TERM PAPER
1D Su-Schrieffer-Heeger model: phases and topology

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Abstract

In this term paper we study 1-D SSH model.When Hopping amplitudes in SSH Hamiltonian are staggered we enter the insulating phase.But the two cases of insulating phase intracell hopping amplitudes < intercell amplitudes and vice versa are topologically not equivalent.The first one is non trivial ,where it harbours localised edge states.This is not the case for the later.The edge states are protected by the chiral symmetry of the Hamiltonian which is roboust to disorders in hopping amplitudes .But addition of onsite potential,breaks the chiral symmetry and we loose the zero eigen states.

1 1D Su-Schrieffer-Heeger model

The Su-Schrieffer-Heeger (SSH) model describes electrons hopping on a chain (one-dimensional lattice), with staggered hopping amplitudes.In this model the interaction between the electrons is neglected,therefore dynamics of each electron is described by single particle Hamiltonian.The model is a 1-D lattice chain of N sites,where each site has two sub lattices A and B. Intra cell hopping is v and Inter cell hopping amplitude is w.

The single particle Hamiltonian is of the form:

$$\hat{H} = v\sum_{m=1}^{N}(|m,B\rangle\langle m,A| + h.c) + w\sum_{m=1}^{N-1}(|m+1,A\rangle\langle m,B| + h.c) \tag{1}$$

$m \in 1,2,...,N$ is the lattice site and A,B are sub lattice sites.Hence $|m,A\rangle$ denotes state of the chain where electron is in A sub lattice of mth latice.

The basis $|m,\alpha\rangle$ can be written as tensor product of two basis $|m\rangle$ and $|\alpha\rangle$.m $\in$ 1,2,....,N and α $\in$A,B.Taking $|A\rangle$ as (1,0) vector and $|B\rangle$ as (0,1) vector, The hamiltonian can be written in terms of pauli matrices.

$$\hat{H} = \sum_{m=1}^{N} v\,|m\rangle\langle m| \otimes \hat{\sigma_x} + w\sum_{m=1}^{N-1}\left[|m+1\rangle\langle m| \otimes \frac{\hat{\sigma_x} + i\hat{\sigma_y}}{2} + h.c\right] \tag{2}$$

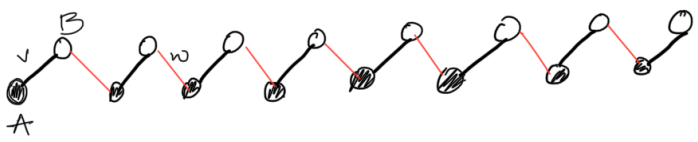

Figure 1: 1D SSH lattice with two sub lattices.

