A. The Rice-Mele model

The Hamiltonian of Rice-Mele model is given by

$$\hat{H}_N^{RM} = \hat{H}_N + \hat{H}_{N,m} \tag{1}$$

where $\hat{H}_N$ is the Hamiltonian of SSH model and $\hat{H}_{N,m}$ is the Hamiltonian of on-site energy.

$$\hat{H}_N = t\sum_{j=1}^{N}(|j,A\rangle\langle j,B| + h.c.) + t'\sum_{j=1}^{N-1}(|j+1,A\rangle\langle j,B| + h.c.) \tag{2}$$

$$\hat{H}_{N,m} = m\sum_{j=1}^{N}(|j,A\rangle\langle j,A| - |j,B\rangle\langle j,B|) \tag{3}$$

We assume $m \neq 0$.

(a) Assuming periodic boundary condition (PBC) by setting $|N+1,\alpha\rangle = |1,\alpha\rangle$ $(\alpha = A, B)$, we can establish the Fourier transform between real space and momentum space and the relevant expressions are given by

$$|\mathbf{k},\alpha\rangle = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{i\mathbf{kja}}|j,\alpha\rangle \quad (\alpha = A, B) \tag{4}$$

$$|j,\alpha\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{kja}}|\mathbf{k},\alpha\rangle \quad (\alpha = A, B) \tag{5}$$

where a is the size of the unit cell.

Therefore, two parts of the Hamiltonian can be written in momentum space

$$\begin{aligned}
\hat{H}_N &= t\sum_{j=1}^{N}(|j,A\rangle\langle j,B| + h.c.) + t'\sum_{j=1}^{N-1}(|j+1,A\rangle\langle j,B| + h.c.) \\
&= t\sum_{j=1}^{N}(\frac{1}{N}\sum_{\mathbf{k,k'}} e^{i(\mathbf{k'}-\mathbf{k})ja}|\mathbf{k},A\rangle\langle\mathbf{k'},B| + h.c.) + t'\sum_{j=1}^{N-1}(\frac{1}{N}\sum_{\mathbf{k,k'}} e^{i(\mathbf{k'}-\mathbf{k})ja}e^{-i\mathbf{k}a}|\mathbf{k},A\rangle\langle\mathbf{k'},B| + h.c.) \\
&= t(\sum_{\mathbf{k,k'}}\delta_{\mathbf{k,k'}}|\mathbf{k},A\rangle\langle\mathbf{k'},B| + h.c.) + t'(\sum_{\mathbf{k,k'}}\delta_{\mathbf{k,k'}}e^{-i\mathbf{k}a}|\mathbf{k},A\rangle\langle\mathbf{k'},B| + h.c.) \\
&= \sum_{\mathbf{k}}(t + t'e^{-i\mathbf{k}a})|\mathbf{k},A\rangle\langle\mathbf{k},B| + h.c.
\end{aligned} \tag{6}$$

Similarly, we can derive

$$\hat{H}_{N,m} = m\sum_{\mathbf{k}}(|\mathbf{k},A\rangle\langle\mathbf{k},A| - |\mathbf{k},B\rangle\langle\mathbf{k},B|) \tag{7}$$

Choose the basis $\{|\mathbf{k}, A\rangle, |\mathbf{k}, B\rangle\}$, then we can rewrite matrix representation of the Hamiltonian in the selected basis:

$$H_N^{RM} = \sum_{\mathbf{k}} H_N^{RM}(\mathbf{k}) = \sum_{\mathbf{k}} H_N(\mathbf{k}) + H_{N,m}(\mathbf{k}) \tag{8}$$

with

$$H_N(\mathbf{k}) = \begin{pmatrix} 0 & t + t'e^{-i\mathbf{k}a} \\ t + t'e^{i\mathbf{k}a} & 0 \end{pmatrix} \tag{9}$$

$$H_{N,m}(\mathbf{k}) = \begin{pmatrix} m & 0 \\ 0 & -m \end{pmatrix} \tag{10}$$

$$H_N^{RM}(\mathbf{k}) = \begin{pmatrix} m & t + t'e^{-i\mathbf{k}a} \\ t + t'e^{i\mathbf{k}a} & -m \end{pmatrix} \tag{11}$$

Diagonalizing the Hamiltonian, we obtain the dispersion relation:

$$E_{\pm}(\mathbf{k}) = \pm\sqrt{m^2 + t^2 + t'^2 + 2tt'\cos(\mathbf{k}a)} \tag{12}$$

with corresponding eigenvectors

$$|u_-\rangle = \begin{pmatrix} \sin(\theta/2) \\ -\mathrm{e}^{i\phi}\cos(\theta/2) \end{pmatrix}; \quad |u_-\rangle = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{i\phi}\sin(\theta/2) \end{pmatrix}. \tag{13}$$

where $\cos\theta = \frac{m}{\sqrt{m^2+t^2+t'^2+2tt'\cos(\mathbf{k}a)}}$, $\sin\theta = \frac{\sqrt{t^2+t'^2+2tt'\cos(\mathbf{k}a)}}{\sqrt{m^2+t^2+t'^2+2tt'\cos(\mathbf{k}a)}}$ and $e^{-i\phi} = \frac{t+t'e^{-i\mathbf{k}a}}{\sqrt{t^2+t'^2+2tt'\cos(\mathbf{k}a)}}$.

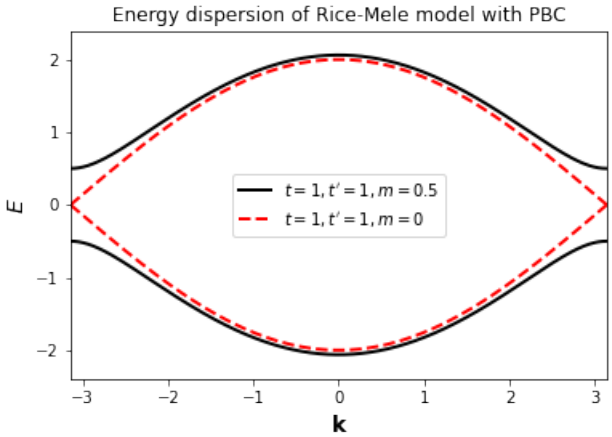

Figure 1: Energy spectrum of Rice-Mele model under PBC. (Red dashed line: on-site energy $m = 0$; Black solid line: on-site energy $m \neq 0$)

The bandstructure is plotted in Fig.(1). The band gap is the smallest energy difference between two bands and therefore given by $\Delta = 2\sqrt{m^2 + (t - t')^2} \neq 0$. The interband transition will not happen easily as a gap (always exists) should be overcome in any case.

In SSH model, we know that for $t < t'$ and $t' < t$ the Zak phases are $-\pi$ and 0, and winding number, which is a topological invariant, is given by 1 and 0. Therefore, a topological

transition happens at $t = t'$. Two topological phases are well distinguished by the winding number. The states which correspond to different winding numbers are strictly topological different.

However, in RM model, the Zak phases are given by

$$\phi_{Zak}^{(\pm)} = -\int_{1BZ} dk \frac{1 \mp \cos(\theta_{\mathbf{k}})}{2} \frac{\partial \phi_k}{\partial k} \tag{14}$$

Let $A = t'/t$ $(A > 0)$, $B = m/t$ $(B > 0)$, one is easy to verify that

$$\frac{\partial \phi_k}{\partial k} = \frac{aA(A + \cos(\mathbf{k}a))}{1 + A^2 + 2A\cos(\mathbf{k}a)} \tag{15}$$

Then we obtain

$$\phi_{Zak}^{\pm} = -\frac{1}{2}\int_{-\pi}^{\pi} dx \frac{A(A + \cos x)}{1 + A^2 + 2A\cos x} \pm \frac{1}{2}\int_{-\pi}^{\pi} dx \frac{B}{\sqrt{1 + A^2 + B^2 + 2A\cos x}} \frac{A(A + \cos x)}{1 + A^2 + 2A\cos x} \tag{16}$$

The phase diagram of the Zak phase $\phi_{Zak}^{(-)}$ is given by Fig.(2) (manually plotted inorder to save time). One is easy to see that when $B = 0$ the Zak phase changes from π to 0 across $A = 1$. But now the gapped band insulators at $B = 0, A > 1$ and $B = 0, A < 1$ can be continuously connected by tracing out a path that has $B \neq 0, A = 1$.

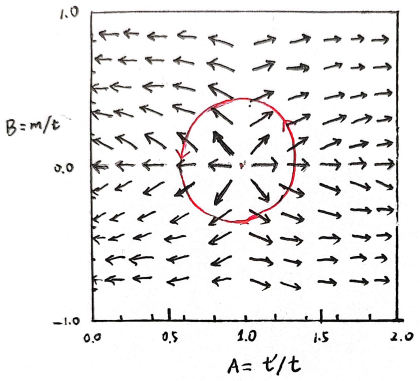

Figure 2: Phase diagram ($A = t'/t$, $B = m/t$) of Zak phase $\phi_{Zak}^{(-)}$.

