Topology in condensed matter physics
Exercise sheet 9

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9.1 Spectrum and Diagonalization of the Su-Schrieffer-Heeger (SSH) Model

The Su-Schrieffer-Heeger (SSH) model is a fundamental (toy) model for a one-dimensional topological insulator. The SSH chain consists of N unit cells, here with periodic boundary conditions, each containing two sites A and B

$$\mathcal{H} = \sum_{j=1}^{N} \left(v\, c_{j,A}^{\dagger} c_{j,B} + w\, c_{j+1,A}^{\dagger} c_{j,B} + \text{h.c.} \right), \tag{1}$$

where $v > 0$ describes the real intracell hopping, $w > 0$ the real intercell hopping, and $c_{j,\alpha}^{\dagger}$ creates a fermion on sublattice $\alpha \in \{A, B\}$ of the j^{th} site.

a. (3 points) Use the Fourier transform of the operators

$$c_{j,\alpha} = \frac{1}{\sqrt{N}} \sum_{k} e^{\mathrm{i}kj} c_{k,\alpha}, \tag{2}$$

where $k = \frac{2\pi m}{N}$ with $m \in \{0, 1, \ldots, N-1\}$ to show that the Hamiltonian can be written as

$$\mathcal{H} = \sum_{k} \Psi_k^{\dagger} H(k) \Psi_k, \tag{3}$$

where $\Psi_k = \begin{pmatrix} c_{k,A} \\ c_{k,B} \end{pmatrix}$ is a two-component spinor, and identify the 2×2 momentum space Hamiltonian $H(k)$.

Solution: By substituting the Fourier representation of the operators into the Hamiltonian, we find:

$$\mathcal{H} = \sum_{j=1}^{N} \Big(v\, c_{j,A}^\dagger c_{j,B} + w\, c_{j+1,A}^\dagger c_{j,B} + v\, c_{j,B}^\dagger c_{j,A} + w\, c_{j,B}^\dagger c_{j+1,A} \Big) \tag{4}$$

$$\Bigg| \quad c_{j,\alpha} = \frac{1}{\sqrt{N}} \sum_k e^{\mathrm{i}kj} c_{k,\alpha}, \quad c_{j,\alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-\mathrm{i}kj} c_{k,\alpha}^\dagger \tag{5}$$

$$= \frac{1}{N} \sum_{k,k'} \sum_{j=1}^{N} \Big[v e^{-\mathrm{i}kj} e^{\mathrm{i}k'j} c_{k,A}^\dagger c_{k',B} + w e^{-\mathrm{i}k(j+1)} e^{\mathrm{i}k'j} c_{k,A}^\dagger c_{k',B} + \text{h.c.} \Big] \tag{6}$$

$$\Bigg| \quad \sum_{j=1}^{N} e^{\mathrm{i}(k'-k)j} = N \delta_{k,k'} \tag{7}$$

$$= \sum_k \Big[\big(v + w e^{-\mathrm{i}k}\big)\, c_{k,A}^\dagger c_{k,B} + \big(v + w e^{\mathrm{i}k}\big)\, c_{k,B}^\dagger c_{k,A} \Big] \tag{8}$$

$$\Bigg| \quad \Psi_k = \begin{pmatrix} c_{k,A} \\ c_{k,B} \end{pmatrix}, \quad \Psi_k^\dagger = \begin{pmatrix} c_{k,A}^\dagger & c_{k,B}^\dagger \end{pmatrix} \tag{9}$$

$$\underline{\underline{= \sum_k \Psi_k^\dagger \begin{pmatrix} 0 & v + w e^{-\mathrm{i}k} \\ v + w e^{\mathrm{i}k} & 0 \end{pmatrix} \Psi_k}} \tag{10}$$

Thus, the bulk Hamiltonian in momentum space is:

$$\underline{\underline{H(k) = \begin{pmatrix} 0 & v + w e^{-\mathrm{i}k} \\ v + w e^{\mathrm{i}k} & 0 \end{pmatrix}}} \tag{11}$$

b. (3 points) Decompose the bulk Hamiltonian $H(k)$ in terms of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12}$$

such that $H(k) = d_0(k) I + \vec{d}(k) \cdot \vec{\sigma}$. Find the coefficients $d_0(k)$, $d_x(k)$, $d_y(k)$, and $d_z(k)$. Show that the energy dispersion relation is $E_\pm(k) = \pm|\vec{d}(k)|$ and determine under which parameters and at which momentum k the band gap closes.