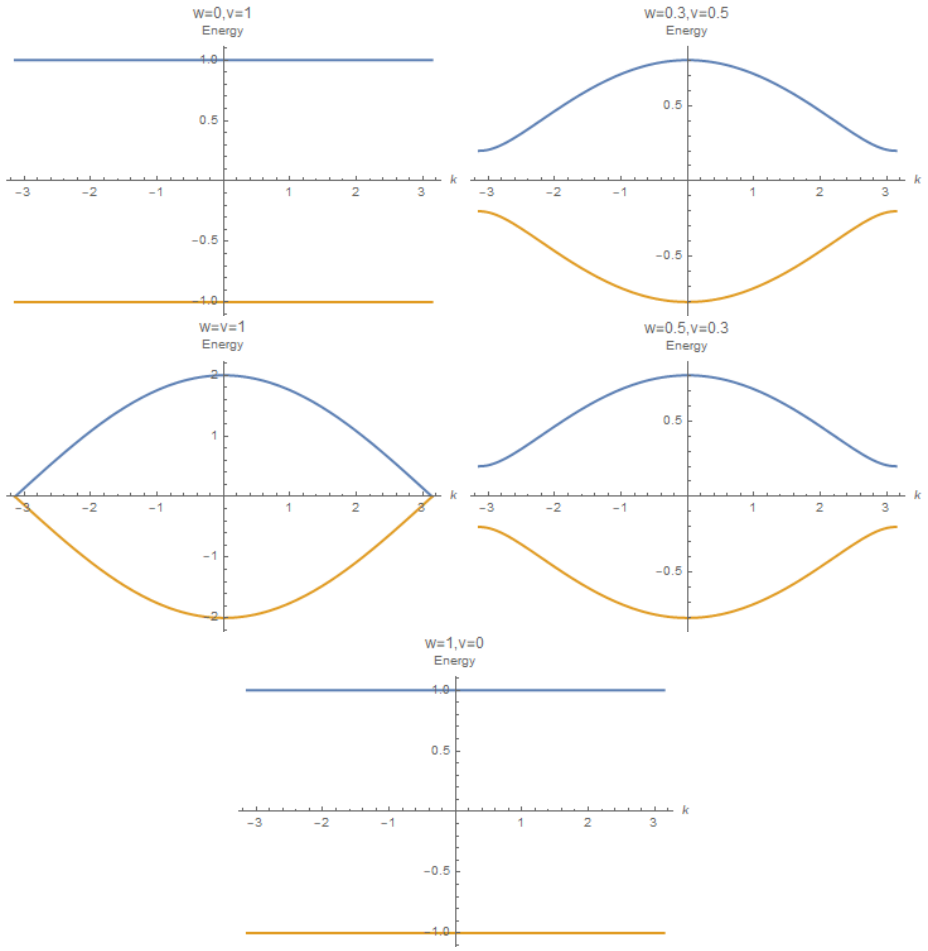

Figure 2: Energy vs k for different values of w and v

2 Periodic boundary Condition:

If we join the two ends of the chain(periodic boundary) ,Then our hamiltonian will have translational invariance, so we can represent it in momentum space using the following fourier transform.

$$|m\rangle = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{-imk} |m\rangle \tag{3}$$

Where $k = \frac{2\pi l}{N}$ for $l \in 1, 2, ..., N-1$.With periodic boundary condition the Hamiltonian in real space is following:

$$\hat{H}_{bulk} = \sum_{m=1}^{N} [v(|m, B\rangle \langle m, A| + h.c)] + \sum_{m=1}^{N} [w(|(m \mod N) + 1, A\rangle \langle m, B| + h.c)] \tag{4}$$

In momentum space:

$$\sum_{m=1}^{N} |m\rangle \langle m| \otimes |B\rangle \langle A| = \sum_{k,k_1 \in BZ} \sum_{m=1}^{N} \frac{e^{imk}.e^{-imk_1}}{N} |k\rangle \langle k_1| \otimes |B\rangle \langle A| = \sum_{k,k_1 \in BZ} \delta_{k,K_1} |k\rangle \langle k_1| \otimes |B\rangle \langle A|$$

$$= \sum_{k} |k\rangle \langle k| \otimes |B\rangle \langle A|$$

$$\sum_{m=1}^{N} |(m \mod N) + 1\rangle \langle m| = \sum_{kk_1 \in BZ} \sum_{m=1}^{N} \frac{e^{i((m \mod N)+1)k}.e^{-imk_1}}{N} |k\rangle \langle k_1|$$

$$= \sum_{k,k_1 \in BZ} \delta_{k,K_1} e^{ik} |k\rangle \langle k_1| \otimes |B\rangle \langle A| = \sum_k e^{ik} |k\rangle \langle k|$$

Using the above relations,

$$\hat{H}_{bulk} = \sum_k v(|k\rangle \langle k| \otimes |B\rangle \langle A| + h.c) + \sum_k w(e^{ik} |k\rangle \langle k| \otimes |A\rangle \langle B| + h.c) \tag{5}$$

To find the eigen states we act $\hat{H}_{bulk}$ on the general state $|\psi(k)\rangle = |k\rangle \otimes (a(k)|A\rangle + b(k)|B\rangle)$.

$$\begin{aligned}\hat{H}_{bulk} |\psi(k)\rangle &= va(k) |k\rangle \otimes |B\rangle + vb(k) |k\rangle \otimes |A\rangle + we^{ik} b(k) |k\rangle \otimes |A\rangle + we^{-ik} a(k) |k\rangle \otimes |B\rangle \\ &= E(k) [(a(k) |k\rangle \otimes |A\rangle + b(k) |k\rangle \times |B\rangle)]\end{aligned}$$

