex systems such as insulators.

3 What is an insulator ?

3.1 Band theory

Before coming to topological insulator, let us first describe briefly how insulating properties of solids are described. Our starting point is the Schrodinger equation

$$-i\hbar\partial_t\psi = H\psi \tag{2}$$

to describe a crystal, that is a set of atoms. Generically, the Hamiltonian can be written as

$$H = -\sum_i \frac{\hbar^2}{2m_N}\nabla^2_{R_i} - \sum_j \frac{\hbar^2}{2m_e}\nabla^2_{r_j} - \frac{q^2}{4\pi\epsilon_0}\sum_{i,j}\left(\frac{1}{r_i - r_j} + \frac{Z_i Z_j}{R_i - R_j} + \frac{Z_i}{R_i - r_j}\right) \tag{3}$$

where R_j is position of nucleus and r_i position of electrons. The Born-Oppenheimer approximation consists in neglecting the motion of nucleus with respect to the one of electrons. Indeed, the mass ratio is about 10^3 while the forces are the same (as they are related to the charge). For the electron, the positions R_j are fixed parameters. We end up with

$$H = -\sum_j \frac{\hbar^2}{2m_e}\nabla^2_{r_j} - \frac{q^2}{4\pi\epsilon_0}\sum_{i,j}\frac{Z_i}{R_i - r_j} + \frac{1}{r_i - r_j} \tag{4}$$

The next step consists in replacing electron-electron interactions by a mean field. The sum over all the electron positions results in a potential $V_m(r_i)$. It is reasonable to think of this potential as having the same periodicity than the nucleus network. Overall, the final Hamiltonian reads

$$H = \sum_j \frac{-\hbar^2}{2m_e}\nabla^2_{r_j} + U(r_i) \tag{5}$$

where $U(r_i)$ is periodic with any discrete translation on the network $U(r + na) = U(r)$. we are left with a sum of independent Hamiltonians. It is enough to consider each Hamiltonian separately

Now we will focus on the tight binding model. The idea is that the electron feels a lot the nearest atom, a bit the two closest neighbors and not the others. The Hamiltonian is set in the form

$$H = \frac{\hbar^2}{2m_e}\nabla^2_r - \frac{\beta}{r} - \beta\left(\frac{1}{r_i + a} + \frac{1}{r_i - a} + ...\right) = H_0 + H_1 \tag{6}$$

From hydrogen atom model, we know that the eigenfunctions of H_0 are localized near $r = 0$ and are labeled by n such that $H_0\phi_n = E_n\phi_n$ with $E_n \sim -1/n^2$. We now aim to build solutions to our problem of the form

$$\psi_n(r) = \sum_j b_n^j \phi_n(r - R_j) \tag{7}$$

We willl formulate this in a more algebraic manner. We define $|j, n\rangle = \phi_n(. - R_j)$. We obtain

$$|\psi_n\rangle = \sum_j b_n^j |j, n\rangle \tag{8}$$

We enforce that this solution respects Bloch theorem that states $\psi_n(x+a) = e^{ika}\psi_n(x)$. Injecting this constrain, we obtain $b_n^{j+1} = e^{ika}b_n^j = e^{ijka}b_n^0$. Therefore, one has

$$|\psi_n\rangle = b_0^n \sum_j e^{ijka} |j, n\rangle \tag{9}$$

We can now inject this ansatz in the Hamitlonian

$$H|\psi_n\rangle = H_0|\psi_n\rangle + H_1|\psi_n\rangle = E|\psi_n\rangle \tag{10}$$

We perform scalar product against $\langle l, m|$. As all functions are orthogonal, we obtain

$$Ee^{ijka}b_m^0 = E_m e^{ijka}b_m^0 + \sum_{j,n} e^{ijka}b_n^0 \langle l, m|H_1|j, n\rangle \tag{11}$$

Rememer that the scalar product measures the overlap between the functions. This overlap is small and assumed to be non-zero only for $j = l \pm 1, n = m$, quantified by $t_m = \langle j \pm 1, m|H_1|j, m\rangle$. We end up with

$$E = E_m + 2t_m \cos ka \tag{12}$$

We see that coupling to neighbors results in degeneracy lifting of the eigenvalues: each k has different energy! It results in band like structure of the energy levels. The metallic or insulating behavior depends on the total amount of electrons in the system compared to this energy structure. Indeed, if one sets an electric force $F = -Vx$ in the material, then electrons can move only if there is some energy state for them.

Important remark: the wavevector k is defined modulo $2\pi/a$, and it is sufficient to consider $k \in [-\pi/a, \pi/a]$ which is called the first Brillouin zone. Also, what we did essentially was to use translation symmetry $x \to x + a$ by performing a Fourier transform of ψ, which allowed to diagonalize H and find its eigenvalues.

