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9. 1. 25

Discussion of the exercises

1)

$$\hat{P}_n(t)\,\hat{P}_m(t) = \delta_{nm}\,\hat{P}_n(t) \qquad (1)$$

$$\hat{P}_n(t) = |u_n(t)\rangle\langle u_n(t)| \qquad (2)$$

$$\hat{P}_n(t) = \sum_{s=1}^{m} |u_{(ns)}(t)\rangle\langle u_{(ns)}(t)| \qquad (3)$$

Excercise:

(1) Show that the $\hat{P}_n$ defined in (2) and (3) satisfy (1).

- $$\hat{P}_n\hat{P}_m = |u_n\rangle\underbrace{\langle u_n|u_m\rangle}_{=\delta_{nm}}\langle u_m| = \delta_{nm}\,|u_n\rangle\langle u_n| = \delta_{nm}\,\hat{P}_n$$

- $$\hat{P}_n\hat{P}_m = \sum_{s,s'} |u_{(ns)}\rangle\underbrace{\langle u_{(ns)}|u_{(ms')}\rangle}_{=\delta_{nm}\delta_{ss'}}\langle u_{(ms')}| = \delta_{nm}\sum_s |u_{(ns)}\rangle\langle u_{(ns)}| = \delta_{nm}\,\hat{P}_n$$

(2) Show that $\hat{P}_n$ in (3) is $U(m)$-gauge invariant using

$$|u_{(ns)}(t)\rangle \longrightarrow \sum_{s'} U_{ss'}(t)\,|u_{(ns')}(t)\rangle .$$

- $U \equiv (U_{ss'}) \in U(n)$

$$\longrightarrow \quad U^\dagger \equiv (U^\dagger_{ss'}) = (\overline{U_{s's}})$$

$$\longrightarrow \quad U^\dagger U = \left(\sum_{s'} U^\dagger_{ss'} U_{s's''}\right) = \mathbb{1}$$

$$\longrightarrow \quad \sum_{s'} \overline{U_{s's}} \, U_{s's''} = \delta_{ss''}$$

- $\langle u_{(ns)}| = \left(|u_{(ns)}\rangle\right)^\dagger$

$$\longrightarrow \quad \left(\sum_{s'} U_{ss'} \, |u_{(ns')}\rangle\right)^\dagger$$

$$= \sum_{s'} \overline{U_{ss'}} \, \langle u_{(ns')}|$$

- $\hat{P}_n = \sum_s |u_{(ns)}\rangle\langle u_{(ns)}|$

$$\longrightarrow \quad \sum_s \sum_{s_1 s_2} U_{ss_1} \, |u_{(ns_1)}\rangle\langle u_{(ns_2)}| \, \overline{U_{ss_2}}$$

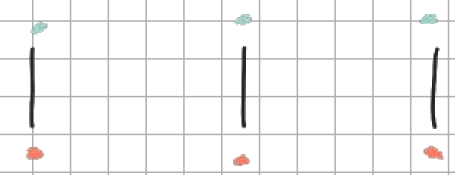
$$= \sum_{s_1 s_2} \delta_{s_1 s_2} \, |u_{(ns_1)}\rangle\langle u_{(ns_2)}|$$

$$= \sum_s |u_{(ns)}\rangle\langle u_{(ns)}|$$

2)

Q: What are the three extreme limits of the SSH model? What are the underlying physical scenarios? How do the eigenstates behave in these cases?

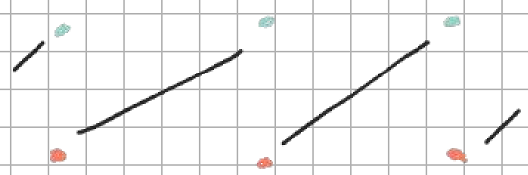
1)



$t = 0$: onsite dimers

$$|u_\pm(k)\rangle = 1/\sqrt{2} \begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$$

2)



$t' = 0$: dimer between different unit cells

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

3)

$t = t'$: simple chain with artifically doubled unit cell

3)

$$\hat{H}(k) = d_0(k) + d(k)\cdot\sigma \qquad (4)$$

$$\hat{P}_\pm(k) = 1/2\,(\mathbb{1}_2 \pm n(k)\cdot\sigma) \qquad (5)$$

Exercise: Prove that (5) is an orthonormal projector and eigenfunction of (4).

- $$\hat{P}_s\,\hat{P}_{s'} = 1/4\,(\mathbb{1}_2 + s\,n\cdot\sigma)(\mathbb{1}_2 + s'\,n\cdot\sigma)$$

$$= 1/4\,\mathbb{1}_2$$

$$+ 1/4\,(s+s')\,n\cdot\sigma$$

$$+ 1/4\,ss'\,\underbrace{(n\cdot\sigma)(n\cdot\sigma)}_{= \underbrace{n\cdot n}_{=1}\mathbb{1}_2 + i\underbrace{(n\times n)}_{=0}\cdot\sigma}$$

$$= 1/4\,(1+ss')\,\mathbb{1}_2 + 1/4\,(s+s')\,n\cdot\sigma$$

$$\longrightarrow\; P_+P_+ = 1/2\,\mathbb{1}_2 + 1/2\,n\cdot\sigma = P_+$$

$$P_-P_- = 1/2\,\mathbb{1}_2 - 1/2\,n\cdot\sigma = P_-$$

$$P_+P_- = 0$$

- $$\hat{H}\hat{P}_\pm = (d_0 + d\cdot\sigma)\,1/2\,\left(1 \pm \frac{d}{|d|}\cdot\sigma\right)$$

$$= d_0\,1/2\,\left(1 \pm \frac{d}{|d|}\cdot\sigma\right)$$

$$+ \tfrac{1}{2}\, d \cdot \sigma$$

$$\pm \tfrac{1}{2} \frac{1}{|d|} \underbrace{(d \cdot \sigma)(d \cdot \sigma)}$$

$$= |d|^2 \mathbb{1} + i \underbrace{(d \times d)}_{=0} \cdot \sigma$$

$$= d_0 \; \tfrac{1}{2} \left(1 \pm \frac{d}{|d|} \cdot \sigma \right)$$

$$\pm |d| \; \tfrac{1}{2} \left(1 \pm \frac{d}{|d|} \cdot \sigma \right)$$

$$= E_\pm \hat{P}_\pm \quad \text{with} \quad E_\pm = d_0 \pm |d|$$

4) Excercise: Show that the two- and three-point functions are sufficient to capture all n-point functions constructed from projectors of non-degenerate bands. For this, first show

$$\mathrm{tr}[P_1 P_2 P_3 P_4]\,\mathrm{tr}[P_3 P_1] = \mathrm{tr}[P_1 P_2 P_3]\,\mathrm{tr}[P_3 P_4 P_1]$$

for $P_i = |u(k_i)\rangle\langle u(k_i)|$.