Solution: We write $H(k) = d_0(k)I + d_x(k)\sigma_x + d_y(k)\sigma_y + d_z(k)\sigma_z$:

$$H(k) = \begin{pmatrix} d_0(k) + d_z(k) & d_x(k) - \mathrm{i}d_y(k) \\ d_x(k) + \mathrm{i}d_y(k) & d_0(k) - d_z(k) \end{pmatrix} \tag{13}$$

Comparing this with $H(k)$ from part (a), we identify:

$$d_x(k) - \mathrm{i}d_y(k) = v + w e^{-\mathrm{i}k} = v + w\cos(k) - \mathrm{i}w\sin(k) \tag{14}$$

$$d_x(k) + \mathrm{i}d_y(k) = v + w e^{\mathrm{i}k} = v + w\cos(k) + \mathrm{i}w\sin(k) \tag{15}$$

Thus, we find:

$$\underline{\underline{d_0(k) = 0, \quad d_x(k) = v + w\cos(k), \quad d_y(k) = w\sin(k), \quad d_z(k) = 0}} \tag{16}$$

The eigenvalues of a general 2×2 matrix of the form $\vec{d} \cdot \vec{\sigma}$ are given by:

$$E_\pm(k) = \pm|\vec{d}(k)| = \pm\sqrt{d_x(k)^2 + d_y(k)^2 + d_z(k)^2} \tag{17}$$

$$= \pm\sqrt{(v + w\cos k)^2 + w^2 \sin^2 k} \tag{18}$$

$$\underline{\underline{= \pm\sqrt{v^2 + w^2 + 2vw\cos(k)}}} \tag{19}$$

The band gap $E_g(k) = E_+(k) - E_-(k) = 2|\vec{d}(k)|$ closes if and only if $E_\pm(k) = 0$, which requires:

$$v^2 + w^2 + 2vw\cos(k) = 0 \tag{20}$$

Since $v, w > 0$, the minimum value of this expression occurs when $\cos(k) = -1$, which corresponds to the Brillouin zone boundary $\underline{\underline{k = \pm\pi}}$. At this point:

$$v^2 + w^2 - 2vw = (v - w)^2 = 0 \implies \underline{\underline{v = w}} \tag{21}$$

Thus, the energy gap closes at $\underline{\underline{k = \pm\pi}}$ at the transition point $\underline{\underline{v = w}}$ between two distinct phases.

9.2 Topology, Vector Visualization, and the Winding Number

Because $d_z(k) = 0$, the vector $\vec{d}(k) = (d_x(k), d_y(k), d_z(k))$ lies in the xy plane. As the momentum k varies continuously across the Brillouin zone $k \in [-\pi, \pi]$, the vector $\vec{d}(k)$ traces a closed curve in this plane.

a. (2 points) Describe the geometric shape of the curve traced by $\vec{d}(k) = (d_x(k), d_y(k))$ in the xy plane. Show how the trajectory behaves for the two phases: (i) $v > w > 0$ and (ii) $w > v > 0$. Geometrically argue whether the origin $(0, 0)$ is enclosed by this curve.

Solution: The trajectory of the vector is parameterized by:

$$d_x(k) = v + w\cos(k), \quad d_y(k) = w\sin(k) \tag{22}$$

This can be rewritten by eliminating k:

$$(d_x(k) - v)^2 + d_y(k)^2 = w^2\cos^2(k) + w^2\sin^2(k) = w^2 \tag{23}$$

This is the algebraic equation for a **circle** of radius w centered at the point $(v, 0)$ in the d_x–d_y plane.

- **Case (i)** $v > w > 0$ **(Trivial Phase):** Since the radius of the circle w is smaller than the distance v of its center from the origin, the entire circle lies to the right of the vertical axis $d_x = 0$. Consequently, the trajectory **does not enclose the origin** $(0, 0)$.
- **Case (ii)** $w > v > 0$ **(Topological Phase):** Here, the radius w is larger than the distance v of the center from the origin. Therefore, the circle crosses the d_y axis and **encloses the origin** $(0, 0)$ exactly once.