(b) For the Hamiltonian $H_N^{RM}(\mathbf{k})$ in Eq.(11), we would like to find a $\mathbf{k}$-independent unitary matrix P such that it anticommutes with $H_N^{RM}(\mathbf{k})$. If P could be found, then we have $PH_N^{RM}P^\dagger = -H_N^{RM}$. Following the argument in TD 4, we know that P reflects the chiral or particle-hole symmetry, which means that if $|\beta\rangle$ is the eigenvector of Hamiltonian H_N^{RM} w.r.t. the eigenvalue E, then $P|\beta\rangle$ is the eivenvector w.r.t. the eigenvalue $-E$.

Suppose there exists a $\mathbf{k}$-independent unitary matrix P that anticommutes with the Hamiltonian and note that a 2×2 unitary matrix can always be written as

$$P = \begin{pmatrix} a & b \\ -e^{i\phi}b^* & e^{i\phi}a^* \end{pmatrix} \tag{17}$$

where a, b are complex numbers, ϕ is a real number between 0 and 2π and all these parameters are $\mathbf{k}$ independent.

Let $PH_N^{RM} = -H_N^{RM}P$, we obtain

$$\begin{cases} 2am + bt - b^*te^{i\phi} + bt'e^{i\mathbf{k}a} - t'b^*e^{i\phi}e^{-i\mathbf{k}a} = 0 \\ at + a^*te^{i\phi} + (at' + a^*e^{i\phi}t')e^{-i\mathbf{k}a} = 0 \\ at + a^*te^{i\phi} + (at' + a^*e^{i\phi}t')e^{i\mathbf{k}a} = 0 \\ 2a^*me^{i\phi} - bt + b^*te^{i\phi} - bt'e^{i\mathbf{k}a} + t'b^*e^{i\phi}e^{-i\mathbf{k}a} = 0 \end{cases} \tag{18}$$

For any $\mathbf{k}$, the four equations in Eq.(18) are always true. Therefore, we have

$$\begin{cases} at' + a^*e^{i\phi}t' = 0 \\ at + a^*e^{i\phi}t = 0 \\ bt' - t'b^*e^{i\phi} = 0 \\ bt' + t'b^*e^{i\phi} = 0 \\ 2am + bt - b^*te^{i\phi} = 0 \\ 2a^*me^{i\phi} - bt + b^*te^{i\phi} = 0 \end{cases} \tag{19}$$

Note that $t, t', m \neq 0$. From the first two equations we have $a + a^*e^{i\phi} = 0$, and we can write $a = i|a|e^{i\phi/2}$. From the thrid and fourth equations we obtain $b = 0$. Then from the fifth and sixth equation we obtain $a = 0$. Finally, we conclude $P = 0$, which suggests that the unitary matrix to be found doesn't exist. **The Hamiltonian doesn't anticommute with any k-independent matrix P.** This implies that Rice-Mele model doesn't have chiral or particle-hole symmetry, and therefore the edge state (if exists), which has zero energy, doesn't need to appear in pairs. **In terms of topological aspects, since the topological invariant of the SSH model is ensured by the chiral symmetry, it is possible to smoothly evolve between states with different topological invariants for the systems in which the chiral symmetry is broken.**

(c) Consider a half-infinite SSH chain defined by $H_\infty = \lim_{N\to\infty} H_N$ $(t, t' > 0)$. Suppose that there is an eigenstate $|\psi_0\rangle$ at zero energy, and we can write it as a combination of states $|n, \alpha\rangle$ with $\alpha = A, B$:

$$|\psi_0\rangle = \sum_{n=1}^{\infty} C_{n,A}\,|n, A\rangle + C_{n,B}\,|n, B\rangle \tag{20}$$

Inserting it in the Schordinger equation $H_\infty\,|\psi_0\rangle = 0$ and do some simplifications, we will obtain

$$tC_{1,B}\,|1, A\rangle + \sum_{n=2}^{\infty}(tC_{n,B} + t'C_{n-1,B})\,|n, A\rangle + \sum_{n=1}^{\infty}(tC_{n,A} + t'C_{n+1,A})\,|n, B\rangle = 0 \tag{21}$$

Therefore, it is obvious to know that

$$\begin{cases} C_{1,B} = 0 \\ C_{n+1,B} = -\frac{t'}{t}C_{n,B} \quad (n \geq 2) \\ C_{n+1,A} = -\frac{t}{t'}C_{n,A} \quad (n \geq 1) \end{cases} \tag{22}$$

Finally we obtain $C_{n,B} = 0$ and $C_{n,A} = C_{1,A}(-\frac{t}{t'})^{n-1}$.

From the normalization condition of $|\psi_0\rangle$, we can write

$$1 = \sum_{n=1}^{\infty} |C_{n,A}|^2 = |C_{1,A}|^2 \sum_{n=1}^{\infty} (\frac{t}{t'})^{2n-2} = |C_{1,A}|^2 \frac{1}{1-(t/t')^2} \tag{23}$$

Then we have $C_{1,A} = \sqrt{1-(t/t')^2}$ and the expression for the zero-energy edge state:

$$|\psi_0\rangle = \sqrt{1-(t/t')^2} \sum_{n=1}^{\infty} (-t/t')^{n-1} |n, A\rangle \tag{24}$$

It is worth noting that the state is valid only when $t < t'$ and the summation will not diverge. This implies the existence regime of the edge states in SSH model, which is consistent with the result we obtain in TD 4.

The probability distribution of electrons is given by the modulus square of the coefficients in the wavefunction. We have $P_{n,B} = 0$ and $P_{n,A} = [1-(t/t')^2](t/t')^{2(n-1)} \sim (t/t')^{2(n-1)}$.

Let $(n-1)a = x$, we have

$$P_{n,A} \sim (t/t')^{2(n-1)} = e^{-\frac{x}{\xi(t,t')}} \tag{25}$$

where the decay length is given by $\xi(t,t') = \frac{a}{2\ln(t'/t)}$. Consider the case $t \lesssim t'$, let $t' = t(1+\delta)$ where $\delta \sim 0$, $\xi(t,t') \sim \frac{a}{2\ln(1+\delta)} \sim \frac{a}{2\delta} \gg a$. The decay length tends to infinity. Such divergence implies that the phase transition appear in the vicinity of $t \lesssim t'$.

We make a further remark here. Note that this edge state occupies only one type of site (here the A sites), in agreement with the general requirement of the chiral symmetry for the state at zero energy: $\hat{P}|\psi_0\rangle \propto |\psi_0\rangle$ (Notice that $\hat{P} = \sum_n |n,A\rangle\langle n,A| - |n,B\rangle\langle n,B|$ is the chiral symmetric operator). And we only have one edge state in this problem.

(d) Consider the exact change in the energy of edge state ($t' > t$) in Rice-Mele model using the perturbation theory. The total Hamiltonian is given by $H_{\infty}^{RM} = H_{\infty} + \lim_{N\to\infty} H_{N,m}$. From Question ($c$) we know the zero-energy edge state of H_{∞} is given by $|\psi_0\rangle$. Consider the second term as a perturbation $V = \lim_{N\to\infty} H_{N,m}$ and use the perturbation theory for non-degenerate systems.

Suppose the eigenvalue of H_{∞} is denoted $\{..., |-E\rangle, ..., |\psi_0\rangle, ..., |E\rangle, ...\}$, where $|-E\rangle = \hat{P}|E\rangle$. The symmetric form of the eigen basis is due to the chiral symmetry. Note that if $|E\rangle = \sum_n c_{n,A}^E |n,A\rangle + c_{n,B}^E |n,B\rangle$, then it is easy to show that $|-E\rangle = \hat{P}|E\rangle = \sum_n c_{n,A}^E |n,A\rangle - c_{n,B}^E |n,B\rangle$, which differ from $|E\rangle$ by the minus sign of coefficients before $|n,B\rangle$. According to the perturbation theory, the first order energy correction is given by

$$\begin{aligned}
\Delta^{(1)} &= \langle\psi_0|\hat{V}|\psi_0\rangle \\
&= (\sqrt{1-(t/t')^2})^2 [\sum_{n=1}^{\infty} (-t/t')^{n-1} \langle n,A|][m\sum_{j=1}^{\infty}(|j,A\rangle\langle j,A| - |j,B\rangle\langle j,B|)][\sum_{n=1}^{\infty}(-t/t')^{n-1}|n,A\rangle] \\
&= (1-(t/t')^2) m \sum_n (t/t')^{2(n-1)} \\
&= m
\end{aligned} \tag{26}$$

The first order wavefunction correction is

$$\begin{aligned}\left|\psi_0^{(1)}\right\rangle &= \sum_{E>0}\{|E\rangle \frac{\left\langle E|\hat{V}|\psi_0\right\rangle}{0-E} + |-E\rangle \frac{\left\langle -E|\hat{V}|\psi_0\right\rangle}{0+E}\} \\ &= \sum_{E>0}\{(\sum_n c_{n,A}^E |n,A\rangle + c_{n,B}^E |n,B\rangle)\frac{\left\langle E|\hat{V}|\psi_0\right\rangle}{-E} + (\sum_n c_{n,A}^E |n,A\rangle - c_{n,B}^E |n,B\rangle)\frac{\left\langle -E|\hat{V}|\psi_0\right\rangle}{E}\} \\ &= \sum_{E>0}\{\sum_n c_{n,A}^E |n,A\rangle \frac{-\left\langle E|\hat{V}|\psi_0\right\rangle + \left\langle -E|\hat{V}|\psi_0\right\rangle}{E} + \sum_n c_{n,B}^E |n,B\rangle \frac{-\left\langle E|\hat{V}|\psi_0\right\rangle - \left\langle -E|\hat{V}|\psi_0\right\rangle}{E}\}\end{aligned} \tag{27}$$

Note that

$$-\left\langle E|\hat{V}|\psi_0\right\rangle + \left\langle -E|\hat{V}|\psi_0\right\rangle = 0 \tag{28}$$

We have

$$\left|\psi_0^{(1)}\right\rangle = -\sum_{E>0}\sum_n \frac{m}{E} S c_{n,B}^E |n,B\rangle \tag{29}$$

where $S = 2\sqrt{1-(t/t')^2}\sum_n c_{n,A}^E(-t/t')^{n-1}$.