3.2 Tight-binding Hamiltonian - SSH model

We have seen above that the role of H_1 is to couple nearest neighbors. The total Hamiltonian can be reframed in our vector language as

$$H = \sum_{j,n} E_n |j, n\rangle \langle j, n| + t_n |j + 1, n\rangle \langle j, n| + t_n |j - 1, n\rangle \langle j, n| = \sum_{n,j} H_n^j \tag{13}$$

Indeed, our previous computation was essentially a computation of the matrix elements of H in the $|j, n\rangle$ basis! The interpretation of this Hamiltonian is fairly simple: there an onsite energy and a jumping term toward neighbors due to tunneling effect.

What if we now have two types of atoms A and B in the media ? According to tight-binding approach, the Hamiltonian now reads

$$H = v \sum_j |A, j\rangle \langle B, j| + w \sum_j |A, j + 1\rangle \langle B, j| + h.c. \tag{14}$$

We now aim to find the energy states of this new Hamiltonian. We perform a Fourier transform by defining

$$|A/B, \hat{k}\rangle = \frac{1}{\sqrt{N}} \sum_j e^{-ijka} |, A/B, j\rangle \tag{15}$$

which can be inverted as

$$|A/B, j\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ijka} |A/B, \hat{k}\rangle \tag{16}$$

In this basis, the Hamiltonian takes the form

$$H = \sum_k (v + e^{-ika}w) |A, \hat{k}\rangle \langle B, \hat{k}| + \sum_k (v + e^{ika}w) |B, \hat{k}\rangle \langle A, \hat{k}| \tag{17}$$

Hence, it is enough to diagonalize the following 2x2 Hamiltonian for each k

$$H_k = \begin{bmatrix} 0 & v + e^{-ika} \\ v + we^{ika} & 0 \end{bmatrix} \tag{18}$$

The eigenvalues of this matrix are

$$E(k) = \pm|v + we^{ika}| = \pm\sqrt{v^2 + w^2 + 2vw\cos(ka)} \tag{19}$$

If $v \neq w$, then the system is gapped around $E = 0$ (=insulator). If $v = w$, the system is not gapped (=conducting metal). As expected, everything is symmetric if one swaps v and w. Or is it really ?

4 What is a topological insulator ?

4.1 Eigenvectors of SSH model

Consider the eigenvectors of the previous Hamiltonian, that are

$$|\pm k\rangle = \begin{bmatrix} \pm e^{i\phi(k)} \\ 1 \end{bmatrix} \tag{20}$$

where $e^{i\phi(k)} = (v + we^{-ika})/E(k)$. In the complex plane, when k goes from $-\pi/a$ to π/a, it describes a circle that winds around the origin for $w > v$ and that does not wind for $w < v$. The only way to go from one to the other is to have it going to zero, where $\phi(k)$ is ill-defined and the material behaves as a conductor. There is something "discontinuous" that occurs between the two insulating states that are not topologically equivalent.

OK, but so what ? Well, consider the two extreme cases $v = 0, w = 1$ (phase W) and $v = 1, w = 0$ (phase V). The energy states are degenerate $E(k) = \pm 1$... but remember that our material has edges. In phase V, the sites $|A, 0\rangle$ and $|B, N\rangle$ are not connected to any other atom. In particular

$$H\,|A, 0\rangle = H\,|B, N\rangle = 0 \tag{21}$$

and both are eigenvectors with zero eigenvalue. These states are edge state, as they only exist due to boundary conditions and correspond to electrons localized on the edge. In phase W, all atoms form dimers and there is no $E = 0$ state.

This picture does not change if one continuously vary v or w unless one meets the origin and goes through the conducting phase. The edge modes are exponentially localized rather than localized on a single site, but the picture is the same. The two different topological phases are associated with (1) different winding number of the bulk eigenvectors and (2) different number of edge states. It is a generic feature of topological insulators: if one goes from one topological phase to another, one must go through a conducting phase, which corresponds to create an edge state. Imagine a chain where $v : 0 \to 1$ and $w : 1 \to 0$. Somewhere in the middle, there is a conducting phase between two gaped phases, which host localized modes. The fact that you can link the number of edge states with a quantity computed in the bulk is called bulk-edge correspondence and is fundamental in topology.

Note that the winding number can be computed as

$$W = \int_{-\pi/a}^{\pi/a} dk \partial_k \phi = i \int dk\, \langle k|\, \partial_k\, |k\rangle \tag{22}$$

where the last equality depends on the Berry connection, which is a fundamental quantity in topological physics. Indeed, it corresponds to the phase acquired by the vector $|k\rangle$ when k is slowly varied along time. Although the Berry connection $\langle k|\, \partial_k\, |k\rangle$ is not invariant when one moves a bit v and w, the winding number is invariant and can only be changed if $v = w$ to cross the origin.

