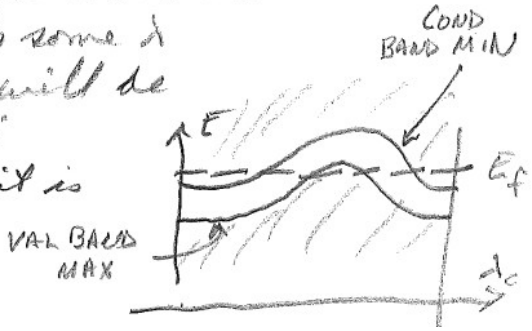
Solutions to problems in
*Berry Phases in Electronic Structure Theory*
David Vanderbilt

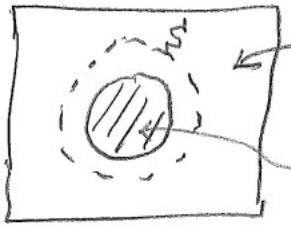
# Chapter 1

## Exercise 1.1

The basic point is that the supercell has to be insulating. If $H_\lambda$ is metallic for some $\lambda$ on the path, then the supercell will be metallic. But it can be metallic even if not (see at right). So it is necessary but not sufficient.




## Exercise 1.2




If this causes $\dot{\rho} \neq 0$, then $\dot{\rho} = -\int_S \underline{J} \cdot d\underline{S}$ by Gauss' Thm

But $\underline{J} = 0$ on dotted surface, so $\dot{\rho} = 0$.

## Exercise 1.3

The two settings are related by a shift of origin and a translation of some atoms by a lattice vector.

In units of $a$:

| | 1st setting | shift origin → | 2nd setting | $\Delta\underline{R}$ → |
|---|---|---|---|---|
| K | $(000)$ | | $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ | $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ |
| Nb | $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ | | $(111)$ | $(000)$ |
| $O_1$ | $(0\frac{1}{2}\frac{1}{2})$ | | $(\frac{1}{2}11)$ | $(\frac{1}{2}00)$ |
| $O_2$ | $(\frac{1}{2}0\frac{1}{2})$ | | $(1\frac{1}{2}1)$ | $(0\frac{1}{2}0)$ |
| $O_3$ | $(\frac{1}{2}\frac{1}{2}0)$ | | $(11\frac{1}{2})$ | $(00\frac{1}{2})$ ✓ |

1st Setting: $P = \frac{e}{a^2}\left[(+1)(000) + (+5)(\frac{1}{2}\frac{1}{2}\frac{1}{2}) - 2(111)\right]$

$= \frac{e}{a^2}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$

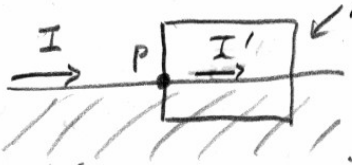
2nd Setting: $P = \frac{e}{a^2}\left[(+1)(\frac{1}{2}\frac{1}{2}\frac{1}{2}) + (+5)(000) - (111)\right]$

$= \frac{e}{a^2}(-\frac{1}{2}-\frac{1}{2}\frac{-1}{2})$

These differ by $\frac{e}{a^3}\underline{R}$ with $\underline{R} = a(111)$, ie, by $\frac{e\underline{R}}{\text{Vcell}}$ ✓

## Exercise 1.4

(a) Eq. (1.24)




Interactions / disorder in region A.

Now change $\phi \to \phi + d\phi$, $I \to I + dI$, $I' = I' + dI'$

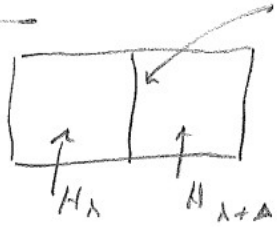
But conservation of charge at P $\Rightarrow \frac{dI}{d\phi} = \frac{dI'}{d\phi}$

(b) Eq. (1.26)

Number $n_{up}$ or $n_{down}$ is necessarily an integer; cannot change gradually, as long as bulk gap remains open.

## Exercise 1.5

1.3.2




FOR SMALL $\Delta\lambda$, THERE IS NO EDGE CHANNEL. SO $G$ CANNOT CHANGE.

OR, ARGUE THAT (# UP-CROSSINGS) − (# DOWN-CROSSINGS) CANNOT CHANGE.