Then second order energy correction is given by

$$\Delta^{(2)} = \langle\psi_0|\hat{V}\left|\psi_0^{(1)}\right\rangle = 0. \tag{30}$$

One can show that higher order energy correction is 0, therefore, **the exact energy change of the edge state is** $\Delta^{(1)} = m$. **The energy of the edge state is** $m \neq 0$, no longer a zero energy mode.

B. Spinful graphene

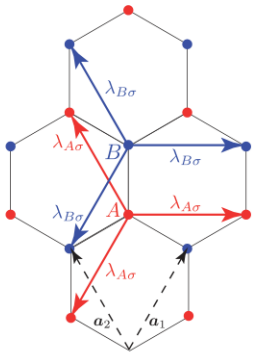

Figure 3: Graphene lattice in real space, with arrow depicting all the spin-dependent next-nearest-neighbor hoppings assigned to one unit-cell.

We use the traditional notation of tight binding model of graphene. Set lattice vector $\vec{a_1} = a(1,0)$, $\vec{a_2} = a(\frac{1}{2}, \frac{\sqrt{3}}{2})$. Three nearest neighbor hopping vectors are given by $\vec{\delta_1} = a(0, \frac{1}{\sqrt{3}})$, $\vec{\delta_2} = a(-\frac{1}{2}, -\frac{1}{2\sqrt{3}})$ and $\vec{\delta_2} = a(\frac{1}{2}, -\frac{1}{2\sqrt{3}})$. Three next-nearest neighbor hoppings are given by $\vec{\gamma_1} = a(1,0)$, $\vec{\gamma_2} = a(-\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $\vec{\gamma_3} = a(-\frac{1}{2}, -\frac{\sqrt{3}}{2})$, as shown in the figure above.

The corresponding lattice vectors for the reciprocal space are given by $\vec{b_1} = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}})$ and $\vec{b_2} = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}})$. Two Dirac points are denoted by $K_D = \frac{4\pi}{3a}(1,0)$ and $-K_D$.

In this problem, the next-nearest neighbor hoppings are added in graphene model, as shown in Fig.(3). The tight binding lattice model Hamiltonian is written as

$$H = H_t + H_m + H_\lambda \tag{31}$$

with

$$H_t = \sum_\sigma \sum_{R,\{\delta\}} t_\sigma c^\dagger_{B,R+\delta,\sigma} c_{A,R,\sigma} + h.c. \tag{32}$$

$$H_m = \sum_\sigma \sum_R m_\sigma (c^\dagger_{A,R,\sigma} c_{A,R,\sigma} - c^\dagger_{B,R,\sigma} c_{B,R,\sigma}) \tag{33}$$

$$H_\lambda = \sum_\sigma \sum_{R,\{\gamma\}} \lambda_{A\sigma} c^\dagger_{A,R+\gamma,\sigma} c_{A,R,\sigma} + h.c. + \lambda_{B\sigma} c^\dagger_{B,R+\gamma,\sigma} c_{B,R,\sigma} + h.c. \tag{34}$$

where $\lambda_{\alpha,\sigma} (\alpha = A, B$ and $\sigma = \uparrow, \downarrow)$ are four spin-dependent next-nearest neighbor hopping parameters and $\lambda_{\alpha,\sigma} \in \mathbb{C}$.

(a) In order to write the Hamiltonian in the momentum space, we define Fourier transform operations

$$c^\dagger_{\alpha,k\sigma} = \frac{1}{\sqrt{N}} \sum_R e^{ikR} c^\dagger_{\alpha,R\sigma} \tag{35}$$

and

$$c^\dagger_{\alpha,R\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{-ikR}c^\dagger_{\alpha,k\sigma} = \int_{1BZ}\frac{d^2k}{(2\pi)^2}e^{-ikR}c^\dagger_{\alpha,k\sigma} \tag{36}$$

Then H_t can be written as

$$\begin{aligned} H_t &= \sum_\sigma\sum_{R,\delta} t_\sigma[\frac{1}{N}\sum_{k,k'} e^{-ik(R+\{\delta\})}c^\dagger_{B,k\sigma}e^{ik'R}c_{A,k'\sigma} + h.c.] \\ &= \sum_\sigma\sum_{k,k'}\sum_R\sum_{\{\delta\}} t_\sigma\frac{1}{N}e^{i(k'-k)R}e^{-ik\delta}c^\dagger_{B,k\sigma}c_{A,k'\sigma} + h.c. \\ &= \sum_\sigma\sum_{\{\delta\}} t_\sigma\sum_{k,k'}\delta_{k,k'}e^{-ik\delta}c^\dagger_{B,k\sigma}c_{A,k'\sigma} + h.c. \\ &= \sum_{k,\sigma} t_\sigma\gamma(k)c^\dagger_{B,k\sigma}c_{A,k\sigma} + h.c. \end{aligned} \tag{37}$$

where $\gamma(k) = \sum_{\{\delta\}} e^{-ik\delta}$.

Similarly, we can prove that

$$H_m = \sum_{k,\sigma} m_\sigma[c^\dagger_{A,k\sigma}c_{A,k\sigma} - c^\dagger_{B,k\sigma}c_{B,k\sigma}] \tag{38}$$

$$H_\lambda = \sum_{k,\sigma}[\lambda_{A,\sigma}\eta(k)c^\dagger_{A,k\sigma}c_{A,k\sigma} + h.c.] + [\lambda_{B,\sigma}\eta(k)c^\dagger_{B,k\sigma}c_{B,k\sigma} + h.c.] \tag{39}$$

The total Hamiltonian is the sum of these partial Hamiltonians, as written in Eq.(31). The matrix representation is given by

$$H = \sum_{k,\sigma}\begin{pmatrix} c^\dagger_{A,k\sigma} & c^\dagger_{B,k\sigma}\end{pmatrix} H^\sigma_k \begin{pmatrix} c_{A,k\sigma} \\ c_{B,k\sigma}\end{pmatrix} \tag{40}$$

$$H^\sigma_k = \begin{pmatrix} m_\sigma + (\lambda_{A,\sigma}\eta(k) + \lambda^*_{A,\sigma}\eta^*(k)) & t^*_\sigma\gamma^*(k) \\ t_\sigma\gamma(k) & -m_\sigma + (\lambda_{B,\sigma}\eta(k) + \lambda^*_{B,\sigma}\eta^*(k))\end{pmatrix} \tag{41}$$

where $\eta(k) = \sum_{\{\gamma\}} e^{-ik\gamma}$.

Now we focus on spin-independent nearest neighbor hopping $t_\sigma = t > 0$ and on-site energy $m_\sigma = m$.

(b) The anti-unitary time reversal operator $\mathcal{T}$ for spin$-\frac{1}{2}$ electrons acts in the following way:

$$\begin{aligned} \mathcal{T}zc_{\alpha,R,\uparrow}\mathcal{T}^\dagger &= z^*c_{\alpha,R,\downarrow} \\ \mathcal{T}zc_{\alpha,R,\downarrow}\mathcal{T}^\dagger &= -z^*c_{\alpha,R,\uparrow} \end{aligned} \tag{42}$$

for a complex number z.

