

Physics with Coffee and Doughnuts*

Understanding the Physics Behind Topological Insulators Through Su-Schrieffer-Heeger Model

Navketan Batra and Goutam Sheet

Topological insulators are a new class of materials that have attracted significant attention in contemporary condensed matter physics. They are different from regular insulators, and they display novel quantum properties that involve the idea of ‘topology’, an area of mathematics. Some of the fundamental concepts behind topological insulators, particularly in low-dimensional condensed matter systems such as poly-acetylene chains, can be understood using a simple one-dimensional toy model popularly known as the Su-Schrieffer-Heeger (SSH) model. This model can also be used as an introduction to the topological insulators of higher dimensions. Here, we give a concise description of the SSH model along with a brief review of the background physics and attempt to understand the ideas of topological invariants, edge states, and bulk-boundary correspondence using the model.

1. Introduction

Topology is a branch of mathematics that deals with different classes of geometries of objects. If you are allowed to bend and stretch an object but not tear it apart or join two regions together, then all the geometries you will be able to make from the given object will be topologically equivalent. A coffee mug is topologically equivalent to a doughnut, see *Figure 1*. Similarly, a football is topologically equivalent to the page of the book you are probably reading this article in. Some of you might have encountered



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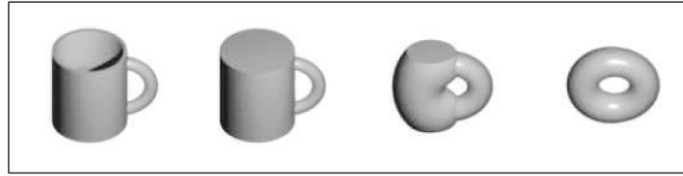


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Figure 1. Topological equivalence of a coffee mug and a doughnut: A coffee mug can be *smoothly* deformed into a doughnut without tearing it apart or joining two regions together.



the Gauss-Bonnet's theorem in mathematics,

$$\frac{1}{4\pi} \int_M \kappa dA = 1 - g. \quad (1)$$

Keywords

Topological insulators, tight-binding model, band insulators.

Here κ is the Gauss curvature of the object M , we are considering. What this statement means is that if we integrate an object's Gaussian curvature over the object's surface, divide it by 4π , the result will be $(1 - g)$ where g is an *integer* representing the number of holes in the object (or a manifold M). Making small deformations on the surface of the manifold will, of course, change the curvature of the object *locally*, however, when we integrate the 'changed' curvature onto the deformed surface, the right side of the equation remains the same! Therefore, the number g is known as a 'topological invariant', meaning it does not change with small deformations on the surface of the manifold.

The exciting thing about topological invariants describing physical properties is that if the *nature* of the physical quantities is tied to the topological invariant, changing the Hamiltonian slightly will not affect those quantities, and hence they will become robust against such changes.

It has recently been discovered that in condensed matter physics, it is possible to realize certain phases of matter that display unique physical properties that can be described by the existence of *physical* quantities analogous to the topological invariant g . One class of such materials is topological insulators. In this article, we shall discuss this connection between the ideas of topology and topological invariants with condensed matter physics in the light of a beautiful toy model called the SSH model [1, 2]. However, before introducing the SSH model, we give a brief review of the background physics and discuss band insulators in section 2. In section 3, we understand how metals and insulators are modeled using quantum mechanics by writing a *tight-binding Hamiltonian*. Then, in section 4, we digress a little to explore Peierls instability, a special case of *charge density waves*. We then introduce the concept of the Berry phase in section 5, which forms the basis



of topological band theory. Finally, in section 6, we present the SSH model and do a detailed analysis before giving concluding remarks in section 7.

2. Band Insulators

To understand the ideas of topological insulators, we first need to understand the band theory. Using a simple analogy with the particle-in-a-potential-well problem, let us explore how energy bands are formed in a solid.

Consider a particle in a finite potential well from quantum mechanics - with certain approximations, it can be seen as a model atom (hydrogen-like), where the potential well is created by the nucleus, and the electron is a particle under that potential [3]. The one-dimensional version of this problem is solved in a standard undergraduate level quantum mechanics course [4]. The energy of such a system is discrete and can be computed to be $E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$, where L is the length of the box, and n is a level index (a non-zero +ve integer). Recall that $n = 1$ corresponds to the ground state energy. Now, if we bring a second such finite well system close to the first, the full system can be treated as a model molecule with two electrons under the influence of the potential due to two nuclei. As per Pauli's exclusion principle, these two electrons cannot be accommodated in a single ground state unless their spins are anti-aligned. In fact, for such a molecule, the states corresponding to isolated particles overlap and we obtain two new energy eigenstates one having *lower* energy than the ground state energy of a single atom (the so-called bonding state for which the wavefunction is symmetric) and the other one having higher energy (the anti-bonding state for which the wavefunction is antisymmetric). In a hydrogen-like molecule, therefore, it makes sense for both the electrons to anti-align and occupy the bonding energy (symmetric) state to lower the energy of the whole system. Consequently, we see that bringing two atoms close to each other can, in principle, reduce the energy of the entire system by the formation of bonding and anti-bonding states. Note that here

Robert Mulliken and Linus Pauling won Nobel Prizes in chemistry for their work on understanding how different elements make bonds with each other.



we have ignored the Coulomb interaction between two charged electrons.

This is the idea behind the formation of *conduction band* and *Valence band*. When the atoms are brought together to form a solid, the discrete energy levels alter into bands.