## Exercise 1.6

(a) $k_i = \sigma_{AH}\,\epsilon_{ij}\,\mathcal{E}_j$ , $\mathcal{E}$ = electric field, $\mathcal{E}_j = -\partial_j \phi$

$= -\sigma_{AH}\,\epsilon_{ij}\,(\partial_j \phi)$

$\epsilon_{ij}$: current is ∥ to contours; $(\partial_j \phi)$: gradient is ⊥ to contours

$-\frac{\partial \rho}{\partial t} = \partial_i k_i = -\sigma_{AH}\,\epsilon_{ij}\,(\partial_i \partial_j \phi) = 0$

$\epsilon_{ij}$ symmetric under $i \leftrightarrow j$ ✓

(b) As part (a), current arriving at AB is

$$\frac{1}{\sigma_{AH}} \int_{x_A}^{x_B} k_y\,dx = \int_{x_A}^{x_B} \mathcal{E}_x\,dx = -\int_{x_A}^{x_B} (\partial_x \phi)\,dx = \phi_A - \phi_B = \Delta\phi$$

$$I = \sigma_{AH}\,\Delta\phi = C\left(\frac{e^2}{h}\right)\Delta\phi$$

(c) $\Delta I = G\,\Delta\phi = C\frac{e^2}{h}\Delta\phi$ = same as (b).

# Chapter 2

## Exercise 2.1

Eq. (2.21); $h_{soc} = \gamma \underline{\sigma} \cdot \underline{\nabla} V \times \underline{p}$ $\quad \gamma = \frac{\hbar}{4m^2c^2}$ $\quad V = -e\phi(r)$

$$h_{soc} = -e\gamma \frac{d\phi}{dr} \underline{\sigma} \cdot \hat{r} \times \underline{p}$$

$$= -\frac{e\gamma}{r} \frac{d\phi}{dr} (\underline{r} \times \underline{p}) \cdot \left(\frac{2}{\hbar} \underline{S}\right) \qquad \underline{S} = \frac{\hbar}{2}\underline{\sigma}$$

$$h_{soc} = \xi(r)\, \underline{L} \cdot \underline{S} \quad , \quad \xi(r) = \frac{\hbar}{4m^2c^2}\left(\frac{-e}{r}\right)\left(\frac{2}{\hbar}\right)$$

$$\xi(r) = \frac{-e}{2m^2c^2} \frac{1}{r} \frac{d\phi}{dr} \quad \checkmark$$

## Exercise 2.2

(a) $\frac{1}{\hbar} \underline{\nabla}_k H_k = \frac{1}{\hbar} \underline{\nabla}_k e^{-i\underline{k}\cdot\underline{r}} H e^{i\underline{k}\cdot\underline{r}}$

$= \frac{1}{\hbar} e^{-i\underline{k}\cdot\underline{r}} (-i\underline{r} H + iH\underline{r}) e^{i\underline{k}\cdot\underline{r}}$

$= \frac{-i}{\hbar} e^{-i\underline{k}\cdot\underline{r}} [\underline{r}, H] e^{i\underline{k}\cdot\underline{r}}$

$= e^{-i\underline{k}\cdot\underline{r}} \underline{v} e^{i\underline{k}\cdot\underline{r}}$

$= \underline{v}_k \quad \checkmark$

(b) $\underline{v} = \frac{-i}{\hbar} [\underline{r}, \frac{1}{2m}(\underline{p} + \frac{e}{c}\underline{A}(r))^2 - e\phi(r)]$

$= \frac{-i}{\hbar} \frac{1}{m} (\underline{p} + \frac{e}{c}\underline{A}(r))(i\hbar)$

$= \frac{1}{m}(\underline{p} + \frac{e}{c}\underline{A}(\underline{r}))$

$\underline{v}_k = \frac{1}{m} e^{-i\underline{k}\cdot\underline{r}} (\underline{p} + \frac{e}{c}\underline{A}) e^{i\underline{k}\cdot\underline{r}}$

$= \frac{1}{m} e^{-i\underline{k}\cdot\underline{r}} e^{+i\underline{k}\cdot\underline{r}} (\underline{p} + \hbar\underline{k} + \frac{e}{c}\underline{A})$

$= \frac{1}{m}(\underline{p} + \hbar\underline{k} + \frac{e}{c}\underline{A})$

Check: $\underline{H}_k = \frac{1}{2m}(\underline{p} + \hbar\underline{k} + \frac{e}{c}\underline{A})^2 - e\phi(\underline{r})$