- $P_i \equiv |i\rangle\langle i|$

$$\rightarrow \mathrm{tr}[P_1 P_2 P_3 P_4]\,\mathrm{tr}[P_3 P_1]$$

$$= \langle 1|2\rangle\langle 2|3\rangle\langle 3|4\rangle\langle 4|1\rangle\langle 3|1\rangle\langle 1|3\rangle$$

1 2 3 4 5 6

$$\mathrm{tr}[P_1 P_2 P_3]\,\mathrm{tr}[P_3 P_4 P_1]$$

$$= \langle 1|2\rangle\langle 2|3\rangle\langle 3|1\rangle\langle 3|4\rangle\langle 4|1\rangle\langle 1|3\rangle$$

1 2 5 3 4 6

- Same proof for general case

$$\mathrm{tr}[P_1 P_2 \ldots P_{k-1} P_k P_{k+1} \ldots P_n]$$

$$= \mathrm{tr}[P_1 P_2 \ldots P_{k-1} P_{k+1} \ldots P_n]\,\frac{\mathrm{tr}[P_{k-1} P_k P_{k+1}]}{\mathrm{tr}[P_{k-1} P_{k+1}]}$$

- apply this formula several times

5)

Ex: In anticipation of the discussion of optical responses, we define

$$e^{mn}_\alpha(k) = i P_m(k)\, \partial_\alpha P_n(k) P_n(k)$$

with band indices n, m.

(1) Show that $e^{nn}(k) = 0$.

(2) Show that $(e^{mn}_\alpha)^+ = e^{nm}_\alpha$.

(3) Show that

$$A^k_\alpha(k) = -\tfrac{1}{2} \sum_{n,m} \left(e^{mn}_\alpha(k) + e^{nm}_\alpha(k) \right)$$

- $$\begin{aligned} e^{nn}_\alpha &= i P_n \partial_\alpha P_n P_n \\ &= i P_n \partial_\alpha P_n^2 P_n \\ &= i P_n (\partial_\alpha P_n P_n + P_n \partial_\alpha P_n) P_n \\ &= i P_n \partial_\alpha P_n P_n + i P_n \partial_\alpha P_n P_n \\ &= 2 e^{nn}_\alpha \end{aligned}$$

$$\longrightarrow e^{nn}_\alpha = 0$$

- $$\begin{aligned} (e^{mn}_\alpha)^+ &= (i P_m \partial_\alpha P_n P_n)^+ \\ &= -i P_n^+ \partial_\alpha P_n^+ P_m^+ \\ &= -i P_n \partial_\alpha P_n P_m \\ &= -i P_n (\partial_\alpha P_n P_m) P_m \end{aligned}$$

$$= -i P_n \left(\partial_\alpha (\underbrace{P_n P_m}_{= \delta_{nm} P_n \to 0}) - P_n \partial_\alpha P_m \right) P_m$$

$$= i P_n \partial_\alpha P_m P_m = e_\alpha^{nm}$$

$$\cdot \; -1/2 \sum_{n,m} \left(e_\alpha^{mn} + e_\alpha^{nm} \right)$$

$$= -i/2 \sum_{n,m} \left(P_m \partial_\alpha P_n P_n + P_n \partial_\alpha P_m P_m \right)$$

$$= -i/2 \sum_n \left(\underbrace{\partial_\alpha P_n P_n}_{= \underbrace{\partial_\alpha P_n}_{\to \partial_\alpha 1 = 0} - P_n \partial_\alpha P_n} + \partial_\alpha P_n P_n \right)$$

$$= i/2 \sum_n \left[P_n , \partial_\alpha P_n \right] = A_\alpha^K$$

6)

Ex: Show that

$$\mathrm{tr}\left[P \partial_\alpha \partial_\beta P\right] = -\mathrm{tr}\left[\partial_\alpha P \partial_\beta P\right]$$

via the projector identity for $\partial_\alpha \partial_\beta P$.

$$\begin{aligned}\partial_\alpha \partial_\beta P &= \partial_\alpha \partial_\beta P^2 \\ &= \partial_\alpha \partial_\beta P \, P + \partial_\alpha P \partial_\beta P \\ &\quad + \partial_\beta P \partial_\alpha P + P \partial_\alpha \partial_\beta P\end{aligned}$$

$$\xrightarrow{\mathrm{tr}} \underbrace{\partial_\alpha \partial_\beta \, \mathrm{tr}\, P}_{=0} = 2\, \mathrm{tr}\left[\partial_\alpha \partial_\beta P \, P\right] + 2\, \mathrm{tr}\left[\partial_\alpha P \, \partial_\beta P\right]$$

7)

The metric is the only quantity with trace, single-band, two derivatives, symmetric, and local.

Ex: (1) Show that by explicit construction.

- 1) $c\, tr[\partial_\alpha P \partial_\beta P] = 2c\, g_{\alpha\beta}$

2) $tr[P \partial_\alpha P \partial_\beta P] + tr[P \partial_\beta P \partial_\alpha P]$

$= tr[(P\partial_\alpha P + \partial_\alpha P P)\partial_\beta P]$

$= tr[\partial_\alpha P \partial_\beta P] = 2 g_{\alpha\beta}$

3) $tr[\partial_\alpha P P \partial_\beta P] = tr[P \partial_\beta P \partial_\alpha P]$

$\longrightarrow g_{\beta\alpha}$

4) $tr[P^n \partial_\alpha P \partial_\beta P] = tr[P \partial_\alpha P \partial_\beta P]$

5) $tr[\partial_\alpha \partial_\beta P] = \partial_\alpha \partial_\beta\, tr P = 0$

6) $tr[P \partial_\alpha \partial_\beta P] = -\, tr[\partial_\alpha P \partial_\beta P] = -2 g_{\alpha\beta}$