When time-reversal symmetry is imposed on the Hamiltonian, we have

$$\mathcal{T}H\mathcal{T}^\dagger = H \tag{43}$$

Define $\mathrm{sgn}(\sigma) = \delta_{\sigma,\uparrow} - \delta_{\sigma,\downarrow}$. First notice that

$$\begin{aligned}
\mathcal{T}H_t\mathcal{T}^\dagger &= \sum_\sigma \mathcal{T}[t\sum_{R,\{\delta\}} c^\dagger_{B,R+\delta,\sigma}c_{A,R,\sigma}]\mathcal{T}^\dagger + h.c. \\
&= \sum_\sigma \sum_{R,\{\delta\}} t^*[\mathrm{sgn}(\sigma)]^2 c^\dagger_{B,R+\delta,\bar{\sigma}}c_{A,R,\bar{\sigma}} + h.c. \\
&= \sum_{\bar{\sigma}} \sum_{R,\{\delta\}} t^* c^\dagger_{B,R+\delta,\bar{\sigma}}c_{A,R,\bar{\sigma}} + h.c. \\
&= \sum_\sigma \sum_{R,\{\delta\}} t^* c^\dagger_{B,R+\delta,\sigma}c_{A,R,\sigma} + h.c. \\
&= \sum_\sigma \sum_{R,\{\delta\}} t c^\dagger_{B,R+\delta,\sigma}c_{A,R,\sigma} + h.c. \\
&= H_t
\end{aligned} \tag{44}$$

We use the condition that t is real so that $t^* = t$. This is obvious, as we only focus on spin-independent $t > 0$.

$$\begin{aligned}
\mathcal{T}H_m\mathcal{T}^\dagger &= \sum_\sigma \sum_R \mathcal{T}[m(c^\dagger_{A,R,\sigma}c_{A,R,\sigma} - c^\dagger_{B,R,\sigma}c_{B,R,\sigma})]\mathcal{T}^\dagger \\
&= \sum_\sigma \sum_R [m^*[\mathrm{sgn}(\sigma)]^2(c^\dagger_{A,R,\bar{\sigma}}c_{A,R,\bar{\sigma}} - c^\dagger_{B,R,\bar{\sigma}}c_{B,R,\bar{\sigma}})] \\
&= \sum_{\bar{\sigma}} \sum_R [m^*(c^\dagger_{A,R,\bar{\sigma}}c_{A,R,\bar{\sigma}} - c^\dagger_{B,R,\bar{\sigma}}c_{B,R,\bar{\sigma}})] \\
&= \sum_\sigma \sum_R [m^*(c^\dagger_{A,R,\bar{\sigma}}c_{A,R,\bar{\sigma}} - c^\dagger_{B,R,\bar{\sigma}}c_{B,R,\bar{\sigma}})]
\end{aligned} \tag{45}$$

Let $\mathcal{T}H_m\mathcal{T}^\dagger = H_m$ we obtain $m^* = m$, which implies that m is a real number.

Now consider the third part

$$\begin{aligned}
\mathcal{T}H_\lambda\mathcal{T}^\dagger &= \sum_\sigma \sum_{R,\{\gamma\}} \mathcal{T}[\lambda_{A\sigma}c^\dagger_{A,R+\gamma,\sigma}c_{A,R,\sigma}]\mathcal{T}^\dagger + h.c. + \mathcal{T}[\lambda_{B\sigma}c^\dagger_{B,R+\gamma,\sigma}c_{B,R,\sigma}]\mathcal{T}^\dagger + h.c. \\
&= \sum_\sigma \sum_{R,\{\gamma\}} \lambda^*_{A\sigma}c^\dagger_{A,R+\gamma,\bar{\sigma}}c_{A,R,\bar{\sigma}} + h.c. + \lambda^*_{B\sigma}c^\dagger_{B,R+\gamma,\bar{\sigma}}c_{B,R,\bar{\sigma}} + h.c. \\
&= \sum_\sigma \sum_{R,\{\gamma\}} \lambda^*_{A\bar{\sigma}}c^\dagger_{A,R+\gamma,\sigma}c_{A,R,\sigma} + h.c. + \lambda^*_{B\bar{\sigma}}c^\dagger_{B,R+\gamma,\sigma}c_{B,R,\sigma} + h.c.
\end{aligned} \tag{46}$$

Imposing $\mathcal{T}H_\lambda\mathcal{T}^\dagger = H_\lambda$ we will obtain

$$\lambda_{\alpha,\sigma} = \lambda^*_{\alpha,\bar{\sigma}} \quad (\alpha = A, B) \tag{47}$$

In summary, the time reversal symmetry requires that $t \in \mathbb{R}$, $m \in \mathbb{R}$ and $\lambda_{\alpha,\sigma} = \lambda^*_{\alpha,\bar{\sigma}}$ $(\alpha = A, B)$.

(c) In question (a) we know the expression for H_k^σ. Imposing time reversal symmetry, we have

$$H_k^\sigma = \begin{pmatrix} m + (\lambda_{A,\sigma}\eta(k) + \lambda_{A,\sigma}^*\eta^*(k)) & t\gamma^*(k) \\ t\gamma(k) & -m + (\lambda_{B,\sigma}\eta(k) + \lambda_{B,\sigma}^*\eta^*(k)) \end{pmatrix} \tag{48}$$

Define $\lambda_{A,\uparrow} = |\lambda_A|e^{i\phi_A}$, $\lambda_{B,\uparrow} = |\lambda_B|e^{i\phi_B}$, then $\lambda_{A,\downarrow} = |\lambda_A|e^{-i\phi_A}$ and $\lambda_{B,\downarrow} = |\lambda_B|e^{-i\phi_B}$ using TRS. It's enough to have ϕ_A and $\phi_B \in [-\pi, \pi)$.

First, we calculate $\gamma(k)$ at $|\vec{q}| \ll |\vec{K_D}|$ near Dirac points $\xi\vec{K_D}, \xi = \pm 1$.

$$\begin{aligned} \gamma(k) &= \sum_{i=1}^{3} e^{-i(\xi\vec{K}_D + \vec{q})\vec{\delta}_i} \approx \frac{\sqrt{3}}{2}a(-\xi q_x - iq_y) \\ \gamma(k)^* &\approx \frac{\sqrt{3}}{2}a(-\xi q_x + iq_y) \end{aligned} \tag{49}$$

Then we consider $I_{A\uparrow}(\xi) = \lambda_{A,\uparrow}\eta(k) + \lambda_{A,\uparrow}^*\eta^*(k)$.

$$\begin{aligned} I_{A\uparrow}(\xi) &= |\lambda_A|[\sum_{i=1}^{3} e^{-i(\xi\vec{K_D} + \vec{q})\vec{\gamma_i}} e^{i\phi_A} + c.c.] \\ &= 2|\lambda_A|\sum_{i=1}^{3}\cos[(\xi\vec{K_D} + \vec{q})\vec{\gamma}_i - \phi_A] \\ &= 2|\lambda_A|[\cos(aq_x - \xi\frac{2\pi}{3} - \phi_A) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} - \phi_A) \\ &+ \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} - \phi_A)] \\ &= 2|\lambda_A|[(\cos(aq_x) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) + \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y))\cos(\xi\frac{2\pi}{3} + \phi_A) \\ &+ (\sin(aq_x) + \sin(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) + \sin(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y))\sin(\xi\frac{2\pi}{3} + \phi_A)] \\ &\approx 2|\lambda_A|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} + \phi_A) + O(q^3)] \end{aligned} \tag{50}$$

$$\begin{aligned} I_{A\downarrow}(\xi) &= 2|\lambda_A|\sum_{i=1}^{3}\cos[(\xi\vec{K_D} + \vec{q})\vec{\gamma}_i + \phi_A] \\ &= 2|\lambda_A|[\cos(aq_x - \xi\frac{2\pi}{3} + \phi_A) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} + \phi_A) \\ &+ \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} + \phi_A)] \\ &\approx 2|\lambda_A|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} - \phi_A) + O(q^3)] \end{aligned} \tag{51}$$

Similarly

$$\begin{aligned} I_{B\uparrow}(\xi) &= \lambda_{B,\uparrow}\eta(k) + \lambda^*_{B,\uparrow}\eta^*(k) \\ &= 2|\lambda_B|\sum_{i=1}^{3}\cos[(\xi\vec{K_D} + \vec{q})\vec{\gamma}_i - \phi_B] \\ &= 2|\lambda_B|[\cos(aq_x - \xi\frac{2\pi}{3} - \phi_B) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} - \phi_B) \\ &+ \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} - \phi_B)] \\ &\approx 2|\lambda_B|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} + \phi_B) + O(q^3)] \end{aligned} \tag{52}$$

$$\begin{aligned} I_{B\downarrow}(\xi) &= 2|\lambda_B|\sum_{i=1}^{3}\cos[(\xi\vec{K_D} + \vec{q})\vec{\gamma}_i + \phi_B] \\ &= 2|\lambda_B|[\cos(aq_x - \xi\frac{2\pi}{3} + \phi_B) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} + \phi_B) \\ &+ \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y) - \xi\frac{2\pi}{3} + \phi_B)] \\ &\approx 2|\lambda_B|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} - \phi_B) + O(q^3)] \end{aligned} \tag{53}$$

Then the Hamiltonian can be rewritten as

$$H_q^{\uparrow}(\xi) = \begin{pmatrix} m + I_{A\uparrow}(\xi) & -\frac{\sqrt{3}}{2}at(\xi q_x - iq_y) \\ -\frac{\sqrt{3}}{2}at(\xi q_x + iq_y) & -m + I_{B\uparrow}(\xi) \end{pmatrix} \tag{54}$$

$$H_q^{\downarrow}(\xi) = \begin{pmatrix} m + I_{A\downarrow}(\xi) & -\frac{\sqrt{3}}{2}at(\xi q_x - iq_y) \\ -\frac{\sqrt{3}}{2}at(\xi q_x + iq_y) & -m + I_{B\downarrow}(\xi) \end{pmatrix} \tag{55}$$

(d) Diagonalizing $H_q^{\sigma}(\xi)$ one can obtain the energy dispersion. This is amount to having

$$\mathbf{Det}\begin{pmatrix} m + I_{A\sigma}(\xi) - \lambda & -\frac{\sqrt{3}}{2}at(\xi q_x - iq_y) \\ -\frac{\sqrt{3}}{2}at(\xi q_x + iq_y) & -m + I_{B\sigma}(\xi) - \lambda \end{pmatrix} = 0 \tag{56}$$

One is easy to show that λs satisfy

$$\lambda_{\pm}^{\sigma,\xi}(q) = \frac{(I_{A\sigma}(\xi) + I_{B\sigma}(\xi)) \pm \sqrt{(I_{A\sigma}(\xi) - I_{B\sigma}(\xi) + 2m)^2 + 3(atq)^2}}{2} \tag{57}$$

These give the energy dispersion when time reversal symmetry is imposed on the Hamiltonian.