By comparing the coefficients, we get:

$$\begin{pmatrix} 0 & v + we^{ik} \\ v + we^{-ik} & 0 \end{pmatrix} \begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = E_k \begin{pmatrix} a(k) \\ b(k) \end{pmatrix} \tag{6}$$

We get the energy,

$$E_k = \pm\sqrt{v^2 + w^2 + 2wv\cos(k)} \tag{7}$$

correspinding eigen vectors:

$$|\pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{i\phi(k)} \\ 1 \end{pmatrix}$$

where $\phi(k) = \tan^{-1}(\frac{w \sin k}{v + w \cos k})$.We plot the energy as function of k,figure 2:

When w and v are not equal,bands are separated,system behaves as insulator.When w=v,the gap closes ,therefore behaves as conductor.From Eigen Energy point of view there is no difference in dispersion relation , between $w < v$ and $w > v$ cases.Let us define $H(k)$ as:

$$H(k) = \langle k| \hat{H}_{bulk} |k\rangle = (v + we^{ik}) |A\rangle \langle B| + (v + we^{-ik}) |B\rangle \langle A| \tag{8}$$

In terms of pauli matrices this can be written as:

$$H(k) = (v + w\cos k)\hat{\sigma}_x + w \sin k \hat{\sigma}_y = h(\vec{k}) \cdot \vec{\sigma} \tag{9}$$

Where $h_x(k) = (v + w\cos k)$,$h_y(k) = w \sin k, h_z = 0$.The eigen states were parameterised by $\phi(k) = \tan^{-1}(\frac{w \sin k}{v + w \cos k}) = \tan^{-1} \frac{h_y(k)}{h_x(k)}$.Therefore in in $h_x - h_y$ space the direction of $h(\vec{k})$ denotes an eigen state and it's magnitude gives eigenvalue.Figure 3 shows that the trajectory of $h(\vec{k})$ on h_x and h_y plane is different for $w < v$ and $w > v$ cases. The vector $h(\vec{k})$ forms a closed loop due to periodicity of Brillouin zone.For one of the insulator behavior case($v < w$) ,the vector $h(\vec{k})$ winds about the origin, where as,for other case ($v > w$) the vector trajectory does not wind about origin.For conductor case,the trajectory passes through origin.We can define this property as winding number ν.For $v < w$,$\nu = 1$.For $v > w$,$\nu = 0$ and for $v = w$,winding number is not defined since the trajectory passes through origin.Hence,winding number distinguishes between $v > w$ and $w > v$ cases.

Now we will take a small diversion and describe the theory of Berry phase:

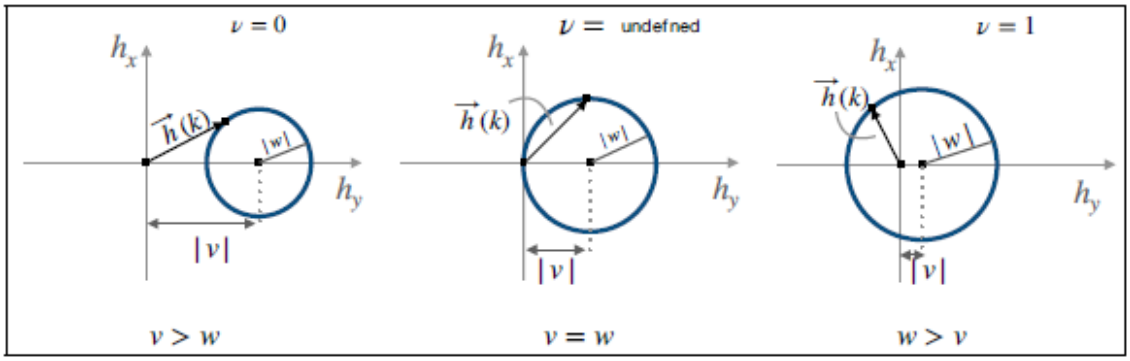

Figure 3: $h(\vec{k})$ as we varry k from 0 to 2π

3 The Berry phase

Suppose the Hamiltonian $\mathcal{H}$of the system is a function of the set of parameters $\mathbf{R}(t) = (\mathcal{R}_1(t), \mathcal{R}_2(t),...)$ which varies with time.Suppose $|n\rangle$ are the eigen states of $\mathcal{H}$

When the Hamiltonian does not depend on the external parameters,the wave functions simply evolve with a dynamical phase factor:

$$|n(t)\rangle = e^{-iE_n t/\hbar} |n(0)\rangle$$

But when $\mathcal{H}$ does depend on $\mathbf{R}(t)$,it is not only the dynamical phase which is picked up.Some other phase factor is also picked up.To Give an example consider the parallel transport of vector on the surface of sphere.Even though locally the direction of vector does not change , after a closed path of transport,the final vector does not align parallel with the initial vector.