(2) Show that $tr[A^k_\alpha(t) A^k_\beta(t)] = \sum_n g^n_{\alpha\beta}(t)$

for arbitrary number of bands. For this, first show

$\sum_m tr[e^{nm}_\alpha e^{mn}_\beta] = tr[P_n \partial_\alpha P_n \partial_\beta P_n]$.

$$\cdot \ \sum_m \mathrm{tr}\left[e_\alpha^{nm} e_\beta^{mn} \right]$$

$$= - \sum_m \mathrm{tr}\left[P_n \, \partial_\alpha P_m \, P_m \, P_m \, \partial_\beta P_n \, P_n \right]$$

$$= - \sum_m \mathrm{tr}\left[P_n \, \underbrace{\partial_\alpha P_m \, P_m}_{\substack{= \partial_\alpha P_m - P_m \partial_\alpha P_m \\ \longrightarrow 0}} \, \partial_\beta P_n \right]$$

$$= \sum_m \mathrm{tr}\left[\underbrace{P_n P_m}_{= \delta_{nm} P_n} \, \partial_\alpha P_m \, \partial_\beta P_n \right]$$

$$= \mathrm{tr}\left[P_n \, \partial_\alpha P_n \, \partial_\beta P_n \right]$$

$$\cdot \ \mathrm{tr}\left[A_\alpha^k \, A_\beta^k \right]$$

$$= 1/4 \sum_{\substack{n_1 m_1 \\ n_2 m_2}} \mathrm{tr}\left[\left(e_\alpha^{m_1 n_1} + e_\alpha^{n_1 m_1} \right) \left(e_\beta^{m_2 n_2} + e_\beta^{n_2 m_2} \right) \right]$$

$$= 1/4 \sum_{\substack{n_1 m_1 \\ n_2 m_2}} \mathrm{tr}\left[e_\alpha^{m_1 n_1} e_\beta^{m_2 n_2} \right] \ \delta_{\underset{n}{m_1 n_2}} \delta_{\underset{m}{n_1 m_2}}$$

$$+ \mathrm{tr}\left[e_\alpha^{m_1 n_1} e_\beta^{n_2 m_2} \right] \ \delta_{\underset{m}{m_1 m_2}} \delta_{\underset{n}{n_1 n_2}}$$

$$+ \mathrm{tr}\left[e_\alpha^{n_1 m_1} e_\beta^{m_2 n_2} \right] \ \delta_{\underset{n}{n_1 n_2}} \delta_{\underset{m}{m_1 m_2}}$$

$$+ \mathrm{tr}\left[e_\alpha^{n_1 m_1} e_\beta^{n_2 m_2} \right] \ \delta_{\underset{m}{n_1 m_2}} \delta_{\underset{n}{m_1 n_2}}$$

$$= 1/4 \sum_{n,m} \mathrm{tr}\left[e_\alpha^{nm} e_\beta^{mn} \right]$$

$$+ \mathrm{tr}\left[e_\alpha^{mn} e_\beta^{nm} \right]$$

$$+\ \mathrm{tr}\left[e_\alpha^{nm}\, e_\beta^{mn}\right]$$

$$+\ \mathrm{tr}\left[e_\alpha^{mn}\, e_\beta^{nm}\right]$$

$$= \tfrac{1}{2} \sum_n \mathrm{tr}\left[P_n\, \partial_\alpha P_n\, \partial_\beta P_n\right] + (\alpha \leftrightarrow \beta)$$

$$= \sum_n g^n_{\alpha\beta}$$

8)

$$d(k) = \left(\cos(\varkappa k), \sin(\varkappa k), 0 \right)$$

Ex: (1) Construct the corresponding tight-binding Hamiltonian.

- $$H(k) = d \cdot \sigma = \begin{pmatrix} 0 & \cos \varkappa k - i \sin \varkappa k \\ \cos \varkappa k + i \sin \varkappa k & 0 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & e^{-i\varkappa k} \\ e^{i\varkappa k} & 0 \end{pmatrix}$$

- $$\hat{H} = \sum_k e^{-i\varkappa k} \, \hat{c}^+_{kA} \hat{c}_{kB} + h.c$$
$$= \sum_{j,j'} \underbrace{\frac{1}{N} \sum_k e^{-i\varkappa k} e^{ikR_j} e^{-ikR_{j'}}}_{= \delta_{j,j'+\varkappa}} \hat{c}^+_{jA} \hat{c}_{jB} + h.c.$$
$$= \sum_j \hat{c}^+_{j+\varkappa, A} \hat{c}_{j,B} + h.c.$$

(2) How can we physically interpret the corresponding quantum metric?

the metric $\varkappa^2/4$ corresponds to the variance of the dimer

9)

Ex: We exemplify the previous concepts for the SSH model setting $t' = 0$.

(1) Show that a Wannier function reads

$$|w_{j,\pm}\rangle = \frac{1}{\sqrt{2}}\left(\pm|j,A\rangle + |j+1,B\rangle\right).$$

- $$|v_\pm(k)\rangle = 1/\sqrt{2}\begin{pmatrix}\pm 1\\ e^{-ik}\end{pmatrix}$$

$$\longrightarrow \quad v_\pm^A = \pm 1/\sqrt{2} \qquad v_\pm^B = 1/\sqrt{2}\, e^{-ik}$$

- $$w_{R,R'}^{A,\pm} = \int_{BZ} e^{ik\cdot(R'-R)} v_\pm^A = \pm 1/\sqrt{2}\, \delta_{R,R'}$$

$$w_{R,R'}^{B,\pm} = \int_{BZ} e^{ik\cdot(R'-R)} v_\pm^B = 1/\sqrt{2}\, \delta_{R',R+1}$$

- $$|w_{j,\pm}\rangle = \sum_\alpha \sum_{R'} w_{R,R'}^{\alpha,\pm} |R',\alpha\rangle$$

$$= 1/\sqrt{2}\left(\pm|j,A\rangle + |j+1,B\rangle\right)$$

(2) Calculate $\langle\hat{x}\rangle \equiv \langle w_{j,\pm}|\hat{x}|w_{j,\pm}\rangle$ and $\langle\hat{x}^2\rangle \equiv \langle w_{j,\pm}|\hat{x}^2|w_{j,\pm}\rangle$ using

$$\hat{x} = \sum_j j\left(|j,A\rangle\langle j,A| + |j,B\rangle\langle j,B|\right)$$

and show that the results agree with the gauge-invariant contributions obtained via the Berry connection and quantum metric.