Now, instead of just two atoms, if we take many such atoms to form a solid, there are several bonding and anti-bonding states. In the case of a real macroscopic solid where the number of atoms is of the order of 10^{23} , these states have to be so closely spaced that the discreteness of their energies can be ignored and instead we will have bands where such states exist. In a more complex solid, where each atom contributes several electrons, many distinct energy bands can form. Two such energy bands can also be separated from each other, giving rise to a range of energies where no electronic states are present. Such an energy range is called a bandgap in solid-state physics and electronics [5, 6]. If the maximum energy up to which all quantum states are filled at zero temperature $T = 0$, which is known as the Fermi energy of a solid, falls within such a bandgap, the solid behaves like an insulator. Such insulators are often termed as the “band insulators”. If the Fermi energy is within a band, the solid behaves like a metal. Notice, this theory, known as the band theory, neglects electronic interactions due to which it may fail for specific materials.

3. Tight Binding Model

The minus sign in defining the overlap inner product ($-t$) is just a convention. It has the dimensions of energy.

Imagine again building up a one-dimensional crystal lattice by arranging hydrogen-like atoms together along a straight line in an ordered fashion. As we discussed before, when atoms are far apart, they can be treated separately as there is no overlap between their respective eigenstates. Once they come close enough, their wave functions will no longer be orthogonal, they mix up and as a consequence, form bonding and anti-bonding states. Now with many atoms together, forming a crystalline lattice, the overlaps help the electron to delocalise on the lattice by tunneling from one atom to the other. This tunneling potential is given by the overlap (inner product integral), denoted by $-t$, between the two states at different sites [3].



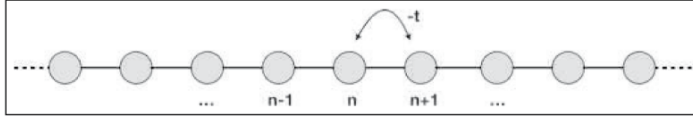


Figure 2. Pictorial representation of a one dimensional tight-binding Hamiltonian.

One can now write down a Hamiltonian describing a particle's motion on a lattice structure—say, a one-dimensional ring with N such lattice points:

$$H = - \sum_{ij} t_{ij} |i\rangle \langle j|. \quad (2)$$

Here, i, j represent the lattice site and $-t_{ij}$ is the overlap integral between the i th and j th site. The sum over i, j runs independently over *all* i, j pairs. Note since going to-and-fro between two lattice points is equivalent, we impose $t_{ij} = t_{ji}$ (this condition makes the Hamiltonian Hermitian) and $t_{ii} = 0$ for all site i . From quantum mechanics, we recall that the translation operator translates site i to $i + 1$ which we represent here as $T = \sum_i |i + 1\rangle \langle i|$. Now if we assume that the overlap integral only depends on the distance between the two sites $t_{i,i+n} \equiv t_n$ then we see that the tight-binding Hamiltonian defined above is just a function of the translation operator and can thus be written as $H = - \sum_n t_n T^n$. Since now $[H, T] = 0$, we can diagonalise the Hamiltonian in the eigenbasis of the translation operator which we know are the plane wave states defined as:

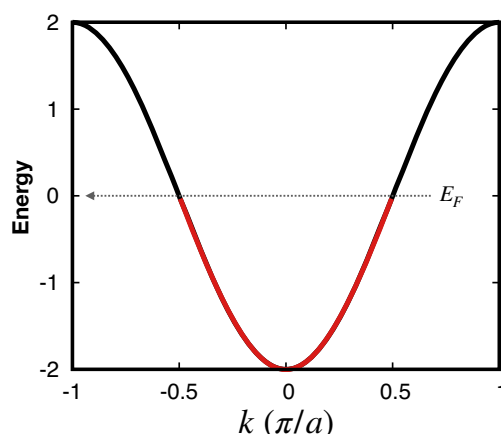
This is not a coincidence: Imposing $t_{i,i+n} \equiv t_n$ is equivalent of assuming translational symmetry in our system since the hopping potential does not depend on the site location. This is exactly why the Hamiltonian becomes a function of the translation operator which allowed us to define a new plane-wave basis.

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ikj} |j\rangle. \quad (3)$$

Action of T^m on $|k\rangle$ gives $T^m |k\rangle = e^{-ikma} |k\rangle$. Therefore, the eigenvalue spectrum for our tight binding Hamiltonian is given by:



Figure 3. Energy dispersion obtained from a 1D nearest neighbour tight binding Hamiltonian. The red portion represent the filled states.



$$\begin{aligned}
 H|k\rangle &= \epsilon(k)|k\rangle. \\
 \epsilon(k) &= -\sum_n t_n e^{-ikna}.
 \end{aligned}
 \quad (4)$$

For a case when we only allow the nearest-neighbor hopping i.e., $t_1 = t \neq 0$ and all others are zero. Then, we obtain $\epsilon(k) = -2t \cos ka$.

By allowing hopping between the orbitals, some of the eigenstates in the band have decreased in energy with respect to the Fermi energy—this is what we discussed in section 2.

Note that if the band were not completely filled, like in our case, the *total* energy of all the electrons would decrease which makes it favourable for the atoms to move together. This is precisely the *binding force* of a metallic bond and explains why solids exist at all in the first place!

This is the dispersion that is followed by a single electron hopping on a lattice made from hydrogen-like atoms. It turns out that this method when applied to the many-electron problem by neglecting the $e^- - e^-$ interaction is not a bad approximation to describe many physical properties like the metallic character. All the allowed k falling in the line from $-\pi/a$ to $+\pi/a$ constitute a Brillouin zone. The edges at $k = \pm\pi/a$ are called the Brillouin zone edges. These have interesting features when weak interactions are introduced. We will come back to this in the next section.