$\frac{1}{\hbar} \underline{\nabla}_k \underline{H}_k = \frac{1}{m}(\underline{p} + \hbar\underline{k} + \frac{e}{c}\underline{A})$ $\quad \checkmark$

## Exercise 2.3

a) $e^{i\beta_n(\underline{k}+\underline{G})} = e^{i\beta_n(\underline{k})}$ to preserve smoothness at BZ boundary

$\Rightarrow \beta_n(\underline{k}+\underline{G}) = \beta_n(\underline{k}) + 2\pi \times \text{int}.$

Recall $\underline{G} = m_1\underline{b}_1 + m_2\underline{b}_2 + m_3\underline{b}_3$ so

$$\beta_n(\underline{k}+\underline{b}_1) = \beta_n(\underline{k}) + 2\pi\, l_1$$
$$\beta_n(\underline{k}+\underline{b}_2) = \beta_n(\underline{k}) + 2\pi\, l_2$$
$$\beta_n(\underline{k}+\underline{b}_3) = \beta_n(\underline{k}) + 2\pi\, l_3$$

in full glory ↓

$$\beta_n(\underline{k}+\underline{G}) = \beta_n(\underline{k}) + 2\pi\,(l_1 m_1 + l_2 m_2 + l_3 m_3)$$

b) $\tilde{\psi}_{n\underline{k}}(\underline{r}) = e^{-i\beta_n(\underline{k})}\psi_{n\underline{k}}(\underline{r})$ ↙ mult each side by $e^{-i\underline{k}\cdot\underline{r}}$

$\Rightarrow \tilde{u}_{n\underline{k}}(\underline{r}) = e^{-i\beta_n(\underline{k})} u_{n\underline{k}}(\underline{r})$

c) $\tilde{A}_{n\underline{k}} = i\langle \tilde{u}_{n\underline{k}} | \partial_{\underline{k}} | \tilde{u}_{n\underline{k}} \rangle$

$= i\langle u_{n\underline{k}} | e^{i\beta_n} \partial_{\underline{k}} e^{-i\beta_n} | u_{n\underline{k}} \rangle$

$= (\partial_{\underline{k}}\beta_n)\langle u_{n\underline{k}} | u_{n\underline{k}} \rangle + i\langle u_{n\underline{k}} | \partial_{\underline{k}} u_{n\underline{k}} \rangle$

$= (\partial_{\underline{k}}\beta_n) + \underline{A}_{n\underline{k}}$

d) $\nabla_{\underline{k}} \times \tilde{\underline{A}}_{n\underline{k}} = \nabla_{\underline{k}} \times \nabla_{\underline{k}}\beta_{n\underline{k}} + \nabla_{\underline{k}} \times \underline{A}_{n\underline{k}} = \nabla_{\underline{k}} \times \underline{A}_{n\underline{k}}$ ✓

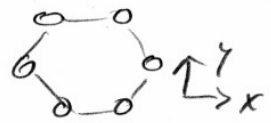
## Exercise 2.4

| (a,b) | | $\underline{r}$ | $\underline{p}$ | $p^2/2m$ | $\underline{v}$ | $\underline{S}$ | $\underline{L}$ |
|---|---|---|---|---|---|---|---|
| | TR | + | − | + | − | − | − |
| | Inv | − | − | + | − | + | + |

| (c) | | $\sigma$ | $\nabla V$ | $\underline{p}$ | Prod. | $\underline{L}$ | $\underline{S}$ | Prod |
|---|---|---|---|---|---|---|---|---|
| | TR | − | + | − | + | − | − | + |
| | Inv | + | − | − | + | + | + | + |

## Exercise 2.5

Apply electric field to benzene molecule:



at high fields, site energies dominate over hoppings.

$E_x$ at high field: separates into groups of 1+2+2+1, corresponding to x coordinate.

$E_y$ at high field: separates into three groups: 2+2+2, corresponding to y coordinates. First + third groups retain $\pm t$ splitting since they are 1st neighbors.

## Exercise 2.6

Now looks like 

For large $|\delta|$, looks like 3 dimers, weakly coupled,

For $\delta = t$, looks like  i.e., 3 uncoupled dimers.

Net 3-fold degeneracies.