We use adiabatic theorem,which states that:For a slowly varying Hamiltonian ,a system initially in the eigenstate will always remain in it's instantaneous eigenstate at any later time.so. If the state is prepared initially in the state $|n(\mathbf{R}(t=0))\rangle$,at later time t we write the evolved state as $|\psi(t)\rangle = e^{-i\theta(t)} |n(\mathbf{R}(t))\rangle$.Using the Schrodinger equation:

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

$$\implies E_n(\mathbf{R}(t)) |n(\mathbf{R}(\mathbf{t}))\rangle = \hbar \frac{d}{dt}(\theta(t)) |n(\mathbf{R}(t))\rangle + i\hbar \frac{d}{dt} |n(\mathbf{R}(t))\rangle$$

We now take scalar product with $\langle n(\mathbf{R}(t))|$ of the above equation, We get.

$$E_n(\mathbf{R}(t)) - i\hbar \langle n(\mathbf{R}(t))| \frac{d}{dt} |n(\mathbf{R}(t))\rangle = \hbar \frac{d}{dt}\theta(t)$$

Solving it We get:

$$\theta(t) = \frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(t'))dt' - i \int_0^t \left\langle n(\mathbf{R}(t'))\right| \frac{d}{dt'} \left|n(\mathbf{R}(t'))\right\rangle dt' \tag{10}$$

The first term is the dynamical phase due to evolution of Hamiltonian.The negative of second term is the extra phase we pick up, known as the Berry phase.So the expression for Berry Phase:

$$\gamma_n = i \int_0^t \left\langle n(\mathbf{R}(t'))\right| \frac{d}{dt'} \left|n(\mathbf{R}(t'))\right\rangle dt' \tag{11}$$

We write it in terms of Parameter space variable $\mathbf{R}$:

$$\gamma_n = i\int_0^t \left\langle n(\mathbf{R}(t^{'}))\right| \boldsymbol{\nabla}_{\mathbf{R}} \left|n(\mathbf{R}(t^{'}))\right\rangle \frac{d\mathbf{R}}{dt^{'}}dt^{'}$$

$$= i\int_{\mathbf{R}_0}^{\mathbf{R}_t} \langle n(\mathbf{R})| \boldsymbol{\nabla}_{\mathbf{R}} |n(\mathbf{R})\rangle \, d\mathbf{R}$$

$$\gamma_n = \int_{\mathbf{R}_0}^{\mathbf{R}_t} \mathbf{A}_n(\mathbf{R}) d\mathbf{R} \tag{12}$$

Where $\mathbf{A}_n(\mathbf{R}) = i\langle n(\mathbf{R})| \boldsymbol{\nabla}_{\mathbf{R}} |n(\mathbf{R})\rangle$ is known as the Berry potential. We can always multiply any quantum state with a global phase factor since it does not change the dynamics of system(Gauge invariance).

$$|n(\mathbf{R})\rangle \to e^{iX(\mathbf{R})} |n(\mathbf{R})\rangle$$

But the Berry potential is not Gauge invariance.It changes as:

$$\mathbf{A}_n(\mathbf{R}) \to \mathbf{A}_n(\mathbf{R}) - \frac{\partial}{\partial \mathbf{R}} X(\mathbf{R}) \tag{13}$$

The change in berry phase if we change parameters over a path $\mathcal{C}$:

$$-\int_{\mathcal{C}} \frac{\partial}{\partial \mathbf{R}} X(\mathbf{R}) d\mathbf{R} = X(\mathbf{R}_0) - X(\mathbf{R}_t)$$

If Path $\mathcal{C}$ is a closed path then , above integral vanish and We get a Gauge invariant Berry Phase.