If we stick to non-interacting particle description and assume every atom has a single loosely bound electron that hops around, then the band formed by the dispersion relation is half-filled (red region in Figure 3). This is because every atomic state contributes one electron, whereas, its maximum occupancy is restricted to two (due to Pauli's principle). Notice that in condensed matter, energies are always measured from the Fermi energy. Hence, it

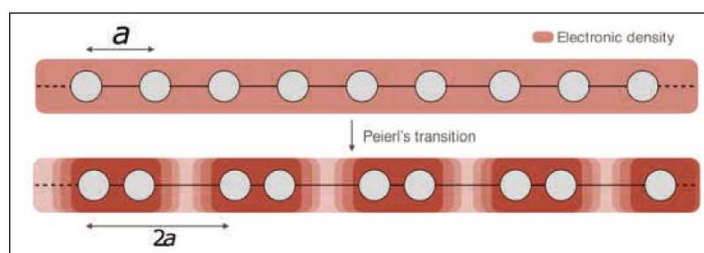


Figure 4. A 1D lattice, lattice constant a , undergoes a Peierls transition and distorts the lattice such the the lattice constant becomes $2a$. The brown region shows the electronic density.

is convenient to set Fermi energy to zero. Since there are states available at arbitrary small energies above Fermi energy, this system thus describes a metal otherwise insulator, as we will see in the next section.

4. Peierls Instability

In the previous problem, we studied a one-dimensional non-interacting tight-binding model that described a metal. When we drew the E vs. k relation in *Figure 3*, we assumed the existence of background lattice, which gives rise to a periodic potential that the electrons can sense. Now, consider several free-electron dispersions (which is just parabolic $E = \frac{\hbar^2 k^2}{2m}$) separated from each other.

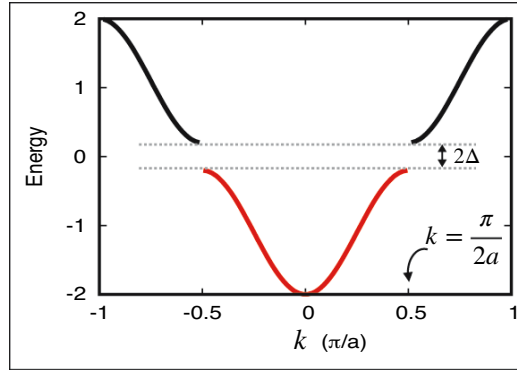
The point where two dispersions cross each other is a point of degeneracy, which will be lifted once weak periodic potential due to the lattice is included. For a similar reason, energy gaps arise in their dispersion relation at the Brillouin zone boundary when a weak periodic potential is considered. If we put just one electron per lattice site, then the states from $-\pi/2a$ to $+\pi/2a$ will be occupied without a bandgap between the occupied and the unoccupied states. Hence, the system will still behave like a metal. However, in the 1930s, Rudolf Peierls proved that a one-dimensional equally spaced chain with one electron per lattice site is unstable, and such a system is prone to distortion. This can be qualitatively understood in the following way.

In *Figure 4*, the brown region shows the electronic density due to the electrons. In the normal case, where the lattice spacing is a , the electronic density is uniform. But if we consider a case

Although the band theory correctly explained the existence of metals and insulators based on how the bands are filled, it was not enough. The discovery of the quantum Hall effect in the 1980s showed that the simple division into band insulators and metals is not the end of the story. Some systems behave as band insulators in the bulk, whereas, at the boundaries, they are metallic.



Figure 5. Due to the distortion in the lattice, the lattice constant is now $2a$ instead of a , therefore, the Brillouin zone boundary is at $k = \pm \frac{\pi}{2a}$.



where every atom distorts itself such as the resulting lattice has two sublattice sites in a unit cell, and the inter-unit cell distance is $2a$. The electronic density will become periodically modulated. This is known as a ‘charge density wave’ [7]. The final energy of the distorted lattice atoms alone will, of course, be higher than the original undistorted case. Estimating this energy per unit length in the elastic approximation gives:

$$\Delta E_{\text{lattice}} = \frac{1}{4} K \delta^2, \quad (5)$$

Rudolf Peierls was working on developing a theory for high- T_c superconductors when he found this result. His idea was that the ‘lattice distortions’ which are responsible for the formation of Cooper pairs in the BCS theory of superconductivity could be replaced by ‘charge distortions’, or the charge density waves, to obtain a similar mechanism of Cooper pairing with higher critical temperature.

which is quadratic in the distortion δ . K is the elastic constant determined by the material. However, if we calculate the electronic energy per unit length of the new charge configuration due to distortion, in the low distortion limit, we get,

$$\Delta E_{\text{electronic}} \approx \frac{A^2 \delta^2}{\pi} \ln |\delta|. \quad (6)$$

the total energy per unit length, $\Delta E_{\text{lattice}} + \Delta E_{\text{electronic}}$ is extremized as,

$$\frac{d}{d\delta} [\Delta E_{\text{lattice}} + \Delta E_{\text{electronic}}] = \frac{1}{2} K \delta + \frac{2A^2}{\pi} \delta \ln |\delta| + \frac{A^2}{\pi} \delta = 0. \quad (7)$$

The solution $\delta = 0$ corresponds to a maxima which can be checked explicitly by calculating the second derivative. The minima cor-

responds to

$$\delta_{\min} = \pm e^{-\frac{1}{2}} e^{-\frac{K}{4\pi}}. \quad (8)$$

It can also be checked, by plugging in δ_{\min} into ΔE_{total} , that total change in energy is negative! This means that the system gains energy by distorting itself by δ_{\min} . Note that it was only possible due to electronic energy that compensated the higher-than-original energy contributed by the lattice due to distortion. This is called ‘Peierls instability’.