## Exercise 2.7

$$H_{ij}^{k} = \langle \chi_i^k | H | \chi_j^k \rangle$$

$$= \frac{1}{N} \left( \sum_R e^{-ik\cdot(R+T_i)} \langle \phi_{R;i} | \right) H \left( \sum_{R'} e^{ik\cdot(R'+T_j)} | \phi_{R';j} \rangle \right)$$

$$= \frac{1}{N} \sum_R \sum_{R'} e^{ik\cdot(R'-R+T_j-T_i)} \langle \phi_{R;i} | H | \phi_{R';j} \rangle \quad \downarrow R'' = R' - R$$

$$= \left( \frac{1}{N} \sum_R \right) \sum_{R''} e^{ik\cdot(R''+T_j-T_i)} H_{ij}(R'') \quad \downarrow R'' \to R$$

$$= \sum_R e^{ik\cdot(R+T_j-T_i)} H_{ij}(R) \quad \checkmark$$

# Exercise 2.8

**Convention I:**

$$|\chi_j^{k+G}\rangle = \sum_R e^{i(k+G)\cdot(R+\tau_j)} |\phi_{Rj}\rangle \quad \Big) e^{iG\cdot R} = 1$$

$$= e^{iG\cdot\tau_j} \sum_R e^{k\cdot\tau_j} |\phi_{Rj}\rangle$$

$$|\chi_j^{k+G}\rangle = e^{iG\cdot\tau_j} |\chi_j^{k}\rangle$$

Periodic gauge: $|\psi_{nk}\rangle = |\psi_{n,k+G}\rangle$

$$\sum_i C_i^{nk} |\chi_i^{k}\rangle = \sum_i C_i^{n,k+G} |\chi_i^{k+G}\rangle$$

$$= \sum_i C_i^{n,k+G} e^{iG\cdot\tau_i} |\chi_i^{k}\rangle$$

$\langle \chi_j^{k}| \cdot \rightarrow$ $\quad C_j^{nk} = e^{iG\cdot\tau_j} C_j^{n,k+G}$

**Convention II**

Same approach $\Rightarrow$ $|\tilde{\chi}_j^{k+G}\rangle = |\tilde{\chi}_j^{k}\rangle$

$\Rightarrow$ $\tilde{C}_j^{nk} = \tilde{C}_j^{n,k+G}$

**Compare**

$|\psi_{n,k+G}\rangle = |\psi_{nk}\rangle \iff \tilde{C}_j^{n,k+G} = \tilde{C}_j^{nk}$ [Conv. II]

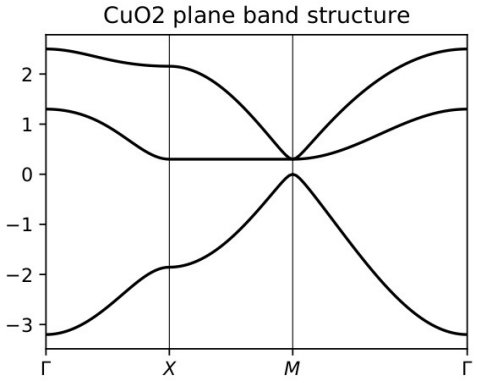
$|u_{n,k+G}\rangle = e^{-iG\cdot r} |u_{nk}\rangle \iff C_j^{n,k+G} = e^{-iG\cdot\tau_j} C_j^{nk}$ [Conv I]

So $|u_{nk}\rangle$ are like Conv. I

$|\psi_{nk}\rangle$ are like Conv. II

## Exercise 2.9

See sample solution program ex-2.9.py




## Exercise 2.10

*This was a free-style question; no solution is provided.*

## Exercise 2.11

*No solution yet.*

## Exercise 2.12

(a) $|\partial_\lambda n\rangle = -iA_n|n\rangle + T_n(\partial_\lambda H)|n\rangle$

$\langle\partial_\lambda n| = iA_n\langle n| + \langle n|(\partial_\lambda H)T_n$ (note $A_n^* = A_n$)

$\partial_\lambda \rho = \sum_n \left( |\partial_\lambda n\rangle\langle n| + |n\rangle\langle\partial_\lambda n| \right)$

Terms involving $A_n$ cancel.

$$\boxed{\partial_\lambda \rho = \sum_n T_n(\partial_\lambda H)|n\rangle\langle n| + \text{h.c.}}$$