- $< w_{j,\pm} | \hat{x} | w_{j,\pm} >$

$$= 1/2 \left(\pm < j, A| + < j+1, B| \right)$$

$$\left[\sum_{j'} j' \left(|j', A><j', A| + |j', B><j', B| \right) \right]$$

$$\left(\pm |j, A> + |j+1, B> \right)$$

$$= 1/2 \left(j + j+1 \right) = j + 1/2$$

compared to

$$A^{\pm} = i < v_{\pm} | \partial_k v_{\pm} >$$

$$= i/2 \left(\pm 1 \quad e^{ik} \right) \begin{pmatrix} 0 \\ -i e^{-ik} \end{pmatrix}$$

$$= 1/2 \quad \longrightarrow \quad \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \, A^{\pm}(k) = 1/2$$

- $< w_{j,\pm} | \hat{x}^2 | w_{j,\pm} >$

$$= 1/2 \left(\pm < j, A| + < j+1, B| \right)$$

$$\left[\sum_{j'} j' \left(|j', A\rangle\langle j', A| + |j', B\rangle\langle j', B| \right) \right]^2$$

$$\left(\pm |j, A\rangle + |j+1, B\rangle \right)$$

$$= 1/2 \left(j^2 + (j+1)^2 \right)$$

$$= 1/2 \left(j^2 + j^2 + 2j + 1 \right)$$

$$= j^2 + j + 1/2$$

$$\longrightarrow \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$$

$$= j^2 + j + 1/2 - (j + 1/2)^2$$

$$= j^2 + j + 1/2 - j^2 - j - 1/4 = 1/4$$

compared to

$$1/2\pi \int_{-\pi}^{\pi} dk \, \underbrace{g(k)}_{= 1/4} = 1/4 .$$

10)

Ex: (1) Proof the relation between Berry curvature and connection by using $P_n = |u_n\rangle\langle u_n|$.

- $$\Omega^n_{\alpha\beta} = i\left(\mathrm{tr}\left[P_n\, \partial_\alpha P_n\, \partial_\beta P_n\right] - (\alpha \leftrightarrow \beta)\right)$$

$$= i\langle u_n|\, \partial_\alpha\left(|u_n\rangle\langle u_n|\right) \partial_\beta\left(|u_n\rangle\langle u_n|\right) |u_n\rangle - (\alpha \leftrightarrow \beta)$$

$$= i\langle u_n|\partial_\alpha u_n\rangle\langle u_n|\partial_\beta u_n\rangle\underbrace{\langle u_n|u_n\rangle}_{=0}$$
$$+ i\langle u_n|\partial_\alpha u_n\rangle\underbrace{\langle u_n|u_n\rangle}_{=1}\underbrace{\langle\partial_\beta u_n|u_n\rangle}_{=-\langle u_n|\partial_\beta u_n\rangle}$$
$$+ i\underbrace{\langle u_n|u_n\rangle}_{=1}\langle\partial_\alpha u_n|\partial_\beta u_n\rangle\underbrace{\langle u_n|u_n\rangle}_{=1}$$
$$+ i\underbrace{\langle u_n|u_n\rangle}_{=1}\langle\partial_\alpha u_n|u_n\rangle\langle\partial_\beta u_n|u_n\rangle$$
$$- (\alpha \leftrightarrow \beta)$$

$$= i\left(\langle\partial_\alpha u_n|\partial_\beta u_n\rangle - \langle\partial_\beta u_n|\partial_\alpha u_n\rangle\right)$$

- $$\partial_\alpha A^n_\beta - \partial_\beta A^n_\alpha$$

$$= i\,\partial_\alpha\langle u_n|\partial_\beta u_n\rangle - (\alpha \leftrightarrow \beta)$$

$$= i\langle\partial_\alpha u_n|\partial_\beta u_n\rangle + i\langle u_n|\partial_\alpha\partial_\beta u_n\rangle - (\alpha \leftrightarrow \beta)$$

$$= \Omega^n_{\alpha\beta}$$

(2) Show that the curl of Berry connection is indeed gauge invariant.

$$\partial_\alpha A^n_\beta - \partial_\beta A^n_\alpha$$

$$\longrightarrow \partial_\alpha \left(A^n_\beta - \partial_\beta \phi \right) - \partial_\beta \left(A^n_\alpha - \partial_\alpha \phi \right)$$

$$= \partial_\alpha A^n_\beta - \partial_\beta A^n_\alpha \underbrace{- \partial_\alpha \partial_\beta \phi + \partial_\beta \partial_\alpha \phi}_{=0}$$

(3) Show that the Berry curvature is additive in contrast to the quantum metric, e.g., $\Omega^{(12)}_{\alpha\beta} = \Omega^1_{\alpha\beta} + \Omega^2_{\alpha\beta}$ for $P_{(12)} = P_1 + P_2$.

$$\Omega^{(12)}_{\alpha\beta} = i \, \mathrm{tr} \left[(P_1 + P_2) \partial_\alpha (P_1 + P_2) \partial_\beta (P_1 + P_2) \right] - (\alpha \leftrightarrow \beta)$$

$$= i \, \mathrm{tr} \left[P_1 \partial_\alpha P_1 \partial_\beta P_1 \right]$$

$$+ i \, \mathrm{tr} \left[P_1 \partial_\alpha P_1 P_2 \partial_\beta P_2 \right] \longrightarrow -i \, \mathrm{tr} \left[(-e^{12}_\alpha)(-e^{21}_\beta) \right] \quad (1)$$

$$+ i \, \mathrm{tr} \left[P_1 \partial_\alpha P_2 P_2 \partial_\beta P_1 \right] \longrightarrow -i \, \mathrm{tr} \left[e^{12}_\alpha \; e^{21}_\beta \right] \quad (2)$$

$$+ i \, \mathrm{tr} \left[P_1 \partial_\alpha P_2 P_2 \partial_\beta P_2 \right] \longrightarrow -i \, \mathrm{tr} \left[e^{12}_\alpha \; (-e^{21}_\beta) \right] \quad (3)$$

$$+ i \, \mathrm{tr} \left[P_2 \partial_\alpha P_1 P_1 \partial_\beta P_1 \right] \longrightarrow -i \, \mathrm{tr} \left[e^{21}_\alpha \; (-e^{12}_\beta) \right] \quad (3)$$

$$+ i \, \mathrm{tr} \left[P_2 \partial_\alpha P_1 P_1 \partial_\beta P_2 \right] \longrightarrow -i \, \mathrm{tr} \left[e^{21}_\alpha \; e^{12}_\beta \right] \quad (2)$$

$$+ i \, \mathrm{tr} \left[P_2 \partial_\alpha P_2 P_1 \partial_\beta P_1 \right] \longrightarrow -i \, \mathrm{tr} \left[(-e^{21}_\alpha)(-e^{12}_\beta) \right] \quad (1)$$

$$+ i \, \mathrm{tr} \left[P_2 \partial_\alpha P_2 \partial_\beta P_2 \right]$$

$$- (\alpha \leftrightarrow \beta) = 0$$

(4) Show that $\Omega^{+}_{\alpha\beta} = - \Omega^{-}_{\alpha\beta}$ for a two-band model.