As illustrated in *Figure 5*, now it is easy to notice that for the distorted lattice, the zone-edges are located at $k = \pm\pi/2a$ instead of at $k = \pm\pi/a$, since now the periodicity of the Brillouin zone is doubled. Doubling the period hence introduces new band gaps in the Brillouin zone, therefore, the system becomes lower in energy corresponding to the states in the vicinity of the new gaps. This transition fills the band completely, and a bandgap (shown as 2Δ in *Figure 5*) opens up separating the empty states from the populated ones at the new edges of the Brillouin zone. This makes the system a band insulator.

5. Berry Phase

Let us digress a little and look at an exciting concept in quantum mechanics that will become necessary at a later stage—the concept of Berry phase. Consider a general Hamiltonian $H(\mathbf{R})$, which is a function of several parameters represented as a vector $\mathbf{R} = (R_1, R_2, \dots)$. At any instant, for a fixed \mathbf{R} , the solutions can be obtained using the time-independent Schrödinger equation as,

$$H(\mathbf{R}) |n(\mathbf{R})\rangle = E_n(\mathbf{R}) |n(\mathbf{R})\rangle. \quad (9)$$

Now as \mathbf{R} changes in the parameter space (starting from $\mathbf{R}(t = 0)$) along some path C , we are interested in knowing how the state changes when the system is initially prepared in the state $|n(\mathbf{R}(t = 0))\rangle$. There is a very useful theorem known as the *adiabatic theorem* that states—for a *slowly* varying Hamiltonian, a

In contrast, rapidly changing conditions prevent the system from acclimatizing its configuration, hence the wavefunction remains unchanged. Typically, there is no eigenstate of the final Hamiltonian with the same form as the initial state. Hence the system ends up in a linear combination state. This is known as quantum quenching.



system initially in the eigenstate will always remain in its *instantaneous* eigenstate at any later time. From this theorem, we have got half the answer to our question. We now know starting from $|n(\mathbf{R}(0))\rangle$, the system will evolve to $|n(\mathbf{R}(t))\rangle$ which is the instantaneous eigenstate of $H(\mathbf{R}(t))$ with slowly varying \mathbf{R} . But what about the phase? We can in general write the evolved state at t as $|\psi(t)\rangle = e^{-i\theta(t)} |n(\mathbf{R}(t))\rangle$. This state will follow the Schrödinger equation,

$$H(\mathbf{R}(t)) |\psi(t)\rangle = i\hbar \frac{d}{dt} |\psi(t)\rangle, \quad (10)$$

which translates into the differential equation,

$$E_n(\mathbf{R}(t)) |n(\mathbf{R}(t))\rangle = \hbar \left(\frac{d}{dt} \theta(t) \right) |n(\mathbf{R}(t))\rangle + i\hbar \frac{d}{dt} |n(\mathbf{R}(t))\rangle. \quad (11)$$

Taking the scalar product with $\langle n(\mathbf{R}(t))|$ and assuming the state is normalised, we get,

$$E_n(\mathbf{R}(t)) - i\hbar \langle n(\mathbf{R}(t))| \frac{d}{dt} |n(\mathbf{R}(t))\rangle = \hbar \left(\frac{d}{dt} \theta(t) \right). \\ \theta(t) = \frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(t')) dt' - i \int_0^t \langle n(\mathbf{R}(t'))| \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle dt'. \quad (12)$$

The first term of the phase is just the conventional dynamical phase that arises due to the time evolution of the Hamiltonian.

The negative of the second term is what is known as the Berry phase γ_n ,

$$\gamma_n = i \int_0^t \langle n(\mathbf{R}(t'))| \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle dt'. \quad (13)$$

This term arises because the states at t and $t+dt$ are not 'identical', and a phase is picked up that depends on the trajectory in the parameter space. From the previous expression,

$$\begin{aligned} \gamma_n &= i \int_0^t \langle n(\mathbf{R}(t'))| \nabla_{\mathbf{R}} |n(\mathbf{R}(t'))\rangle \frac{d\mathbf{R}}{dt'} dt' \\ &= i \int_{\mathbf{R}_0}^{\mathbf{R}_t} \langle n(\mathbf{R})| \nabla_{\mathbf{R}} |n(\mathbf{R})\rangle d\mathbf{R} \\ &= \int_{\mathbf{R}_0}^{\mathbf{R}_t} \mathbf{A}_n(\mathbf{R}) d\mathbf{R}. \end{aligned} \quad (14)$$

A similar-in-spirit angle shows up in the problem of *parallel transport* along curved surfaces. This angle measures the amount of *intrinsic curvature* when one is embedded in the surface. For instance, to measure the curvature of the Earth, one need not go to space, but by making large enough (closed-loop) round trips on Earth, one can deduce the curvature of the Earth.

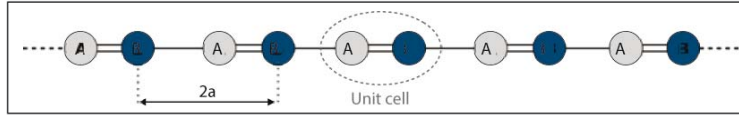


Figure 6. Visual representation of the SSH Model.

where we define Berry potential as,

$$\mathbf{A}_n(\mathbf{R}) = i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle. \quad (15)$$

From quantum mechanics, we know that by multiplying the states by an overall *global* phase factor,

$$|n(\mathbf{R})\rangle \rightarrow |\tilde{n}(\mathbf{R})\rangle = e^{i\chi(\mathbf{R})} |n(\mathbf{R})\rangle. \quad (16)$$

the dynamics of the system does not change—this is known as *gauge invariance*. However, we see that the Berry Potential $\mathbf{A}_n(\mathbf{R})$, is not a gauge invariant quantity. Under gauge transformation it changes as

$$\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) - \frac{\partial}{\partial \mathbf{R}} \chi(\mathbf{R}). \quad (17)$$

Consequently, Berry phase will change by, $-\int_C \frac{\partial}{\partial \mathbf{R}} \chi(\mathbf{R}) d\mathbf{R} = \chi(\mathbf{R}_0) - \chi(\mathbf{R}_1)$. Therefore, we can have Berry phase to be gauge invariant as long as the path C is closed. This quantity shows up in many areas of physics, one classic example is the Aharonov-Bohm effect [8].