The phase transition occurs at $v = w$, where the circle passes directly through the origin. At this point, the Hamiltonian becomes gapped out only at other parts of the zone but is gapless at $k = \pm\pi$, rendering the winding number ill-defined.

b. (4 points) The topological invariant characterizing this one-dimensional system is the winding number ν. It measures the number of times the vector $\vec{d}(k)$ wraps around the origin as k sweeps through the Brillouin zone:

$$\nu = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{d_x(k)\frac{d}{dk}d_y(k) - d_y(k)\frac{d}{dk}d_x(k)}{d_x(k)^2 + d_y(k)^2} dk \tag{24}$$

By defining a complex number $z(k) = d_x(k) + \mathrm{i}d_y(k)$, show that Eq. (24) can be written in the form

$$\nu = \frac{1}{2\pi \mathrm{i}}\int_{-\pi}^{\pi} \frac{1}{z(k)}\frac{dz(k)}{dk} dk \tag{25}$$

Solution: Let $z(k) = d_x(k) + \mathrm{i}d_y(k)$. The derivative of $z(k)$ with respect to k is:

$$\frac{dz}{dk} = \frac{dd_x}{dk} + \mathrm{i}\frac{dd_y}{dk} \tag{26}$$

We evaluate the integrand $\frac{1}{z}\frac{dz}{dk}$:

$$\frac{1}{z}\frac{dz}{dk} = \frac{1}{d_x + \mathrm{i}d_y}\left(\frac{dd_x}{dk} + \mathrm{i}\frac{dd_y}{dk}\right) \tag{27}$$

$$\left| \quad \frac{1}{d_x + \mathrm{i}d_y} = \frac{d_x - \mathrm{i}d_y}{d_x^2 + d_y^2} \right. \tag{28}$$

$$= \frac{d_x - \mathrm{i}d_y}{d_x^2 + d_y^2}\left(\frac{dd_x}{dk} + \mathrm{i}\frac{dd_y}{dk}\right) \tag{29}$$

$$= \frac{\left(d_x\frac{dd_x}{dk} + d_y\frac{dd_y}{dk}\right) + \mathrm{i}\left(d_x\frac{dd_y}{dk} - d_y\frac{dd_x}{dk}\right)}{d_x^2 + d_y^2} \tag{30}$$

Dividing this by i (which is equivalent to multiplying by $-\mathrm{i}$) yields:

$$\frac{1}{\mathrm{i}}\frac{1}{z}\frac{dz}{dk} = \frac{d_x\frac{dd_y}{dk} - d_y\frac{dd_x}{dk}}{d_x^2 + d_y^2} - \mathrm{i}\frac{d_x\frac{dd_x}{dk} + d_y\frac{dd_y}{dk}}{d_x^2 + d_y^2} \tag{31}$$

Now we integrate this expression over the Brillouin zone $k \in [-\pi, \pi]$:

$$\frac{1}{2\pi \mathrm{i}}\int_{-\pi}^{\pi} \frac{1}{z(k)}\frac{dz(k)}{dk} dk = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{d_x\frac{dd_y}{dk} - d_y\frac{dd_x}{dk}}{d_x^2 + d_y^2} dk - \frac{\mathrm{i}}{4\pi}\int_{-\pi}^{\pi} \frac{d}{dk}\ln\left(d_x^2 + d_y^2\right) dk \tag{32}$$

The second term is the integral of a total derivative of a periodic, non-vanishing function (since the system is gapped, $d_x^2 + d_y^2 = E(k)^2 > 0$ for all k). Thus, it vanishes:

$$\int_{-\pi}^{\pi} \frac{d}{dk}\ln\left(d_x^2 + d_y^2\right) dk = \ln\left[E(\pi)^2\right] - \ln\left[E(-\pi)^2\right] = 0 \tag{33}$$

Therefore, we are left only with the real part:

$$\underline{\underline{\frac{1}{2\pi \mathrm{i}}\int_{-\pi}^{\pi} \frac{1}{z(k)}\frac{dz(k)}{dk} dk = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{d_x\frac{dd_y}{dk} - d_y\frac{dd_x}{dk}}{d_x^2 + d_y^2} dk = \nu}} \tag{34}$$

c. (4 points) Evaluate the winding number ν analytically for the two phases

(i) $v > w > 0$

(ii) $w > v > 0$

Hint: Write $z(k)$ in a form where you can pull out the dominant amplitude and use the expansion $\ln(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} x^n$ *for* $|x| < 1$.