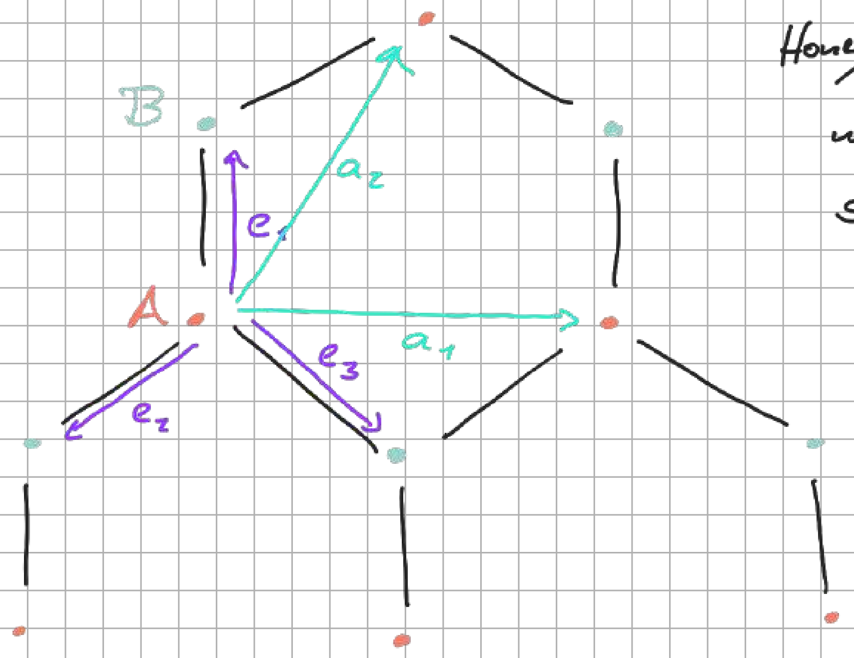
$$\Omega^{+}_{\alpha\beta} = i \,\mathrm{tr}\left[P_+ \partial_\alpha P_+ \partial_\beta P_+ \right] - (\alpha \leftrightarrow \beta)$$

$$= i \,\mathrm{tr}\left[(1 - P_-) \partial_\alpha (1 - P_-) \partial_\beta (1 - P_-) \right] - (\alpha \leftrightarrow \beta)$$

$$= i \,\mathrm{tr}\left[\partial_\alpha P_- \partial_\beta P_- \right] - i \,\mathrm{tr}\left[P_- \partial_\alpha P_- \partial_\beta P_- \right] - (\alpha \leftrightarrow \beta)$$

$$= - \Omega^{-}_{\alpha\beta}$$

11)



Honeycomb lattice with A and B sites

Ex: (1) Construct tight-binding Hamiltonian including equal hopping in e_i directions and show that linear band crossings occur at K and K'.

- $$\hat{H} = \sum_R \sum_{i=1}^{3} \hat{c}^+_{R+e_i B} \hat{c}_{RA} + h.c.$$

$$= \sum_k \sum_{i=1}^{3} e^{-ik\cdot e_1} \hat{c}^+_{kB} \hat{c}_{kA} + h.c$$

$$\longrightarrow \hat{H}(k) = \begin{array}{cc} A & B \\ \left(\begin{array}{cc} 0 & \sum_{i=1}^{3} e^{ik\cdot e_1} \\ \sum_{i=1}^{3} e^{-ik\cdot e_1} & 0 \end{array}\right) & \begin{array}{c} A \\ B \end{array} \end{array}$$

with

$$e_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad e_2 = \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ -1/2 \end{pmatrix} \quad e_3 = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -1/2 \end{pmatrix}$$

- Diagonalizing $\hat{H}(k)$ leads to

$$E_\pm(k) = \pm\sqrt{3 + 2\cos(\sqrt{3}\,k_x) + 4\cos\left(\frac{\sqrt{3}}{2}k_x\right)\cos\left(\frac{3}{2}k_y\right)}$$

The coordinates of the high symmetry points are

$$K = \left(\frac{2\pi}{3\sqrt{3}}, \frac{2\pi}{3}, 0\right)$$

$$K' = \left(\frac{4\pi}{3\sqrt{3}}, 0, 0\right)$$

$\longrightarrow$ expansion of dispersion shows the linear dispersion around K and K'.

(2) Show that a energy shift between A and B sites, e.g., $\mu\left(c^+_{jA}c_{jA} - c^+_{jB}c_{jB}\right)$, gaps the band crossings.

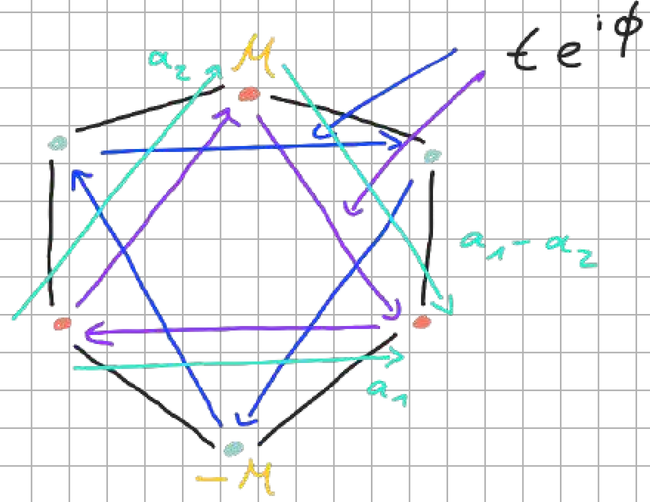
$$\longrightarrow \quad \hat{H}(k) = \begin{array}{cc} & \begin{array}{cc} A & B \end{array} \\ \begin{array}{c} A \\ B \end{array} & \begin{pmatrix} \mu & \sum_{i=1}^{3} e^{ik\cdot e_i} \\ \sum_{i=1}^{3} e^{-ik\cdot e_i} & -\mu \end{pmatrix} \end{array}$$

$\longrightarrow$ diagonalize Hamiltonian and evaluate $E_\pm$ at K and K'.