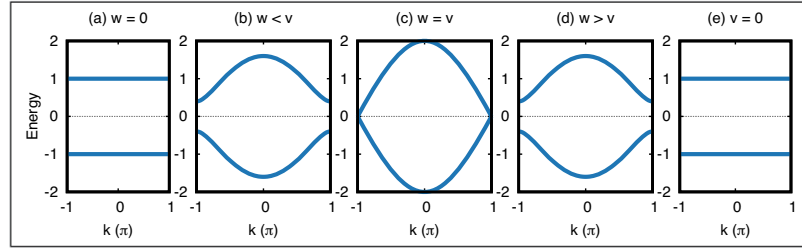
6. The SSH model

We now move onto a slightly more complicated version of the previous Hamiltonian, where instead of a single site unit cell, we have a two-site unit cell as shown in *Figure 6*, as if the lattice has been distorted due to Peierls instability. The Su-Schrieffer-Heeger (SSH) model is a tight-binding model that describes a single spin-less electron on a two-site unit cell 1D lattice. The two sites in a unit cell are labeled as A and B . From here, we will set the lattice constant, $2a = 1$.

We will work with one particle per unit cell that corresponds to a half-filled lattice since we are considering spin-less particles.

When we say spin-less particles, we mean that the spin degree of freedom does not contribute to the dynamics, therefore, one may think of it as a spin-polarized system, say due to constant external magnetic field.

Figure 7. Dispersion relation obtained from bulk Hamiltonian plotted for different parameter cases



Thus the only degree of freedom the electrons have is that they can hop around from one site to other. Let us call the hopping potentials as v (for hopping within the unit cell) and w (for hopping connecting neighboring unit cells), and write the tight-binding Hamiltonian as:

$$H = v \sum_{n=1}^N (|n, B\rangle \langle n, A| + \text{H.c.}) + w \sum_{n=1}^N (|n+1, A\rangle \langle n, B| + \text{H.c.}) \quad (18)$$

In reality, a material will always be finite, and hence it will break the translational symmetry.

However, since the number of particles is so large, the physics of the bulk of the material can be closely approximated to a translationally invariant system since it is much easier to solve.

Here ‘H.c.’ denotes the Hermitian conjugate of the term before it. The basis we have used to define the Hamiltonian can also be written as $|n, A(\text{or } B)\rangle = |n\rangle \otimes |A(\text{or } B)\rangle$. This representation tells us that the full Hilbert space is made of two parts— $\mathcal{H}_{\text{external}} \otimes \mathcal{H}_{\text{internal}}$. The internal Hilbert space is due to the two sub-lattice sites (A and B) in the unit cell, and the external is due to the repetition of the unit cells N times.

6.1 The Band Hamiltonian

The two-site unit cell adds another band to the band structure we explored previously. To see this, we need to solve for its dispersion relation by only focusing on the bulk part of the chain, that is to say, assuming the chain forms a loop (periodic boundary). Because the system is translationally invariant, it allows us to perform Fourier transform in the external Hilbert space similar to what we did earlier.

$$|n\rangle \otimes |A(\text{or } B)\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ikn} |k\rangle \otimes |A(\text{or } B)\rangle. \quad (19)$$

Plugging this back into the Hamiltonian (with periodic boundaries), we get:

$$H = \sum_k (v + e^{-ik}w) |k, B\rangle \langle k, A| + (v + e^{ik}w) |k, A\rangle \langle k, B|. \quad (20)$$

The external and internal parts can be separated and this can further be reduced to:

$$H = |k\rangle \langle k| \otimes [(v + e^{ik}w) |A\rangle \langle B| + (v + e^{-ik}w) |B\rangle \langle A|]. \quad (21)$$

In a compact form, $H = \sum_k |k\rangle H(k) \langle k|$.

$$H(k) = \begin{pmatrix} 0 & v + e^{ik}w \\ v + e^{-ik}w & 0 \end{pmatrix}. \quad (22)$$

$H(k)$ is the band Hamiltonian that acts on the internal Hilbert space [9]. With the help of Fourier transform, we have block diagonalized the full Hamiltonian into N such 2×2 band Hamiltonians for each k . Now our task is simply to diagonalize this two-dimensional matrix that will give us the bulk dispersion relation in terms of the energy eigenvalues:

$$E(k) = \pm \sqrt{v^2 + w^2 + 2vw \cos(k)}. \quad (23)$$

Likewise, the eigenstates (eigenvectors) look like,

$$|\pm(k)\rangle = \begin{pmatrix} \pm e^{-i\phi(k)} \\ 1 \end{pmatrix},$$

$$\phi(k) = \tan^{-1} \left(\frac{w \sin k}{v + w \cos k} \right). \quad (24)$$

We would not have been able to simplify the problem without assuming translational invariance. However, soon you will see that due to translational invariance we are missing out an important piece of information—the physics of the edge!

Note that our Hamiltonian has two parameters: v and w . It is clear that different choices of these parameters will lead to different dispersion relations. Let us try to see what these band structures look like and conclude from the dispersion. Note that we have considered the Fermi energy to be the zero energy level—this is the origin in our energy scale relative to which all other energies are measured here.

This is the *only* information that can be extracted from the typical band theory of solids.