Solution: For the SSH model, we have $z(k) = v + we^{\mathrm{i}k}$. Let us compute the winding number using the logarithmic derivative form $\nu = \frac{1}{2\pi\mathrm{i}} \int_{-\pi}^{\pi} \frac{d}{dk} [\ln z(k)]\, dk$.

- **Case (i)** $v > w > 0$**:** Since $w/v < 1$, we can pull out v:

$$z(k) = v\left(1 + \frac{w}{v} e^{\mathrm{i}k}\right) \tag{35}$$

$$\ln z(k) = \ln(v) + \ln\left(1 + \frac{w}{v} e^{\mathrm{i}k}\right) \tag{36}$$

$$\ln(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} x^n \text{ for } |x| < 1 \tag{37}$$

$$= \ln(v) + \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \left(\frac{w}{v}\right)^n e^{\mathrm{i}nk} \tag{38}$$

Now we take the derivative with respect to k:

$$\frac{d}{dk} [\ln z(k)] = \sum_{n=1}^{\infty} \mathrm{i}(-1)^{n-1} \left(\frac{w}{v}\right)^n e^{\mathrm{i}nk} \tag{39}$$

Integrating this expression over $k \in [-\pi, \pi]$:

$$\nu = \frac{1}{2\pi\mathrm{i}} \int_{-\pi}^{\pi} \sum_{n=1}^{\infty} \mathrm{i}(-1)^{n-1} \left(\frac{w}{v}\right)^n e^{\mathrm{i}nk} dk \tag{40}$$

$$= \frac{1}{2\pi} \sum_{n=1}^{\infty} (-1)^{n-1} \left(\frac{w}{v}\right)^n \underbrace{\int_{-\pi}^{\pi} e^{\mathrm{i}nk} dk}_{=0 \text{ for all } n \geq 1} \tag{41}$$

$$\underline{\underline{= 0}} \tag{42}$$

- **Case (ii)** $w > v > 0$**:** Since $v/w < 1$, we pull out the dominant term $we^{\mathrm{i}k}$:

$$z(k) = we^{\mathrm{i}k}\left(1 + \frac{v}{w} e^{-\mathrm{i}k}\right) \tag{43}$$

$$\ln z(k) = \ln(w) + \mathrm{i}k + \ln\left(1 + \frac{v}{w} e^{-\mathrm{i}k}\right) \tag{44}$$

$$= \ln(w) + \mathrm{i}k + \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \left(\frac{v}{w}\right)^n e^{-\mathrm{i}nk} \tag{45}$$

Taking the derivative with respect to k:

$$\frac{d}{dk} [\ln z(k)] = \mathrm{i} + \sum_{n=1}^{\infty} \mathrm{i}(-1)^n \left(\frac{v}{w}\right)^n e^{-\mathrm{i}nk} \tag{46}$$

Integrating this over $k \in [-\pi, \pi]$:

$$\nu = \frac{1}{2\pi \mathrm{i}} \int_{-\pi}^{\pi} \left(\mathrm{i} + \sum_{n=1}^{\infty} \mathrm{i}(-1)^n \left(\frac{v}{w}\right)^n e^{-\mathrm{i}nk} \right) dk \tag{47}$$

$$= \frac{1}{2\pi \mathrm{i}} \int_{-\pi}^{\pi} \mathrm{i}\, dk + \frac{1}{2\pi} \sum_{n=1}^{\infty} (-1)^n \left(\frac{v}{w}\right)^n \underbrace{\int_{-\pi}^{\pi} e^{-\mathrm{i}nk} dk}_{=0 \text{ for all } n \geq 1} \tag{48}$$

$$= \frac{1}{2\pi \mathrm{i}} (\mathrm{i} \cdot 2\pi) \tag{49}$$

$$\underline{\underline{= 1}} \tag{50}$$

Thus, we analytically prove that the topological invariant ν is a step function of the hopping parameters:

$$\nu = \begin{cases} 0 & \text{for } v > w \quad \text{(Trivial phase)} \\ 1 & \text{for } v < w \quad \text{(Topological phase)} \end{cases} \tag{51}$$

End