(e) The unitary spatial inversion operator is geven by $\mathcal{I}$ for the spin$-\frac{1}{2}$ electrons is defined as

$$\mathcal{I}zc_{A/B,k\sigma}\mathcal{I}^{\dagger} = zc_{B/A,-k\sigma} \tag{58}$$

If the Hamiltonian H_k^σ satisfies both time-reversal symmetry and inversion symmetry, let $\mathcal{I}H\mathcal{I}^\dagger = H$ we will obtain further constraints on t, m and $\lambda_{\alpha\sigma}$.

First verify $\mathcal{I}H_t\mathcal{I}^\dagger = H_t$.

$$\begin{aligned}
\mathcal{I}H_t\mathcal{I}^\dagger &= \sum_{k,\sigma} \mathcal{I}[t\gamma(k)c^\dagger_{B,k\sigma}c_{A,k\sigma}]\mathcal{I}^\dagger + h.c. \\
&= \sum_{k,\sigma} t\gamma(k)c^\dagger_{A,-k\sigma}c_{B,-k\sigma} + h.c. \\
&= \sum_{k,\sigma} t\gamma(-k)c^\dagger_{A,k\sigma}c_{B,k\sigma} + h.c. \\
&= \sum_{k,\sigma} t\gamma^*(k)c^\dagger_{A,k\sigma}c_{B,k\sigma} + h.c. \\
&= H_t
\end{aligned} \tag{59}$$

Here we only use the condition that $t \in \mathcal{R}$.

Second check $\mathcal{I}H_m\mathcal{I}^\dagger = H_m$.

$$\begin{aligned}
\mathcal{I}H_m\mathcal{I}^\dagger &= \sum_{k,\sigma} \mathcal{I}[m(c^\dagger_{A,k\sigma}c_{A,k\sigma} - c^\dagger_{B,k\sigma}c_{B,k\sigma})]\mathcal{I}^\dagger \\
&= \sum_{k,\sigma} m(c^\dagger_{B,-k\sigma}c_{B,-k\sigma} - c^\dagger_{A,-k\sigma}c_{A,-k\sigma}) \\
&= \sum_{k,\sigma} m(c^\dagger_{B,k\sigma}c_{B,k\sigma} - c^\dagger_{A,k\sigma}c_{A,k\sigma}) \\
&= H_m
\end{aligned} \tag{60}$$

Therefore, we have $m = -m$, which inplies that $m = 0$.

Third, calculate

$$\begin{aligned}
\mathcal{I}H_\lambda\mathcal{I}^\dagger &= \sum_{k,\sigma} \mathcal{I}[\lambda_{A,\sigma}\eta(k)c^\dagger_{A,k\sigma}c_{A,k\sigma} + h.c.]\mathcal{I}^\dagger + \mathcal{I}[\lambda_{B,\sigma}\eta(k)c^\dagger_{B,k\sigma}c_{B,k\sigma} + h.c.]\mathcal{I}^\dagger \\
&= \sum_{k,\sigma} (\lambda_{A,\sigma}\eta^*(k)c^\dagger_{B,k\sigma}c_{B,k\sigma} + h.c.) + (\lambda_{B,\sigma}\eta^*(k)c^\dagger_{A,k\sigma}c_{A,k\sigma} + h.c.) \\
&= H_\lambda
\end{aligned} \tag{61}$$

This implies that $\lambda_{A\sigma} = \lambda^*_{B\sigma}$. This constraint can be written further as $|\lambda_A| = |\lambda_B| = |\lambda|$ and $\phi_A = -\phi_B = \phi$.

To summarize here, time-reversal symmetry and inversion symmetry being imposed to the Hamiltonian, one is able to show that $t \in \mathbb{R}$, $m = 0$ and $\lambda_{A\sigma} = \lambda^*_{B\sigma}$.

Thus one can further simplify the expression for $I_{\alpha\sigma}$.

$$\begin{aligned}
I_{A\uparrow}(\xi) = I_{B\downarrow}(\xi) &= 2|\lambda|[(\cos(aq_x) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) + \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y))\cos(\xi\frac{2\pi}{3} + \phi) \\
&\quad + (\sin(aq_x) + \sin(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) + \sin(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y))\sin(\xi\frac{2\pi}{3} + \phi)] \\
&\approx 2|\lambda|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} + \phi) + O(q^3)]
\end{aligned} \tag{62}$$

$$\begin{aligned} I_{A\downarrow}(\xi) = I_{B\uparrow}(\xi) &= 2|\lambda|[(\cos(aq_x) + \cos(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) + \cos(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y))\cos(\xi\frac{2\pi}{3} - \phi) \\ &+ (\sin(aq_x) + \sin(a(-\frac{1}{2}q_x + \frac{\sqrt{3}}{2}q_y) + \sin(a(-\frac{1}{2}q_x - \frac{\sqrt{3}}{2}q_y))\sin(\xi\frac{2\pi}{3} - \phi)] \\ &\approx 2|\lambda|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} - \phi) + O(q^3)] \end{aligned} \tag{63}$$

The low energy Hamiltonian is written as

$$H_q^{\uparrow}(\xi) = \begin{pmatrix} 2|\lambda|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} + \phi)] & -\frac{\sqrt{3}}{2}at(\xi q_x - iq_y) \\ -\frac{\sqrt{3}}{2}at(\xi q_x + iq_y) & 2|\lambda|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} - \phi)] \end{pmatrix} \tag{64}$$

$$H_q^{\downarrow}(\xi) = \begin{pmatrix} 2|\lambda|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} - \phi)] & -\frac{\sqrt{3}}{2}at(\xi q_x - iq_y) \\ -\frac{\sqrt{3}}{2}at(\xi q_x + iq_y) & 2|\lambda|[(3 - \frac{3}{4}q^2a^2)\cos(\xi\frac{2\pi}{3} + \phi)] \end{pmatrix} \tag{65}$$

Keep until $O(q)$, the Hamiltonian can be written in a compact form

$$H_q^{\sigma}(\xi) = \begin{pmatrix} -3|\lambda|\cos\phi & 0 \\ 0 & -3|\lambda|\cos\phi \end{pmatrix} - \underbrace{\begin{pmatrix} 3\sqrt{3}\sigma\xi|\lambda|\sin\phi & \frac{\sqrt{3}}{2}at(\xi q_x - iq_y) \\ \frac{\sqrt{3}}{2}at(\xi q_x + iq_y) & -3\sqrt{3}|\lambda|\sigma\xi\sin\phi \end{pmatrix}}_{H_0^{\sigma,\xi}(q)} \tag{66}$$

where σ is the index for spin and define $\sigma(\uparrow) = +1$.

The energy dispersion now becomes

$$\lambda_{\pm}^{\sigma,\xi}(q) = \lambda_{\pm}(q) \approx -3|\lambda|\cos\phi - (\pm\sqrt{\frac{3}{4}a^2t^2q^2 + 27|\lambda|^2(\sin\phi)^2}) \tag{67}$$

Note that the dispersion relation is independent of spin and valley indexes.

At Dirac points, $q = 0$ and the dispersion relation becomes

$$\lambda_{\pm}(q = 0) = -3|\lambda|\cos\phi \pm 3\sqrt{3}|\lambda||\sin\phi| \tag{68}$$

The gap is given by $2\Delta = 6\sqrt{3}|\lambda||\sin\phi|$. The gap closes when $\phi = 0$ or $-\pi$ (Note that we restrict $\phi \in [-\pi, \pi)$). Otherwise, the gap will open.

In the presence of spin, Dirac cones still can not be protected by time-reversal symmetry and spatial inversion symmetry, as there is a tunable parameter ϕ which will create the gap at Dirac points.

(f) A topological band transition (TBT) leading to the topological properties of the bands can occur when bands touch at certain momentum k_0. Furthermore, the information about the topology is hidden in the eigenfunctions.

In the case of spinful graphene, high energy and low energy bands will touch only when $q = 0$ and $\phi = 0, -\pi$. In order to discuss about the topological different phases, eigenfunctions of the low energy Hamiltonian have to be calculated.