The plots in *Figure 7* suggest that when there is staggering, $v \neq w$, in the Hamiltonian, the dispersion is gapped. Hence a staggered case would describe an insulator. Only in the case of $v = w$ the gap closes, and there are states available at arbitrary low energies above the Fermi level, therefore, $v = w$ case describes a metal.

6.2 Beyond Energy-band Description

From the bulk Hamiltonian, it seems like the problem is symmetric about the $v = w$ case. By symmetric we mean that $v > w$ case is exactly the same as $w > v$ case. But this is not quite right. The information obtained from the ‘eigenvalues’ is not complete! We need to also look at the eigenvectors to get complete information about these cases. Interestingly, the topological aspect of this problem is hidden in the eigenvectors.

This is an incredibly useful reminder to us that classification of phases should be done not only by looking at their energy spectrum but also via eigenstate spectrum!

Since the band Hamiltonian is a two-dimensional Hermitian matrix, it can be written in a more insightful notation as,

$$H(k) = \vec{h}(k) \cdot \vec{\sigma}, \quad (25)$$

Notice that we are able to claim that the trajectories for the two cases are *qualitatively* different because both loops lie in a two-dimensional $h_x - h_y$ plane. Again, the co-planar condition is due to the fact that the on-site potential is set to zero.

using Pauli’s matrices, $\{\sigma_i\}$, as the basis for a two dimensional Hermitian matrix [10]. By comparing terms we get,

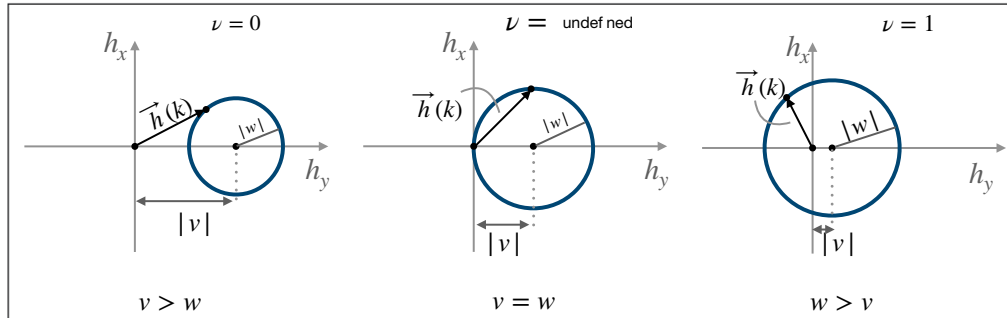
$$h_x(k) = v + w \cos k, \quad (26)$$

$$h_y(k) = w \sin k, \quad (27)$$

$$h_z(k) = 0. \quad (28)$$

As we saw earlier, the eigenstates are parametrised by $\phi = \tan^{-1}(\frac{w \sin k}{v + w \cos k}) = \tan^{-1} \frac{h_y(k)}{h_x(k)}$. Therefore, in the $h_x - h_y$ space, the direction of the





vector $\vec{h}(k)$ denotes an eigenstate, and the magnitude of the vector will give its eigenvalue. A plot of the trajectory of $\vec{h}(k)$ over the first Brillouin zone $\{-\pi \rightarrow \pi\}$ gives the full set of eigenstates. If we plot the trajectories for the two seemingly equivalent cases: $v < w$ and $v > w$ we observe, see Figure 8, that even though their dispersions are identical, these trajectories on the $h_x - h_y$ plane are very different!

The vector $\vec{h}(k)$ that denotes the eigenstates will necessarily form a closed-loop due to the periodicity of the Brillouin zone. For one of the insulating cases ($v < w$), the vector $\vec{h}(k)$ winds about the origin, and for the other case ($v > w$), it does not. Notice that the origin is the point where $\vec{h}(k) = 0$, that corresponds to the gap-less condition. Therefore, a loop plotted for the $v = w$ case would pass through the origin indicating a metallic state. We can call this as a *winding number* ν that tells whether the trajectory of $\vec{h}(k)$ winds about the origin or not. The winding number distinguishes the two seemingly equivalent cases.

Notice that the bulk Hamiltonian we are looking at, $H(k)$, is also a function of some parameter, in this case, k , which is known as the crystal momentum. Therefore, Berry potential for an energy band can be defined. The Brillouin zone is periodic and has a topology of a ring. If we consider the Brillouin zone as a parameter space as we did in section 5., and since it is periodic, integrating the Berry potential for the filled band over the Brillouin zone will correspond to tracing a closed loop in this parameter space and therefore will result in a gauge-invariant berry phase. Let us now

Figure 8. Trajectories of $\vec{h}(k)$ over the Brillouin zone in the $h_x - h_y$ space for different parameter values.

One can also think of the Berry phase in solids as a quantity that calculates the *curvature* of the abstract state-space. A space of collection of all the wavefunctions of the Hamiltonian at each k point.

calculate the Berry phase [9],

$$A_-(k) = i \langle -(k) | \frac{d}{dk} | -(k) \rangle = -\frac{1}{2} \frac{d\phi}{dk}. \quad (29)$$

Now if we integrate this quantity in the Brillouin zone, and put appropriate factors, we get,

$$\frac{-1}{\pi} \oint A_-(k) dk = \begin{cases} 1 & \text{if } \nu < w \\ 0 & \text{if } \nu > w \\ \text{undefined} & \text{if } \nu = w \end{cases} \quad (30)$$

In the case of Quantum Hall effect, using what is known as the *kubo formula*, it was explicitly shown that the Berry phase is responsible for the characterization of such seemingly identical cases.