Zak phase:

The Berry phase calculated over a non-contractible loop L of the Brillouin zone torus is known as the Zak phase.

$$\gamma_n^{zak} = \oint_L d\mathbf{k} \cdot \mathbf{A}_{\mathbf{n}}(\mathbf{k}) \tag{14}$$

For one dimensional system, the interval 0 to $\frac{2\pi}{a}$ is usually used, where a is the lattice constant.

4 Berry Phase in periodic SSH:

We calculate the Berry phase for the ground state $|-\rangle$ of $H(k)$,equation:8,9.Here the external parameter role is played by k.By using equation 12 ,Berry potential is:

$$|-(k)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{i\phi(k)} \\ 1 \end{pmatrix}$$

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

We integrate it over Brillouin zone:

$$\gamma_- = \oint A_-(k) dk = \begin{cases} -\pi & \text{v} < \text{w} \\ 0 & \text{v} > \text{w} \end{cases} \tag{15}$$

We can relate the Winding number to Berry phase as:

$$\nu = -\frac{1}{\pi}(\gamma_-)$$

Suppose we were to transform the Hamiltonian,by changing the parameters w or v.We want to get from one kind($v < w$) insulating phase to another kind($v > w$).We then realize that it is not possible without making the $\vec{h}(k)$ vector trajectory passing through the origin(conducting phase) since h_z is zero.Hence there is no smooth transition between these two phases.So these two phases are adiabatically not connected.In terms of winding numbers,since these have different winding numbers they are adiabatically not equivalent.Where as Two Hamiltonians with same winding number are adiabatically connected.

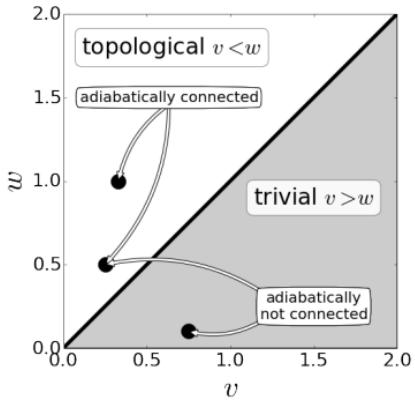

Figure 4: Two hamiltonians in same phase are adiabatically connected.

5 Finite SSH chain

There is no translational invariance in the open case. So we can not do Fourier transform.Therefore we calculate the eigenvalues and eigen vectors computationally.Hamiltonian with four lattice sites look like following:

$$H = \begin{pmatrix} 0 & v & 0 & 0 & 0 & 0 & 0 & 0 \\ v & 0 & w & 0 & 0 & 0 & 0 & 0 \\ 0 & w & 0 & v & 0 & 0 & 0 & 0 \\ 0 & 0 & v & 0 & w & 0 & 0 & 0 \\ 0 & 0 & 0 & w & 0 & v & 0 & 0 \\ 0 & 0 & 0 & 0 & v & 0 & w & 0 \\ 0 & 0 & 0 & 0 & 0 & w & 0 & v \\ 0 & 0 & 0 & 0 & 0 & 0 & v & 0 \end{pmatrix} \tag{16}$$

Eigen value as a function of v and w:

figure 5:We see that zero energy states exist at v=0.But also at very small values of v we have eigen values which are very close to zero.But as we increase the lattice size,these eigenvalues become even more close to zero. **figure 6**:when w is larger than v the close to zero eigen energy starts to appear.