Let $\Delta = 3\sqrt{3}|\lambda|\sin\phi \in \mathbb{R}$ and $b = -\frac{\sqrt{3}}{2}at(q_x - iq_y) \in \mathbb{C}$. Denote the eigenfunction of $H_0^{\sigma,\xi}(q)$ corresponding to $\lambda_{\pm}^{\sigma,\xi}$ by $\left|\lambda_{\pm}^{\sigma,\xi}\right\rangle$. One can calculate the Chern number for each state

$\tilde{C}^{\sigma}_{\lambda,\xi} = -\frac{1}{2}\lambda\xi\mathrm{sgn}(\sigma\xi\Delta) = -\frac{1}{2}\lambda\mathrm{sgn}(\sigma\phi)$ (λ is band index). For each valley, we know that if $\phi > 0$, $\tilde{C}^{\sigma=\uparrow}_{\lambda=-} = 1/2$,$\tilde{C}^{\sigma=\downarrow}_{\lambda=-} = -1/2$,$\tilde{C}^{\sigma=\uparrow}_{\lambda=+} = -1/2$,$\tilde{C}^{\sigma=\downarrow}_{\lambda=+} = 1/2$; if $\phi < 0$, $\tilde{C}^{\sigma=\uparrow}_{\lambda=-} = -1/2$,$\tilde{C}^{\sigma=\downarrow}_{\lambda=-} = 1/2$,$\tilde{C}^{\sigma=\uparrow}_{\lambda=+} = 1/2$,$\tilde{C}^{\sigma=\downarrow}_{\lambda=+} = -1/2$. There are two different cases, which we denote as $\phi > 0$ and $\phi < 0$.

So the combination of ϕ and ξ will give three topological different cases.

- $\phi > 0$ for $-\vec{K}_D$, $\phi > 0$ for $\vec{K}_D$. We have $C^{\sigma=\uparrow}_{\lambda=-} = C^{\sigma=\downarrow}_{\lambda=+} = 1$, $C^{\sigma=\downarrow}_{\lambda=-} = C^{\sigma=\uparrow}_{\lambda=+} = -1$.
- $\phi < 0$ for $-\vec{K}_D$, $\phi < 0$ for $\vec{K}_D$. We have $C^{\sigma=\uparrow}_{\lambda=-} = C^{\sigma=\downarrow}_{\lambda=+} = -1$, $C^{\sigma=\downarrow}_{\lambda=-} = C^{\sigma=\uparrow}_{\lambda=+} = 1$.
- $\phi > 0$ for $-\vec{K}_D$, $\phi < 0$ for $\vec{K}_D$ or $\phi < 0$ for $-\vec{K}_D$, $\phi > 0$ for $\vec{K}_D$. We have $C^{\sigma=\uparrow}_{\lambda=-} = C^{\sigma=\downarrow}_{\lambda=+} = 0$, $C^{\sigma=\downarrow}_{\lambda=-} = C^{\sigma=\uparrow}_{\lambda=+} = 0$.

C. Green's functions

(a) Consider a one-dimensional chain of Hydrogen atoms with periodic boundary conditions within the tight binding approximation.

The Hamiltonian is given by

$$H = t\sum_{i=1}^{N}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + h.c.) \tag{69}$$

Use the Fourier transform

$$c_{k\sigma}^{\dagger} = \frac{1}{\sqrt{N}}\sum_{m=1}^{N} e^{ikma}c_{m\sigma}^{\dagger} \tag{70}$$

$$c_{m\sigma}^{\dagger} = \frac{1}{\sqrt{N}}\sum_{k} e^{-ikma}c_{k\sigma}^{\dagger} \tag{71}$$

One is able to show that

$$H^{int} = H - \mu N = \sum_{k\sigma}(\varepsilon_k - \mu)c_{k\sigma}^{\dagger}c_{k\sigma} \tag{72}$$

where $\varepsilon_k = 2t\cos(ka)$. We don't consider any Coulomb interactions.

The retarded Green's function is given by

$$G^R(k,\sigma,t) = -i\theta(t)\left\langle\{c_{k,\sigma}(t), c_{k,\sigma}^{\dagger}(0)\}\right\rangle \tag{73}$$

To calculate

$$G^R(k,\sigma,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}G^R(k,\sigma,t) \tag{74}$$

here we show two methods.

Method 1 In the non-interacting 1D chain case, we are able to write down the analytic expression for $c_{k,\sigma}(t)$ by using Baker–Campbell–Hausdorff formula.

$$c_{k\sigma}(t) = c_{k\sigma}e^{-i\varepsilon_k t/\hbar} \tag{75}$$

Therefore, we can further calculate

$$\begin{aligned} G^R(k,\sigma,t) &= -i\theta(t)\left\langle c_{k\sigma}(t)c_{k\sigma}^{\dagger}(0) + c_{k\sigma}^{\dagger}(0)c_{k\sigma}(t)\right\rangle \\ &= -i\theta(t)e^{-i(\varepsilon_k-\mu)t/\hbar}\left\langle c_{k\sigma}c_{k\sigma}^{\dagger} + c_{k\sigma}^{\dagger}c_{k\sigma}\right\rangle \\ &= -i\theta(t)e^{-i(\varepsilon_k-\mu)t/hbar} \end{aligned} \tag{76}$$

Then do the Fourier transform to the frequency space, we have

$$G^R(k,\sigma,\omega) = -i\int_{-\infty}^{\infty}\theta(t)e^{-\eta t}e^{-i(\varepsilon_k-\mu)t/\hbar}dt = \frac{1}{\omega + i\eta - (\varepsilon_k-\mu)/\hbar} \tag{77}$$

Method 2 Calculate by using Lehmann representation directly.

$$\begin{aligned}
G^R(k,\sigma,t) &= -i\theta(t)[\left\langle c_{k\sigma}(t)c_{k\sigma}^\dagger \right\rangle + \left\langle c_{k\sigma}^\dagger c_{k\sigma}(t) \right\rangle] \\
&= -i\theta(t)[\frac{1}{Z}e^{-\beta E_n}\sum_{n,m}\langle n|c_{k\sigma}(t)|m\rangle \left\langle m|c_{k\sigma}^\dagger|n \right\rangle + \frac{1}{Z}\sum_{n,m}e^{-\beta E_n}\left\langle n|c_{k\sigma}^\dagger|m \right\rangle \langle m|c_{k\sigma}(t)|n\rangle] \\
&= -i\theta(t)[\frac{1}{Z}\sum_{n,m}e^{-\beta E_n}e^{-i(\varepsilon_k-\mu)t/\hbar}\langle n|c_{k\sigma}|m\rangle \left\langle m|c_{k\sigma}^\dagger|n \right\rangle \\
&\quad + \frac{1}{Z}\sum_{n,m}e^{-\beta E_n}e^{-i(\varepsilon_k-\mu)t/\hbar}\left\langle n|c_{k\sigma}^\dagger|m \right\rangle \langle m|c_{k\sigma}|n\rangle \\
&= -i\theta(t)\frac{1}{Z}\sum_{n}e^{-\beta E_n}e^{-i(\varepsilon_k-\mu)t/\hbar}\left\langle n|c_{k\sigma}c_{k\sigma}^\dagger + c_{k\sigma}^\dagger c_{k\sigma}|n \right\rangle \\
&= -i\theta(t)e^{-i(\varepsilon_k-\mu)t/\hbar}
\end{aligned} \tag{78}$$

Using Fourier transform as shown in **Method 1**, we can also prove Eq.(77).

The spectral function is given by

$$A(k,\omega) = -\frac{1}{\pi}G^R(k,\sigma,\omega) = \delta(\omega-(\varepsilon_k-\mu)/\hbar) \tag{79}$$

The spectral function is shown in Fig.(4).

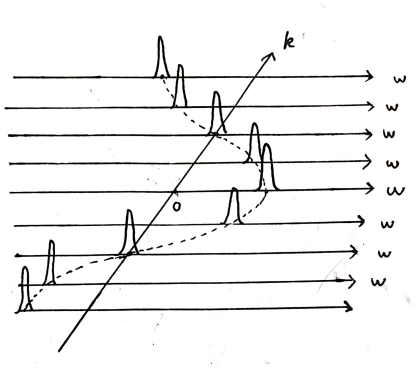

Figure 4: Spectral function of non-interacting 1D chain.

(b) Consider now a single-site problem with an isolated atom whose electrons are described by $H = \epsilon(n_\uparrow+n_\downarrow)+U(n_\uparrow-1/2)(n_\downarrow-1/2)$. The first term is the on-site energy for an electron (either $\uparrow$ or $\downarrow$) occupying the site, and the second term is the on-site Coulomb interaction between a $\uparrow$ spin electron and a $\downarrow$ spin electron occupying the same site, rewritten in the particle-hole symmetry form.

One can show that for $\epsilon = 0$ the system is half filled. This amounts to show $\langle N\rangle = 1$ with $N = c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow$. First solve the single site problem, $E(|0\rangle) = U/4$, $E(|\uparrow\rangle) = E(|\downarrow\rangle) = \epsilon - U/4$

and $E(|\uparrow\downarrow\rangle) = 2\epsilon + U/4$. Then write

$$\begin{aligned}\langle N\rangle &= \frac{1}{Z}\sum_n e^{-\beta E_n}\langle n|N|n\rangle \\ &= \frac{2e^{-\beta(\epsilon-U/4)} + 2e^{-\beta(2\epsilon+U/4)}}{e^{-\beta U/4} + 2e^{-\beta(\epsilon-U/4)} + e^{-\beta(2\epsilon+U/4)}}\end{aligned} \tag{80}$$

Set $\epsilon = 0$ we have $\langle N\rangle = 1$.