(3) Show that the Chern number vanishes.

- Numerically obtain band projectors
- Calculate the Berry curvature
- Perform the integral over the BZ

12)



Ex: Construct the corresponding tight-binding and Bloch Hamiltonian.

The additional term is

$$
\begin{aligned}
\hat{H}_2 = \sum_R \; & t e^{-i\phi} \hat{c}^\dagger_{R+a_1 A} \hat{c}_{RA} \\
& + t e^{i\phi} \hat{c}^\dagger_{R+a_2 A} \hat{c}_{RA} \\
& + t e^{i\phi} \hat{c}^\dagger_{R+a_1-a_2} \hat{c}_{RA} \\
& + t e^{i\phi} \hat{c}^\dagger_{R+a_1 B} \hat{c}_{RB} \\
& + t e^{-i\phi} \hat{c}^\dagger_{R+a_2 B} \hat{c}_{RB} \\
& + t e^{-i\phi} \hat{c}^\dagger_{R+a_1-a_2 B} \hat{c}_{RB} \\
& + h.c
\end{aligned}
$$

$$
\longrightarrow \quad \hat{H}_2(k) = \begin{pmatrix} H_{AA}(k) & 0 \\ 0 & H_{BB}(k) \end{pmatrix}
$$

with

$$
\begin{aligned}
H_{AA}(k) = t \Big(& e^{-i\phi} e^{-ik\cdot a_1} \\
& + e^{i\phi} e^{-ik\cdot a_2} \\
& + e^{i\phi} e^{-ik\cdot (a_1 - a_2)} \Big) + h.c.
\end{aligned}
$$

$$
\begin{aligned}
H_{BB}(k) = t \Big(& e^{i\phi} e^{-ik\cdot a_1} \\
& + e^{-i\phi} e^{-ik\cdot a_2} \\
& + e^{-i\phi} e^{-ik\cdot (a_1 - a_2)} \Big) + h.c.
\end{aligned}
$$

13)

Ex: (1) Show that the particle number operator commutes, i.e., $[\hat n_j, \hat n_{j'}] = 0$.

- for $j = j'$:

$$[\hat n_j, \hat n_j] = \hat n_j \hat n_j - \hat n_j \hat n_j = 0$$

- for $j \neq j'$:

$$\hat n_j \hat n_{j'} = \hat c_j^+ \underbrace{\hat c_j \hat c_{j'}^+}_{= -\hat c_{j'}^+ \hat c_j \text{ and so on}} \hat c_{j'}$$

$$= \hat c_{j'}^+ \hat c_j^+ \hat c_j \hat c_{j'}$$

$$= \hat c_{j'}^+ \hat c_{j'} \hat c_j^+ \hat c_j = \hat n_{j'} \hat n_j$$

$$\longrightarrow [\hat n_j, \hat n_{j'}] = 0$$

(2) Show that $\hat c_j^+ \hat c_j^+ = 0$ and $\hat c_j \hat c_j = 0$.

$$2 \hat c_j^+ \hat c_j^+ = \hat c_j^+ \hat c_j^+ + \hat c_j^+ \hat c_j^+$$

$$= \hat c_j^+ \hat c_j^+ - \hat c_j^+ \hat c_j^+ = 0$$

and the same steps for $\hat c_j \hat c_j$.

(3) Show that $\hat n_j^s = \hat n_j$ for all $s \in \mathbb{N}$.

$$\hat n_j^2 = \hat n_j \hat n_j = \hat c_j^+ \underbrace{\hat c_j \hat c_j^+}_{= 1 - \hat c_j^+ \hat c_j} \hat c_j = \hat c_j^+ \hat c_j = \hat n_j$$

and then iterate.

(4) Show that $\hat{n}_j \hat{c}_j^+ = \hat{c}_j^+$.

$$\hat{n}_j \hat{c}_j^+ = \hat{c}_j^+ \underbrace{\hat{c}_j \hat{c}_j^+}_{= 1 - \hat{c}_j^+ c_j} = \hat{c}_j^+$$

(5) Show the identity

$$e^{i\alpha \hat{n}_j} = 1 - (1 - e^{i\alpha}) \hat{n}_j$$

for $\alpha \in \mathbb{R}$ using the Taylor series of the exponential function.

$$e^{i\alpha \hat{n}_j} = \sum_{s=0}^{\infty} \frac{(i\alpha \hat{n}_j)^s}{s!}$$

$$= 1 + \sum_{s=1}^{\infty} \frac{(i\alpha)^s}{s!} \underbrace{\hat{n}_j^s}_{= \hat{n}_j}$$

$$= 1 + \hat{n}_j \left(\sum_{s=0}^{\infty} \frac{(i\alpha)^s}{s!} - 1 \right)$$

$$= 1 - (1 - e^{i\alpha}) \hat{n}_j$$

(6) Show that $\hat{c}_j^+ e^{i\alpha \hat{n}_j} = \hat{c}_j^+$.

$$\hat{c}_j^+ e^{i\alpha \hat{n}_j}$$

$$= \hat{c}_j^+ \left[1 - (1 - e^{i\alpha}) \hat{n}_j \right]$$

$$= \hat{c}_j^+ - (1 - e^{i\alpha}) \underbrace{\hat{c}_j^+ \hat{c}_j^+}_{=0} c_j$$

$$= \hat{c}_j^+$$

(7) Show that $e^{i\alpha \hat{n}_j} \hat{c}^{+}_{j'} = \hat{c}^{+}_{j'} e^{i\alpha \hat{n}_j}$ for $j \neq j'$.

$$e^{i\alpha \hat{n}_j} \hat{c}^{+}_{j'}$$

$$= \left[1 - (1 - e^{i\alpha}) \hat{c}^{+}_{j} \hat{c}_{j} \right] \hat{c}^{+}_{j'}$$

$$= \hat{c}^{+}_{j'} e^{i\alpha \hat{n}_j}$$

14)

Ex: We focus on the case with $n \neq m$.