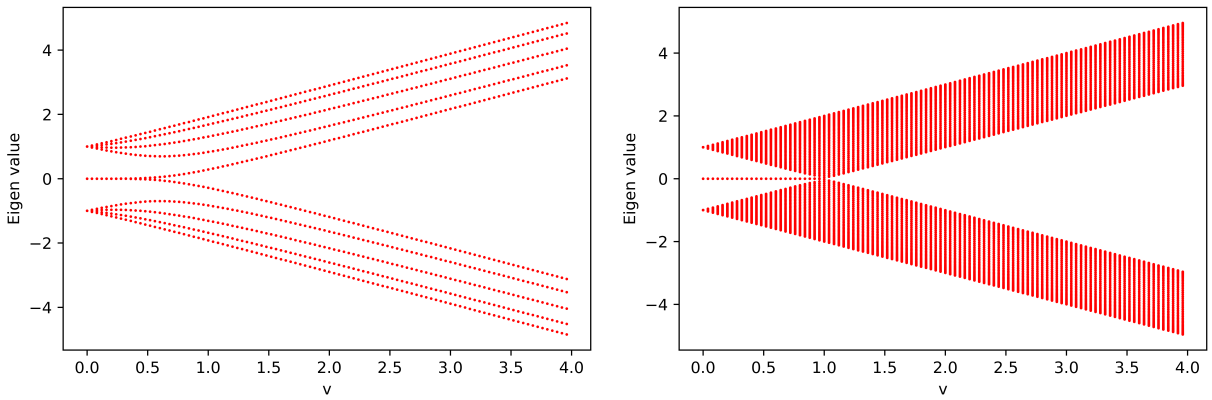

Figure 5: w=1,Lattice size=5 and 50 respectively

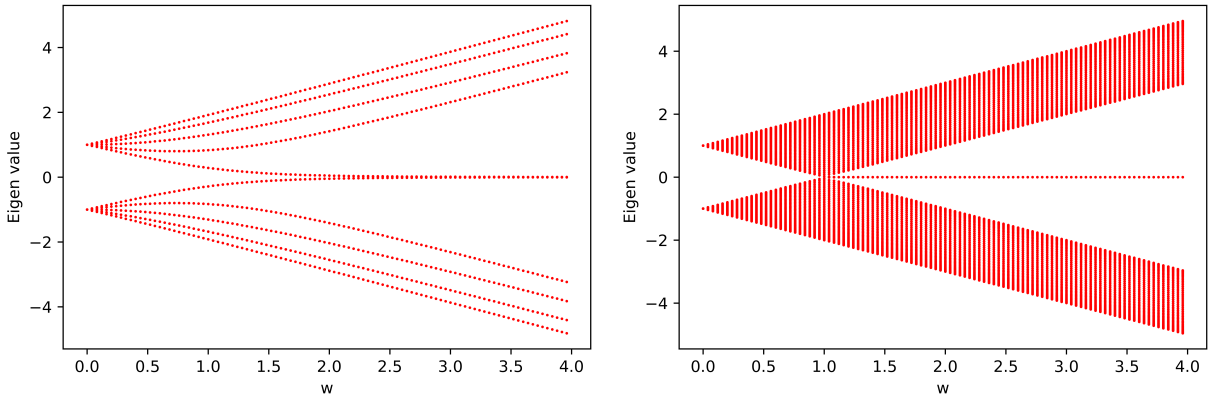

Figure 6: v=1,Lattice size=5 and 50 respectively

Fully Dimerized case:

To understand more about these zero eigen energy state consider the fully dimerized case w=1,v=0. Here there can be zero eigen state corresponding to the state where electrons are on the edge sites.There wave function will be localized to edges.Since there is no on site potential and no where to hop ,this will have zero energy. Where as for w=0,v=1 case there can always be intracell hopping, So there is no zero eigen states are present. So $v < w$ is the non trivial phase where there is presence of localized eigenstates with zero eigen values.

Putting Disorder in Hopping amplitudes:

We put some disorder in the hopping amplitudes.We add the term $d * u$ into all hopping amplitudes ($v \to v(1 + d * u)$ and ($w \to w(1 + d * u)$). Where d denotes the disorder strength $\in [0, 1]$, and u is a uniform random number from -1 to 1. Every hopping amplitude now has some randomness hence different.We calculate the eigen energies and plot as function of disorder strength.We also do similar thing with on site energy.we put onsite random energy fluctuations $d * u$. Where d denotes the disorder strength $\in [0, 1]$, and u is a uniform random number from -1 to 1.We observe that in case of hopping disorder zero energy states are still present,figure 11, but in case of onsite energy fluctuation the zero energy states no longer remains at zero,figure 12, as we increase the disorder strength.So disorder in hopping amplitude still protects the zero eigen states but not in onsite energy.