Now calculate the retarded Green's function of the system

$$\begin{aligned}G^R(\sigma,t) &= -i\theta(t)\left\langle\{c_\sigma(t), c_\sigma^\dagger\}\right\rangle \\ &= -i\theta(t)\frac{1}{Z}\sum_n e^{-\beta E_n}\left\langle n|\{c_\sigma(t), c_\sigma^\dagger\}|n\right\rangle \\ &= -i\theta(t)\frac{1}{Z}[(e^{-\beta U/4} + e^{-\beta(\epsilon-U/4)})e^{i(U/2-\epsilon)t} + (e^{-\beta(\epsilon-U/4)} + e^{-\beta(2\epsilon+U/4)})e^{i(-U/2-\epsilon)t}]\end{aligned} \tag{81}$$

where $Z = e^{-\beta U/4} + 2e^{-\beta(\epsilon-U/4)} + e^{-\beta(2\epsilon+U/4)}$.

The retarded Green's function in frequency space is given by

$$G^R(\sigma,\omega) = A_1\frac{1}{\omega + i\eta - (\epsilon - U/2)} + A_2\frac{1}{\omega + i\eta - (\epsilon + U/2)} \tag{82}$$

where $A_1 = \frac{1}{Z}(e^{-\beta U/4} + e^{-\beta(\epsilon-U/4)})$ and $A_2 = \frac{1}{Z}(e^{-\beta(\epsilon-U/4)} + e^{-\beta(2\epsilon+U/4)})$.

Setting $U = 0$, the retarded Green's function for the non-interacting case is

$$G_0^R(\sigma,\omega) = \frac{1}{\omega + i\eta - \epsilon} \tag{83}$$

Therefore, the self energy is

$$\begin{aligned}\Sigma^R(\sigma,\omega) &= [G_0^R(\sigma,\omega)]^{-1} - [G^R(\sigma,\omega)]^{-1} \\ &= \frac{U}{2}(A_2 - A_1) + \frac{U^2}{4}\frac{1 - (A_2 - A_1)^2}{\omega + i\eta - \epsilon + \frac{U}{2}(A_2 - A_1)}\end{aligned} \tag{84}$$

The spectral function is

$$A(\sigma,\omega) = A_1\delta(\omega - (\epsilon - U/2)) + A_2\delta(\omega - (\epsilon + U/2)) \tag{85}$$

At half filling, we know that $\epsilon = 0$ and $A_1 = A_2 = 1/2$. Therefore, the Green's function is given by

$$G^R(\sigma,\omega) = \frac{1}{2}(\frac{1}{\omega + i\eta - U/2} + \frac{1}{\omega + i\eta + U/2}). \tag{86}$$

The non-interacting Green's function, the self energy and spectral function are given by

$$G_0^R(\sigma,\omega) = \frac{1}{\omega + i\eta} \tag{87}$$

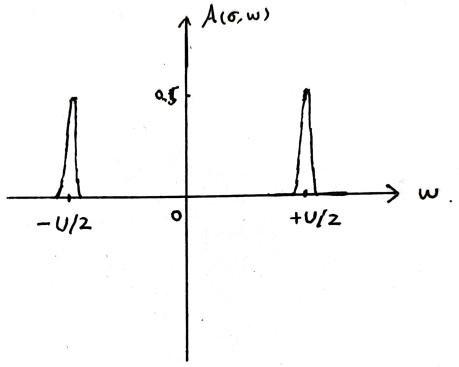

Figure 5: Spectral function of single-site atomic model

$$\Sigma^R(\sigma,\omega) = \frac{U^2}{4}\frac{1}{\omega+i\eta} \tag{88}$$

$$A(\sigma,\omega) = \frac{1}{2}\delta(\omega - U/2) + \frac{1}{2}\delta(\omega + U/2) \tag{89}$$

The spectral function is sketched below in Fig.(5).

(c) Assuming that the self energy calculated in question (b) can be used as an approximation to the self energy of an interacting 1D chain problem at half-filling ($\mu = 0$), the retarded Green's function can now be written as (set $\hbar = 1$)

$$[G^R(k,\sigma,\omega)]^{-1} = [\frac{1}{\omega+i\eta-\varepsilon_k}]^{-1} - \Sigma^R(\sigma,\omega) \tag{90}$$

Then one obtains

$$\begin{aligned} G^R(k,\sigma,\omega) &= \frac{1}{\omega+i\eta-\varepsilon_k-\frac{U^2}{4}\frac{1}{\omega+i\eta}} \\ &= \frac{1}{\omega+i\eta-\varepsilon_k-\mathrm{P}\frac{U^2}{4}\frac{1}{\omega}+i\pi\frac{U^2}{4}\delta(\omega)} \\ &= \frac{1}{[\omega-\varepsilon_k-\mathrm{P}\frac{U^2}{4}\frac{1}{\omega}]+i[\eta+\pi\frac{U^2}{4}\delta(\omega)]} \end{aligned} \tag{91}$$

Now calculate the poles of the Green's function. Let $\omega - \varepsilon_k\omega - \frac{U^2}{4}\frac{1}{\omega} = 0$, we will obtain

$$\omega_{1,2} = \frac{\varepsilon_k \pm \sqrt{\varepsilon_k^2+U^2}}{2} \tag{92}$$

Two poles of the Green's function are positioned at $\omega_{1,2} = \frac{\varepsilon_k \pm \sqrt{\varepsilon_k^2+U^2}}{2}$.

By inspection, we know the spectral function at $\omega = 0$ is 0. Moreover, at $\omega \neq 0$ the Green's function is given by

$$\begin{aligned} G^R(k,\sigma,\omega) &= \frac{1}{\omega - \varepsilon_k - \frac{U^2}{4}\frac{1}{\omega} + i\eta} \\ &= \frac{1}{\omega - \varepsilon_k - \frac{U^2}{4}\frac{1}{\omega}} - i\frac{\eta}{\eta^2 + (\omega - \varepsilon_k - \frac{U^2}{4}\frac{1}{\omega})} \\ &= \frac{M}{\omega - \omega_1} + \frac{N}{\omega - \omega_2} - i\pi\delta(\omega - \varepsilon_k - \frac{U^2}{4}\frac{1}{\omega}) \end{aligned} \tag{93}$$

The spectral function is therefore

$$\begin{aligned} A(k,\omega) &= -\frac{1}{\pi}G^R(k,\sigma,\omega) = \delta(\omega - \varepsilon_k - \frac{U^2}{4}\frac{1}{\omega}) \\ &= \frac{1}{1 + \frac{U^2}{4}\frac{1}{\omega_1^2}}\delta(\omega - \omega_1) + \frac{1}{1 + \frac{U^2}{4}\frac{1}{\omega_2^2}}\delta(\omega - \omega_2) \\ &= \frac{(\varepsilon_k + \sqrt{\varepsilon_k^2 + U^2})^2}{U^2 + (\varepsilon_k + \sqrt{\varepsilon_k^2 + U^2})^2}\delta(\omega - \omega_1) + \frac{(\varepsilon_k - \sqrt{\varepsilon_k^2 + U^2})^2}{U^2 + (\varepsilon_k - \sqrt{\varepsilon_k^2 + U^2})^2}\delta(\omega - \omega_2) \end{aligned} \tag{94}$$

Note that we use the property of Dirac delta function $\delta(g(x)) = \sum_i \frac{\delta(x - x_i}{|g'(x_i)|}$. One can check that the sum of weights of two peaks is 1.

The spectral function is plotted in Fig.(6) for different U values at fixed t.

The approximation used here assumes that the self energy of 1D chain problem is purely local so that k dependence is dropped out. This is the prototype of DMFT. It can qualitatively describe the system in which on-site interaction term and hopping term both play some role, especially can capture the main characteristic of metal-insulator transition process.

(d) Now make a different approximation to the self energy of the retarded Green's function. Assume that $\Sigma^R(k,\omega) = C + Z_k^{-1}\omega - i\Gamma\omega^2$. Using dimension analysis, we know $C \sim [s^{-1}]$, which has the dimension of frequency (or energy). Z_k has the dimension of 1, i.e. $Z_k \sim 1$. Γ has the dimension of inverse of frequency or time, namely, $\Gamma \sim [s]$.

The retarded Green's function of 1D chain problem is given by

$$\begin{aligned} G^R(k,\sigma,\omega) &= \frac{1}{\omega + i\eta + \mu - \varepsilon_k - C - Z_k^{-1}\omega + i\Gamma\omega^2} \\ &= \frac{1}{(1 - Z_k^{-1})\omega + \mu - C - \varepsilon_k + i(\Gamma\omega^2 + \eta)} \end{aligned} \tag{95}$$

The spectral function if given by the imaginary part the the retarded Green's function, thus $A(k,\sigma) \propto -(-\Gamma\omega^2) = \Gamma\omega^2 > 0$. Γ is a positive quantity which captures the lifetime of the quasi-particle.