(1) Show that $Q^{nm}_{\alpha\beta} = Q^{mn}_{\beta\alpha}$.

$$Q^{nm}_{\alpha\beta} = -\operatorname{tr}\left[\hat{e}^{nm}_{\alpha}\,\hat{e}^{nm}_{\beta}\right]$$
$$= -\operatorname{tr}\left[\hat{e}^{nm}_{\beta}\,\hat{e}^{mn}_{\alpha}\right]$$
$$= Q^{mn}_{\beta\alpha}$$

(2) Show that $\overline{Q^{mn}_{\alpha\beta}} = Q^{mn}_{\beta\alpha}$, where the overline denotes complex conjugation.

$$\overline{Q^{mn}_{\alpha\beta}} = -\overline{\operatorname{tr}\left[\left(\hat{e}^{nm}_{\alpha}\,\hat{e}^{mn}_{\beta}\right)^{t5}\right]}$$
$$= -\operatorname{tr}\left[\left(\hat{e}^{nm}_{\alpha}\,\hat{e}^{mn}_{\beta}\right)^{+}\right]$$
$$= -\operatorname{tr}\left[\left(\hat{e}^{mn}_{\beta}\right)^{+}\left(\hat{e}^{nm}_{\alpha}\right)^{+}\right]$$
$$= -\operatorname{tr}\left[\hat{e}^{nm}_{\beta}\,\hat{e}^{mn}_{\alpha}\right]$$
$$= Q^{mn}_{\beta\alpha}$$

(3) Show that $g^{mn}_{\alpha\beta} = g^{(mn)}_{(\alpha\beta)}$ and $\Omega^{mn}_{\alpha\beta} = \Omega^{[mn]}_{[\alpha\beta]}$

with $O_{(ab)} = \frac{1}{2}\left(O_{ab} + O_{ba}\right)$ and

$O_{[ab]} = \frac{1}{2}\left(O_{ab} - O_{ba}\right)$.

- $g^{mn}_{\alpha\beta} = \operatorname{Re} Q^{mn}_{\alpha\beta}$

$$= 1/2 \left(Q^{mn}_{\alpha\beta} + \overline{Q^{mn}_{\alpha\beta}} \right)$$

$$= 1/2 \left(Q^{mn}_{\alpha\beta} + Q^{mn}_{\beta\alpha} \right)$$

$$\longrightarrow g^{mn}_{\beta\alpha} = 1/2 \left(Q^{mn}_{\beta\alpha} + Q^{mn}_{\alpha\beta} \right) = g^{mn}_{\alpha\beta}$$

$$g^{nm}_{\alpha\beta} = 1/2 \left(Q^{nm}_{\alpha\beta} + Q^{nm}_{\beta\alpha} \right)$$

$$= 1/2 \left(Q^{mn}_{\beta\alpha} + Q^{mn}_{\alpha\beta} \right) = g^{mn}_{\alpha\beta}$$

- $\Omega^{mn}_{\alpha\beta} = -2 \operatorname{Im} Q^{mn}_{\alpha\beta}$

$$= -i \left(Q^{mn}_{\alpha\beta} - \overline{Q^{mn}_{\alpha\beta}} \right)$$

$$= i \left(Q^{mn}_{\beta\alpha} - Q^{mn}_{\alpha\beta} \right)$$

$$\longrightarrow \Omega^{mn}_{\beta\alpha} = i \left(Q^{mn}_{\alpha\beta} - Q^{mn}_{\beta\alpha} \right) = -\Omega^{mn}_{\alpha\beta}$$

$$\Omega^{nm}_{\alpha\beta} = i \left(Q^{nm}_{\beta\alpha} - Q^{nm}_{\alpha\beta} \right)$$

$$= i \left(Q^{mn}_{\alpha\beta} - Q^{mn}_{\beta\alpha} \right) = -\Omega^{mn}_{\alpha\beta}$$

15)

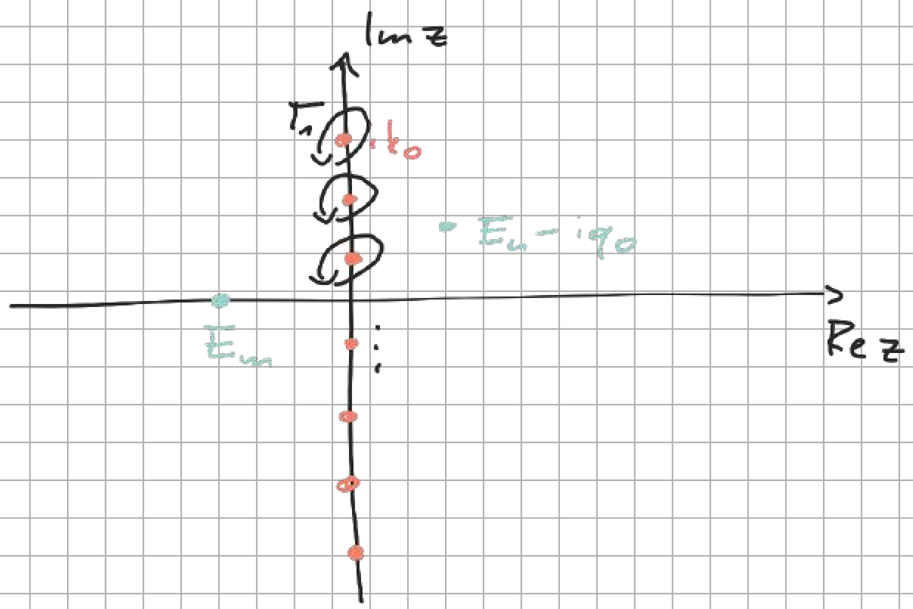
$$S^{(2)}(E_n - iq_0, E_m)$$

$$= k_B T \sum_{ik_0} \frac{1}{ik_0 + iq_0 - E_n} \frac{1}{ik_0 - E_m}$$

$$= \begin{cases} \dfrac{f_n - f_m}{-iq_0 + E_n - E_m} & n \neq m \\ f_n' \, \delta_{iq_0,0} & n = m \end{cases}$$

Ex: Prove this result via the residue theorem. The fermionic Matsubara frequencies are defined as $ik_0 = \frac{(2n+1)i\pi}{\beta}$ and the bosonic Matsubara frequencies are defined as $iq_0 = \frac{2ni\pi}{\beta}$. The Fermi function on the complex plane $f(z) = \frac{1}{e^{\beta z}+1}$ has poles at the fermionic Matsubara frequencies with residue $-1/\beta$ for $\beta = 1/k_B T$.