4.2 Symmetries and topological invariant

Let us discuss a bit the role of symmetries. First, we need the projectors on sites A and B

$$P_{A/B} = \sum_j |A/B, j\rangle\, \langle A/B, j| \tag{23}$$

One has $P_A + P_B = \mathbb{I}$. We now define $\Sigma = P_A - P_B$ called chiral symmetry. Clearly, one has $\Sigma^2 = \mathbb{I}$, $\Sigma = \Sigma^\dagger$. Moreover, one has

$$\Sigma\, |A, j\rangle\, \langle B, j'|\, \Sigma^\dagger = -\,|A, j\rangle\, \langle B, j'| \qquad \text{such that} \qquad \Sigma H \Sigma^\dagger = -H \tag{24}$$

Note that this symmetry is robust, in the sense that it still holds if v, w coupling now depend on space. It holds because the chiral symmetry is local (it is defined using local operators on site j).

This symmetry has important consequences. If there is an eigenstate $H\,|\psi\rangle = E\,|\psi\rangle$, then $H\Sigma\,|\psi\rangle = -\Sigma H\,|\psi\rangle = -E\Sigma\,|\psi\rangle$. If $E \neq 0$, one immediately get a partner of energy $-E$. We therefore expect the non-zero spectrum to be symmetric. Moreover, since $E \neq -E$, their eigenvectors are orthogonal

$$\langle\psi|\, \Sigma\, |\psi\rangle = 0 = \langle\psi|\, P_A\, |\psi\rangle - \langle\psi|\, P_B\, |\psi\rangle \tag{25}$$

This means that any non-zero mode has equal population on the A and B sublattice.

For $E = 0$, $H(1 + \Sigma)|\psi\rangle = P_A|\psi\rangle = 0$ and $H(1 - \Sigma)|\psi\rangle = P_B|\psi\rangle = 0$. Therefore, one can create two orthogonal partners with zero energy on different sublattices from a single zero-state.

Importantly, we have shown that only the zero-energy states have support on one of the two sublattice, while non-zero states are equally distributed on the two sub-lattices.

4.3 Bulk-edge correspondence

Consider now a deformation of a Hamiltonian that (1) respects the chiral symmetry and (2) does not close the gap. One writes $H_k(\lambda) = H_k + H_1(k, \lambda)$. Since H_1 respects chiral symmetry, it is of the form $H_1 = a(\lambda, k)\sigma_x + b(\lambda, k)\sigma_y$. Due to the imposed properties, one cannot change the winding number of our topological insulator (=bulk invariant). Let us now denote N_A and N_B the number of zero-energy states on the left side with support on A and B in a semi-infinite insulator. Note that these modes are edge modes, because they cannot exist in the bulk. Besides, $N_A - N_B$ is also a topological invariant. Indeed, what can happen upon deformations ?

- A state $|\psi\rangle$ of energy $E > 0$ can be taken to zero energy. But then, its chiral partner $\Gamma|\psi\rangle$ will also come to zero, such that $(1 + \Gamma)|\psi\rangle = P_A|\psi\rangle$ and $(1 - \Gamma)|\psi\rangle = P_B|\psi\rangle$ are new zero eigenstates. Then $N_A \to N_A + 1$, $N_B \to N_B + 1$ and $N_A - N_B$ is invariant.
- Conversely, a zero energy state can get strictly positive energy. But then its chiral partner must also get strictly negative energy. Hence both N_A and N_B have lost a unit.

Last, one can remark that for $w = 0$, there is one edge state carried by A. This edge state must remain whatever the deformation on v and w. The only way to get rid of it is to turn it into a bulk state i.e. to take $v = w$. Thus, we see that $N_A - N_B$ (=edge quantity) has the same behavior as a bulk quantity (=winding number computed on eigenstates).

If you now have a long segment of SSH insulator, you have also a B-state on the right. There, one may think that maybe the left and right state could leave the zero-energy level at the same time ? Actually, it is not possible because your eigenstates will display some discontinuity. For instance, your left-edge mode will suddenly turn to a (left+right)-edge mode, and the mass on the right has appeared suddenly. In other words, the two edges cannot talk to each other because of the insulating bulk. Note that the total number of edge states is exactly equal to the winding difference $W_+ - W_-$ between the two bands in the bulk.

4.4 Be careful on your deformations

However, if one adds a perturbation that does not respect the symmetries, then everything is possible ! For instance consider $H_1(\lambda) = E(\lambda)\sigma_z$. Then $E(k) = \pm|E(\lambda) + v + we^{ika}|$. The gap does not close anymore for $v = w$, one can perform a perturbation that removes the winding without going through the origin.

5 Take-home message

- Topology is used to compute things that resists against continuous deformations
- Not all insulators are topologically equivalent: one must go through a conducting phase to go from one to the other
- These insulators are characterized by topological invariants
- You can break these states either by closing the gap or breaking the symmetry
- Depending on the symmetries of the problem, there exist a classification of topological insulators (see https://arxiv.org/pdf/0905.2029). How do we do that ? Well, you have to wonder how many "elementary" Hamiltonian are needed to obtain all possible Hamiltonian through continuous deformations. There is only a finite number of them, resulting in full classification of topological insulators.