Looking at this result immediately reminds us of the winding number ν . In fact, eq. (30) is a proper way to calculate the winding number. Notice that it is undefined for the $\nu = w$ case since the notion of a filled band itself is undefined. Notice that the form of eq. (30) is similar to eq. (1)—let us try to see its analogy with the eq. (1). The role of Gaussian curvature is played by Berry potential, and the role of the manifold we integrate it over is played by the Brillouin zone. Notice that the topological invariant g , which does not change with small deformations on the manifold, is analogous to the winding number. Small changes in the Berry potential (or in the Hamiltonian via the parameters ν or w) will indeed change the Berry potential locally, however, when it is integrated over the entire Brillouin zone, the winding number remains invariant! In other words, small changes to $h(k)$ will change the trajectory of the vector $\vec{h}(k)$, and the trajectory will no longer remain a perfect circle, but the winding number will still be defined and remains unchanged.

Due to this incredible similarity to the theory of topology, the study of such non-trivial phases, characterized by topological invariants, is known as *topological band theory*.

We have seen that the two seemingly equivalent insulating cases are ‘topologically’ different, which is concluded by exploiting the information of wavefunctions in these two cases. But how do these different behaviors of the eigenvectors make the two insulating cases different physically? In other words, we are looking for a physical consequence of the winding number in the seemingly similar insulating cases. But before answering that in its



full glory, let us note one physical consequence that can be drawn from this distinct behavior. If we were to transform the Hamiltonian smoothly, in other words, change any of the parameters v or w , then since $h_z = 0$, the only possible way to get from the insulating phase described by the case $v < w$ to the insulating phase described by the case $v > w$ (or the other way round), is via crossing the origin! This means that somewhere in the middle, we have to get to the solution of eigenstates corresponding to a trajectory, $h(\vec{k})$, in the $h_x - h_y$ space, that passes through the origin in that space. Therefore, a smooth transition from one insulating phase to another is impossible without closing the energy gap (or crossing the metallic phase) at least once. This is the hallmark of a ‘topological phase transition’ [11]. An analogy can be drawn here with a 3D topological insulator (TI) like Bi_2Se_3 . In a 3D TI, the bulk is an insulator topologically distinct (has different winding number) from the vacuum (outside of the TI). Note that vacuum can be thought of like a band insulator with the particle (like an electron) and the antiparticle (like a hole) states separated by a “band gap”. In order to smoothly transit from the TI phase to the band insulator phase, one must cross a point (the interface between the two) where the band gap is zero. That gives rise to conducting surface states at the surface of 3D TIs. We will now explore these conducting states, known as *edge states* in 1D, that appear in the SSH model.

The 2016 Nobel Prize in Physics was awarded to David J. Thouless, Duncan Haldane, and J. Michael Kosterlitz ‘for theoretical discoveries of topological phase transitions and topological phases of matter’.

6.3 A Finite SSH Chain

Till now, we looked at the solutions of a 1D SSH chain with periodic boundaries (i.e., a ring). To answer the question posed in the last section on what physical consequence does the winding number has, let us look at the version of the SSH chain with open boundaries. The problem is not trivial— since there is no translational invariance, we cannot make use of the Fourier transformation to diagonalize the Hamiltonian. We, therefore, feed the Hamiltonian into our computers and explicitly solve the Hamiltonian for its eigenvalues and eigenfunctions.

But before this, let us first try to look at the extreme cases and



Figure 9. Open SSH chain in the limit $w = 0$ and $v \neq 0$

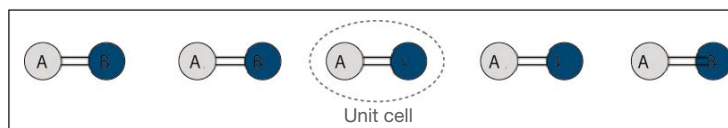
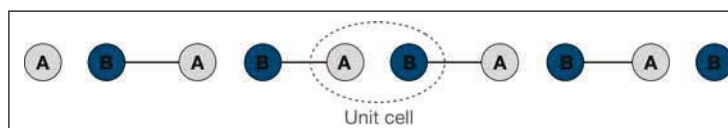


Figure 10. Open SSH chain in the limit $v = 0$ and $w \neq 0$.



guess what could be the solutions. There are two extreme cases— $w = 0, v \neq 0$ and $v = 0, w \neq 0$. These are called the dimerized limits, as this would correspond to breaking the chain into dimers. The first case, $w = 0$, for a chain with $N = 10$, looks like what is shown in *Figure 9*. This seems like a repetitive problem of a dimer, which is, of course, easy to solve. We know the solutions should be the superposition of the A site and B site for each dimer. We can even guess that this should correspond to an insulating state as the chain is now broken, and no particle can hop from one end of the chain to another.

Notice that for each value of v and w , we have a different Hamiltonian. However, from the plots in *Figure 11*, it is clear that all the states vary in energy except for the one with zero (or close to zero) energy! This is an example of the robustness of the physical property we discussed earlier.

Let us now look at the other extreme case of $v = 0$. Similar to the previous case, we get a few dimers, but since the chain has open boundaries, we now have two single sites at the end of the chain, see *Figure 10*. If these two sites, one at each end, carry an electron, the energy should be zero because, in the SSH model, there is no energy contribution for an electron to be held fixed at one site. So we should expect two zero energy states in the system localized at the edges of the chain. Again going by the same argument as in the previous case, we expect this case to describe an insulator as well.