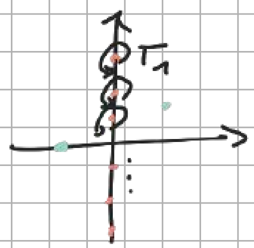
a)



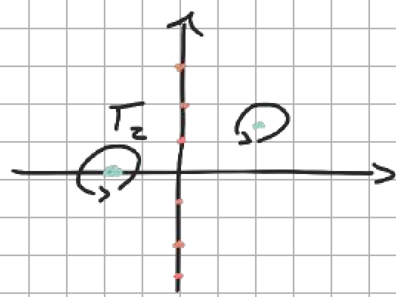
$$k_B T \sum_{ik_0} \frac{1}{ik_0 + iq_0 - E_n} \frac{1}{ik_0 - E_m}$$

$$= -\frac{1}{2\pi i} \oint_{T_1} dz \, \frac{1}{z + iq_0 - E_n} \frac{1}{z - E_m} f(z)$$

b)



$\longrightarrow$ $-$



since integral vanishes at infinity.

$$\longrightarrow \frac{1}{2\pi i} \oint_{T_2} dz \, \frac{1}{z + iq_0 - E_n} \frac{1}{z - E_m} f(z)$$

$$= \frac{1}{z - E_m} f(z) \Big|_{z = E_n - iq_0}$$

$$+ \frac{1}{z + iq_0 - E_n} f(z) \Big|_{z = E_m}$$

using $f(z+iq_0) = f(z)$ for Fermi function f and bosonic Matsubara frequencies

$$= \frac{f_n}{E_n - iq_0 - E_m} + \frac{f_m}{E_m + iq_0 - E_n}$$

$$= \frac{f_n - f_m}{-iq_0 + E_n - E_m}$$

c) The case of $n=m$ can be obtained by the limit $\lim\limits_{E_m \to E_n}$ leading to

$iq_0 \neq 0 \Rightarrow 0$

$iq_0 = 0 \Rightarrow f_n'$

16)

$$\sigma^{\alpha\beta}_{\text{intra}}(0) = \tau e^2 \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n \frac{f_n(k)}{m_n^{\alpha\beta}(k)} \qquad (1)$$

Ex: Show (1) by first showing that

$$f_n'(k)\, v_n^\alpha(k) = \partial_\alpha f_n(k).$$

- $$\partial_\alpha f_n(k) = \partial_\alpha f(E_n(k))$$
$$= f'(E_n(k))\, \partial_\alpha E_n(k)$$
$$= f_n'(k)\, v_n^\alpha(k)$$

- $$\sigma^{\alpha\beta}_{\text{intra}}(\omega) = \frac{e^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n \frac{f_n'(k)\, v_n^\alpha(k)\, v_n^\beta(k)}{i(\omega + i\eta)}$$

with $\omega = 0$ and $\eta = \hbar/\tau$

$$\longrightarrow \sigma^{\alpha\beta}_{\text{intra}}(0) = -\frac{\tau e^2}{\hbar^2} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n f_n'(k)\, v_n^\alpha(k)\, v_n^\beta(k)$$

$$= -\frac{\tau e^2}{\hbar^2} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n \partial_\alpha f_n(k)\, \partial_\beta E_n(k)$$

$$= \tau e^2 \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n f_n(k)\, \underbrace{\frac{\partial_\alpha \partial_\beta E_n(k)}{\hbar^2}}_{= 1/m_n^{\alpha\beta}(k)}$$

17)

Ex: (1) Show that $g^{mn}_{\alpha\beta} \equiv Q^{mn}_{(\alpha\beta)} = \frac{1}{2}\,\mathrm{tr}\,[\partial_\alpha \hat{P}_m \partial_\beta \hat{P}_n]$.

- for $n = m$ by definition
- for $n \neq m$:

$$
\begin{aligned}
g^{mn}_{\alpha\beta} &= Q^{mn}_{(\alpha\beta)} \\
&= \tfrac{1}{2}\,\mathrm{tr}\,[P_n \partial_\alpha P_m \partial_\beta P_n] \\
&\quad + \tfrac{1}{2}\,\mathrm{tr}\,[P_n \partial_\beta P_m \partial_\alpha P_n] \\
&= \tfrac{1}{2}\,\mathrm{tr}\,[\partial_\alpha P_m \partial_\beta P_n] \\
&\quad - \tfrac{1}{2}\,\mathrm{tr}\,[\partial_\alpha P_m P_n \partial_\beta P_n P_m] \\
&\quad + \tfrac{1}{2}\,\mathrm{tr}\,[P_n \partial_\beta P_m P_m \partial_\alpha P_n] \\
&= \tfrac{1}{2}\,\mathrm{tr}\,[\partial_\alpha P_m \partial_\beta P_n] \\
&\quad + \tfrac{1}{2}\,\mathrm{tr}\,[e^{mn}_\alpha e^{nm}_\beta] \\
&\quad - \tfrac{1}{2}\,\mathrm{tr}\,[e^{nm}_\beta e^{mn}_\alpha] \\
&= \tfrac{1}{2}\,\mathrm{tr}\,[\partial_\alpha P_m \partial_\beta P_n]
\end{aligned}
$$

(2) Show that

$$\sum_{n \in occ} \sum_{m \in unocc} g_{\alpha\beta}^{mn} = - g_{\alpha\beta}^{occ} ,$$

which is the quantum metric of the occupied states with projectors $\hat{P}_{occ} = \sum_{n \in occ} \hat{P}_n$.

$$\sum_{n \in occ} \sum_{m \in unocc} g_{\alpha\beta}^{mn}$$

$$= \sum_{n \in occ} \sum_{m \in unocc} 1/2 \; tr \left[\partial_\alpha P_m \, \partial_\beta P_n \right]$$

$$= 1/2 \; tr \left[\partial_\alpha \left(1 - P_{occ} \right) \partial_\beta P_{occ} \right]$$

$$= - g_{\alpha\beta}^{occ}$$