Assuming the system is in the normal Fermi liquid regime, redefine $\tilde{Z}_k = (1 - Z_k^{-1})^{-1}$, $\tilde{\varepsilon_k} = \tilde{Z}(C + \varepsilon_k - \mu)$ and $\frac{1}{2\tau_k(\omega)} = \tilde{Z}_k(\Gamma\omega^2 + \eta)$ and the retarded Green's function can be written as

$$G^R(k,\sigma,\omega) = \frac{\tilde{Z}_k}{\omega - \tilde{\varepsilon_k} + \frac{i}{2\tau_k(\omega)}} \tag{96}$$

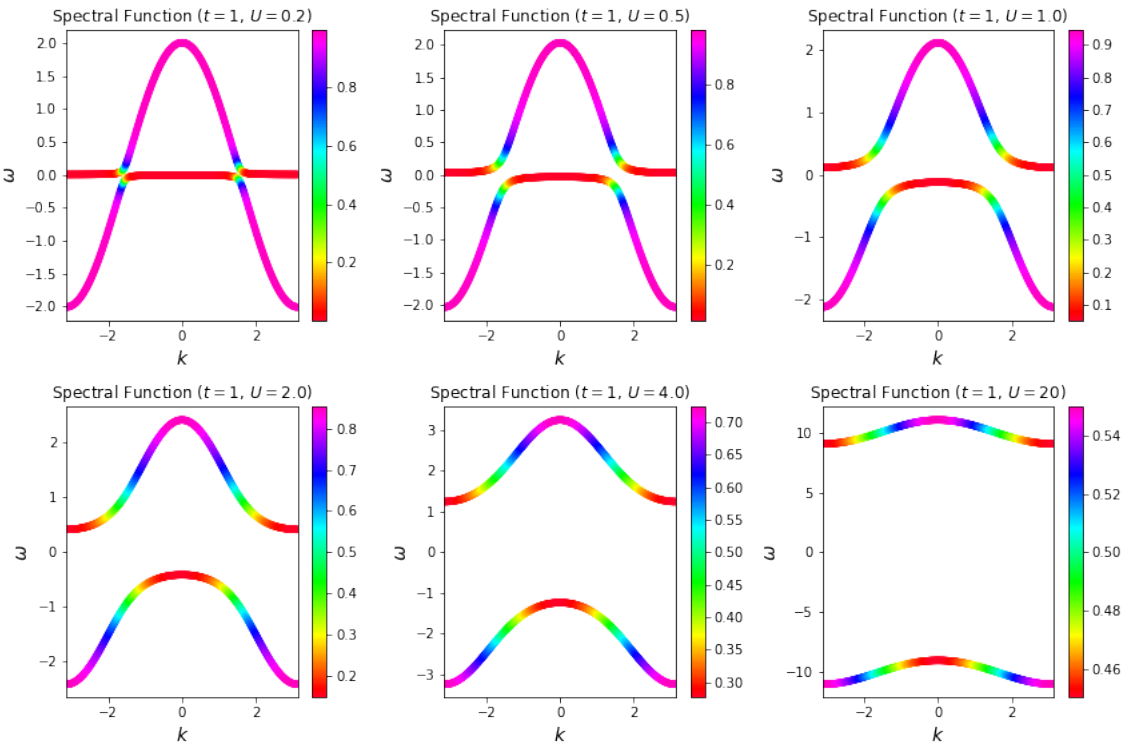

Figure 6: Spectral function of Hubbard-1 approximation 1D chain for different U values at fixed t. The color represents the weight of the peak at corresponding energy and momentum.

The coefficient C is related to the energy shift due to the real part of the self energy term, and Z_k is related to the quasi-particle weight.

The spectral function is given by

$$A(k, \sigma, \omega) = \frac{1}{\pi} \tilde{Z}_k \frac{\frac{1}{2\tau_k(\omega)}}{(\omega - \tilde{\varepsilon}_k)^2 + (\frac{1}{2\tau_k(\omega)})^2} \tag{97}$$

which is a Lorentzian. The width of the spectral function $\tau_k(\omega)$ gives the information about the lifetime of the quasi-particle, and the quasiparticle weight is given by $\tilde{Z}$.

Appendix A: Perturbation theory for non-degenerate time-independent systems

Consider a time-independent Hamiltonian $\hat{H}$ whose eigenfunctions are not degenerate. $\hat{H}$ can be written as the sum of two parts:

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{98}$$

where $\hat{H}_0$ is the system which can be solved,

$$\hat{H}_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle \tag{99}$$

$\hat{V}$ is the perturbation term.

The Schordinger equation can be written as

$$(\hat{H}_0 + \lambda\hat{V}) \left|n\right\rangle = E_n \left|n\right\rangle \tag{100}$$

where λ is a parameter that characterizes the strength of the perturbation. We know that E_n and $|n\rangle$ is a function of λ. When λ changes continuously from 0 to 1, the solution to the Schordinger equation changes from $E_n^{(0)}$, $\left|n^{(0)}\right\rangle$ to E_n and $|n\rangle$. Write $E_n = E_n^{(0)} + \Delta_n$ and the Schordinger equation can be rewritten as

$$(E_n^{(0)} - \hat{H}_0) \left|n\right\rangle = (\lambda\hat{V} - \Delta_n) \left|n\right\rangle \tag{101}$$

Projecting it on $\left|n^{(0)}\right\rangle$ we obtain

$$\left\langle n^{(0)}\right| (\lambda\hat{V} - \Delta_n) \left|n\right\rangle = 0 \tag{102}$$

which indicates that $(\lambda\hat{H}' - \Delta_n) \left|n\right\rangle$ does not contain information of the state $\left|n^{(0)}\right\rangle$. Define the projector operator $\hat{P}_n = \hat{1} - \left|n^{(0)}\right\rangle \left\langle n^{(0)}\right| = \sum_{k\neq n} \left|k^{(0)}\right\rangle \left\langle k^{(0)}\right|$, then Eq.(101) becomes

$$(E_n^{(0)} - \hat{H}_0) \left|n\right\rangle = \hat{P}_n(\lambda\hat{V} - \Delta_n) \left|n\right\rangle \tag{103}$$

Write the formal solution as

$$\left|n\right\rangle = \left|n^{(0)}\right\rangle + (E_n^{(0)} - \hat{H}_0)^{-1}\hat{P}_n(\lambda\hat{V} - \Delta_n) \left|n\right\rangle \tag{104}$$

One can check this satisfies Eq.(101).

Use the intermediate normalization

$$\left\langle n^{(0)}|n\right\rangle = 1 \tag{105}$$

from Eq.(102) we obtain

$$\Delta_n = \lambda \left\langle n^{(0)}|\hat{V}|n\right\rangle \tag{106}$$

Eq.(104) and Eq.(106) are the formal solution of Eq.(101), which must be solved by iterations.

Write $|n\rangle = \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + ...$ and $\Delta_n = \lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + ...$ and substitute them into Eq.(106), we obtain

$$\lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + ... = \lambda \left\langle n^{(0)}\right| \hat{V}(\left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + ...) \tag{107}$$

Compare both sides and let the terms which are of the same order of λ be equal

$$\Delta_n^{(1)} = \left\langle n^{(0)}|\hat{V}|n^{(0)}\right\rangle \tag{108}$$

$$\begin{aligned} &\Delta_n^{(2)} = \left\langle n^{(0)}|\hat{V}|n^{(1)}\right\rangle \\ &... \\ &\Delta_n^{(N)} = \left\langle n^{(0)}|\hat{V}|n^{(N-1)}\right\rangle \end{aligned} \tag{109}$$

These are energy correction terms of order 1 to N.

Similarly, substitute the expansion expression into Eq.(104), we obtain

$$\begin{aligned} \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + ... = \left|n^{(0)}\right\rangle + (E_n^{(0)} - \hat{H}_0)^{-1}\hat{P}_n(\lambda\hat{V} - \lambda\Delta_n^{(1)} - \lambda^2\Delta_n^{(2)} - ...) \\ \times (\left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + ...) \end{aligned} \tag{110}$$

Compare both sides and let the terms which are of the same order of λ be equal. The first order wavefunction correction is

$$\left|n^{(1)}\right\rangle = (E_n^{(0)} - \hat{H}_0)^{-1}\hat{P}_n\hat{V} \left|n^{(0)}\right\rangle \tag{111}$$

The second order wavefunction correction is

$$\left|n^{(2)}\right\rangle = (E_n^{(0)} - \hat{H}_0)^{-1}\hat{P}_n(\hat{V} - \Delta_n^{(1)}) \left|n^{(1)}\right\rangle \tag{112}$$

The rest can be written similarly and will not be shown here.

Note that the N^{th} order energy correction $\Delta_n^{(N)}$ requires the information of $\left|n^{(N-1)}\right\rangle$ and that the N^{th} order wavefunction correction requires the information of $\Delta_n^{(N-1)}$.