Figure 7: v=0

Figure 8: w=0

6 Symmetries of 1-D SSH Hamiltonian:

chiral symmetry:

A Hamiltonian $\hat{H}$ has chiral symmetry if

$$\hat{\Gamma}\hat{H}\hat{\Gamma} = -\hat{H} \tag{17}$$

With the chiral symmetry operator $\hat{\Gamma}$ which has to be unitary as well as hermitian. Consequence of Chiral symmetry in spectrum:The spectrum of chiral symmetric hamiltonian is symmetric.For any state with energy E ,there is a chiral symmetric partner with energy -E.If we have

$$\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

Then:

$$\hat{H}\hat{\Gamma}\left|\psi_n\right\rangle = -\hat{\Gamma}\hat{H}\left|\psi_n\right\rangle = -E_n\hat{\Gamma}\left|\psi_n\right\rangle$$

The orthogonal sublattice projectors $\hat{P}_A$ and $\hat{P}_B$ are defined in terms of chiral symmetry operator as:

$$\hat{P}_A = \frac{1}{2}(1+\hat{\Gamma}) \tag{18}$$

$$\hat{P}_B = \frac{1}{2}(1-\hat{\Gamma}) \tag{19}$$

Since there is no term in SSH hamiltonian which incudes transition between sites with same sublattice index we take The projectors for the sublattices for SSH model as:

$$\hat{P}_A = \sum_{m=1}^{N}\left|m,A\right\rangle\left\langle n,A\right| \tag{20}$$

$$\hat{P}_B = \sum_{m=1}^{N}\left|m,B\right\rangle\left\langle n,B\right| \tag{21}$$

So, the chiral symmetry operator for SSH model :

$$\hat{\Gamma}_z = \hat{P}_A - \hat{P}_B \tag{22}$$

Since Hamiltonian of SSH only contains terms of the form $\left|m,A\right\rangle\left\langle m^{'},B\right|$ or $\left|m,B\right\rangle\left\langle m^{'},A\right|$,The following Holds:

$$\hat{\Gamma}_z\hat{H}\hat{\Gamma}_z = -\hat{H} \tag{23}$$

We note that,above relation will still hold even if hopping amplitudes depend on position of lattice sites.Therefore chiral symmetry of SSH model is robust to disorder in hopping

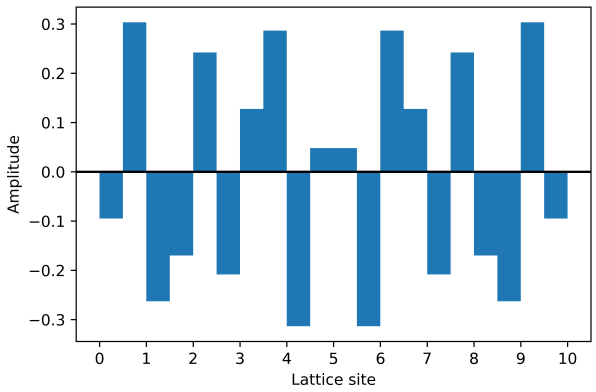

Figure 9: wavefunction corresponding to a non zero eigen value.N=10.v=0.3,w=1.

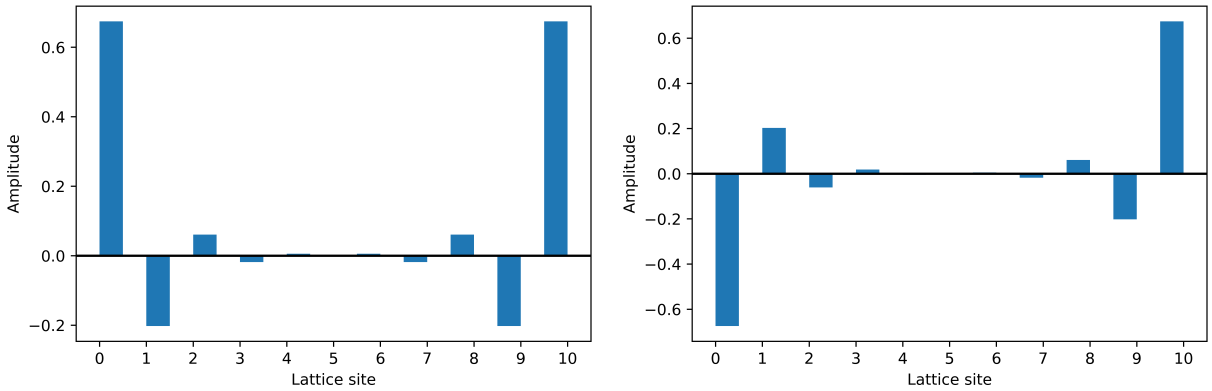

Figure 10: Wave function corresponding to zero eigen state.N=10.v=0.3,w=1.The wavefunctions are exponentially localized to edges.