Let us now solve the Hamiltonian for an open SSH chain and try to see the solutions for different parameter values. The plots in *Figure 11* show the energy spectrum of the eigenstates as we vary the parameter (a) v and (b) w . For the dimerized case, our expected solutions match perfectly well, and we indeed see zero



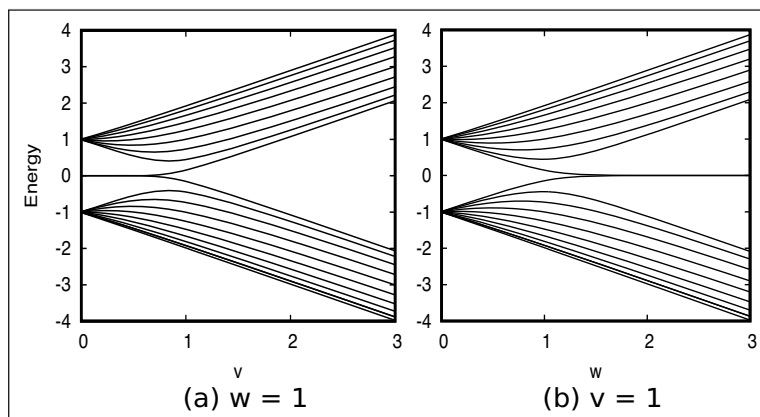


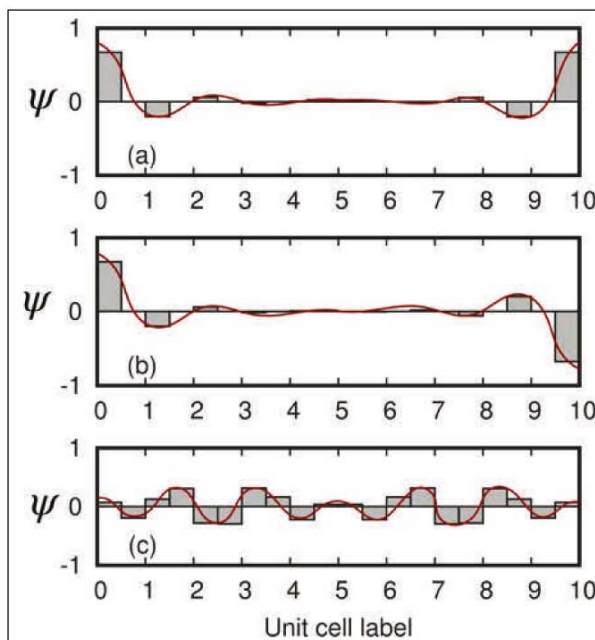
Figure 11. Eigenvalue spectrum as a function of model parameter ν (case (a)) when w is held fixed at $w = 1$ and w (case(b)) when ν is held fixed at $\nu = 1$.

energy states in the case where $w = 0$ and no zero energy states in the other $\nu = 0$ case. One interesting feature we see here is that the zero energy states not only exist in the extreme limit but even for non-zero ν , however, the zero energy states are not quite zero energy states but are very close to zero. Here again, our Fermi energy lies at zero, so we see that the spectrum is gapped in the case $w = 0$. However, due to the presence of zero energy states in the $\nu = 0$ case, we cannot be entirely sure about its insulating behavior. But intuitively, a dimerized chain should not be conducting, and also the zero-energy states should be localized at the boundary. Therefore, let us look at the corresponding wavefunctions of these energy eigenstates [12].

Plots (a) and (b) in Figure 12 shows the (close to) zero energy states for the case when $\nu = 0.3$ and $w = 1.0$ and for reference plot (c), Figure 12 shows an arbitrary non-zero energy state for the same case. We see that the non-zero energy state is delocalized throughout the chain. On the contrary, the zero energy states are exponentially localized at the edges of the chain which we expected from the dimerized limit. These states are called the ‘edge states’ because they live on the edges of the chain. Also, notice that these edge states only remain zero-energy edge states as long as $\nu < w$. Once $\nu > w$, there are no zero energy states, and all states are delocalized throughout the lattice. The existence of these edge states in the $\nu < w$ case makes this case different from

Since we are working with $N = 10$ site lattice, the exponential localization of the edge states is not crystal clear. However, if one increases the lattice sites, which will require greater computational power, the wave functions of the zero energy states become more and more exponentially localized. Since in any realistic material, the number of sites is numerous, one can be sure of their existence only at the edges.

Figure 12. Wavefunction amplitude at each site corresponding to (a) and (b) zero energy edge states and (c) non-zero energy eigenstate.



the case when $v > w$. Otherwise, in the bulk, for both these cases, the system behaves like an insulator.

We have found a physical consequence of the distinct bulk ‘topological’ properties we saw earlier—the existence of ‘edge states’. The case when the winding number is 1 is known as a topologically non-trivial case. Whereas the other is known as a trivial case. These two cases are related via a topological phase transition that corresponds to closing the bandgap that gives rise to the conducting edge states. This is no coincidence! This is a simple example of the ‘bulk-boundary correspondence’: by looking at the bulk and calculating its topological invariants, in our case, the winding number v , we can predict the existence of edge states at the boundaries or the other way around.

7. Conclusions

We started by solving the SSH model in the periodic boundary case, which resulted in a bulk dispersion relation followed by the



electrons. From there, we concluded that there are two different solutions: The metallic phase, when $v = w$ and the insulating phase, when $v \neq w$, which is possible when $w > v$ or $w < v$. From the bulk dispersion, however, these two insulating phases seem to be equivalent. Then we argued that the information from the dispersion relation is incomplete! We then looked at an ‘abstract’ quantity called the winding number governed by the *bulk eigenstates* of the Hamiltonian, which attained different values for the two insulating cases. The winding number was then connected to the existence of the edge states at the boundaries of the model—this indeed proved that the two seemingly equivalent insulating phases are not quite equivalent at the boundaries. This non-trivial phase, where there exist some boundary states, and correspondingly a non-zero winding number in the bulk, is known as a topologically non-trivial insulator. In contrast to the other insulating phase, which has zero winding number, and correspondingly zero edge-states, is a trivial insulator. Despite being simple, the SSH model captures all the essential features of topological insulators that are also encountered in higher dimensional topological condensed matter.

8. Acknowledgements

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Suggested Reading

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