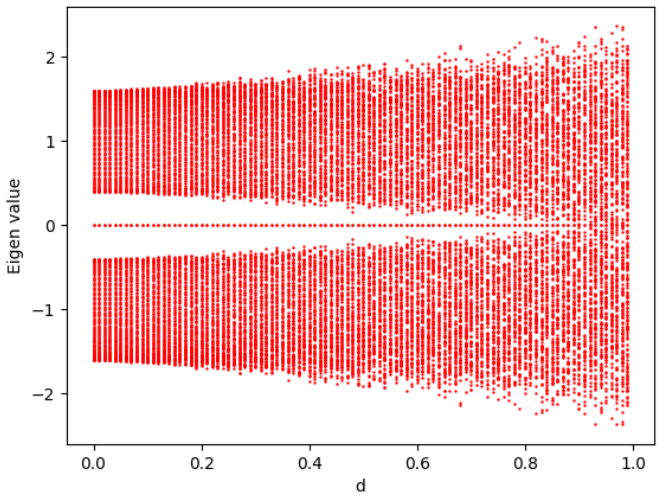

Figure 11: v=0.6,w=1,N=100.x-axis is disorder strength d hopping disorders.

amplitudes.That is the reason why we still get zero energy states in figure 11,Where we have introduced the hopping disorders.The chiral symmetry protects the edge states.But if we put onsite energy then there will be terms of the form $|m, A\rangle \langle m', A|$.The above relation for chiral symmetry will not hold anymore.Therefore in addition of on site enregy ,figure 12, We

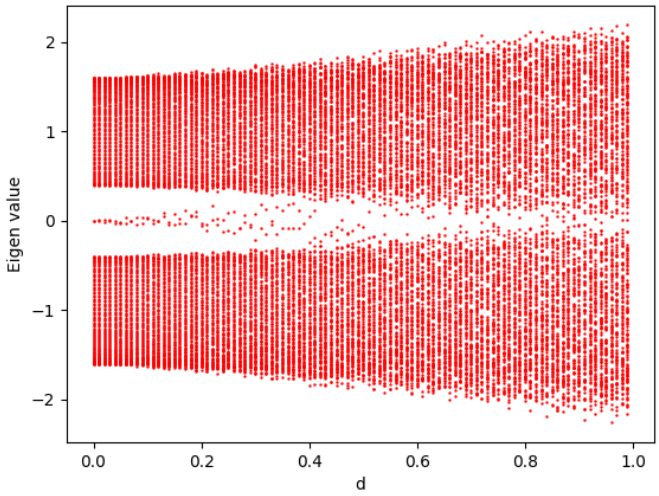

Figure 12: v=0.6,w=1,N=100.x-axis is disorder strength d in onsite energy disorder.

started the loose the zero energy states.

In terms of pauli matrices we had written the SSH model. In general if we have :

$$H(k) = h(k)_x\hat{\sigma}_x + h(k)_y\hat{\sigma}_y + h(k)_z\hat{\sigma}_z + \epsilon\hat{\sigma}_0$$

then

$$\sigma_z\left[h(k)_x\hat{\sigma}_x + h(k)_y\hat{\sigma}_y + h(k)_z\hat{\sigma}_z + \epsilon\hat{\sigma}_0\right]\sigma_z = -h(k)_x\hat{\sigma}_x - h(k)_y\hat{\sigma}_y + h(k)_z\hat{\sigma}_z + \epsilon\hat{\sigma}_0$$

So,Chiral symmetry with with σ_z implies that z-component $h(k)_z$ vanish and $\epsilon = -\epsilon$(protection of zero eigen state).This is what we have in SSH model .We don't have z-component of $h(\vec{k})$ in Hamiltonian and therefore we have Chiral symmetry in SSH model.But addition of onsite potential brings the z-component and We loose the chiral symmetry ,So,In figure 12 we start to loose the zero eigen states.