(b) $\partial_\lambda\langle O\rangle = \mathrm{Tr}\left[(\partial_\lambda\rho)O\right]$

$= \sum_n \mathrm{Tr}\left[T_n(\partial_\lambda H)|n\rangle\langle n|O\right]$

$+ \sum_n \mathrm{Tr}\left[|n\rangle\langle n|(\partial_\lambda H)T_n O\right]$

Use cyclic property of trace and that $\mathrm{tr}\left[\hat{A}|n\rangle\langle n|\right] = \langle n|\hat{A}|n\rangle$ (obvious?)

to get $\partial_\lambda\langle O\rangle = \sum_n \langle n|OT_n(\partial_\lambda H) + (\partial_\lambda H)T_n O|n\rangle$

$$\boxed{\partial_\lambda\langle O\rangle = 2\,\mathrm{Re}\sum_n \langle n|OT_n(\partial_\lambda H)|n\rangle}$$

# Chapter 3

## Exercise 3.1

(a) $\gamma_{ij} = -\mathrm{Im}\ln\langle u_i | u_j\rangle$

Here $\gamma_{01} = \gamma_{12} = \gamma_{30} = 0 \qquad \gamma_{23} = -\mathrm{Im}\ln\left(\frac{i}{\sqrt{2}}\right) = -\frac{\pi}{2}$

$\boxed{\phi = -\pi/2}$

(b) Parallel transport gauge (PTG):

$$|\tilde{u}_0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad |\tilde{u}_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad |\tilde{u}_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-i\\1\end{pmatrix} \quad |\tilde{u}_4\rangle = \begin{pmatrix}-i\\0\end{pmatrix}$$

$$\phi = -\mathrm{Im}\ln\langle\tilde{u}_4|\tilde{u}_0\rangle = -\mathrm{Im}\ln\begin{pmatrix}i & 0\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix} = -\pi/2$$

(c) Twisted PTG:

$$|\tilde{\tilde{u}}_0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad |\tilde{\tilde{u}}_1\rangle = e^{i\pi/8}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad |\tilde{\tilde{u}}_2\rangle = e^{i\pi/4}\begin{pmatrix}0\\1\end{pmatrix}$$

$$|\tilde{\tilde{u}}_3\rangle = e^{3i\pi/8}\frac{1}{\sqrt{2}}\begin{pmatrix}-i\\1\end{pmatrix} \quad |\tilde{\tilde{u}}_4\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

## Exercise 3.2

*Note that the statement of this problem was incorrect in the published book; it was corrected in the Errata.*

$\gamma_{ij} = -\mathrm{Im}\ln\langle u_i | u_j\rangle$

$$\gamma_{ab} = -\mathrm{Im}\ln\begin{pmatrix}1 & 1\end{pmatrix}\cdot\begin{pmatrix}1\\e^{2\pi i/3}\end{pmatrix} = -\mathrm{Im}\ln\left(1+e^{2\pi i/3}\right)$$

$$= -\mathrm{Im}\ln e^{i\pi/3}\left(e^{-i\pi/3}+e^{i\pi/3}\right)$$

$$= -\mathrm{Im}\ln e^{i\pi/3}\,2\cos(\pi/3) = -\pi/3$$

$\gamma_{bc}$ and $\gamma_{ca}$ work in a similar way: all 3 $= -\pi/3$.

Others? (1) $|u_a\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

$$|u_b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{2\pi i/3}\\e^{-2\pi i/3}\end{pmatrix}$$

$$|u_c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-2\pi i/3}\\e^{2\pi i/3}\end{pmatrix}$$

$\gamma_{ab} = \gamma_{bc} = \gamma_{ca} = -\pi = \pi$

(2) $|u_a\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

$$|u_b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-2\pi i/3}\\1\end{pmatrix}$$

$$|u_c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{2\pi i/3}\\1\end{pmatrix}$$

$\gamma_{ab} = \gamma_{bc} = \gamma_{ca} = \pi/3$

## Exercise 3.3

*No solution yet*

Exercise 3.4

(a) φ=0.
(b) φ=−0.079
(c) Yes, it reverses sign

See sample solution program ex-3.4.py

Note the line

n_phi=12

specifying the number of sampling points along the path; increase this number and rerun it until convergence is obtained.

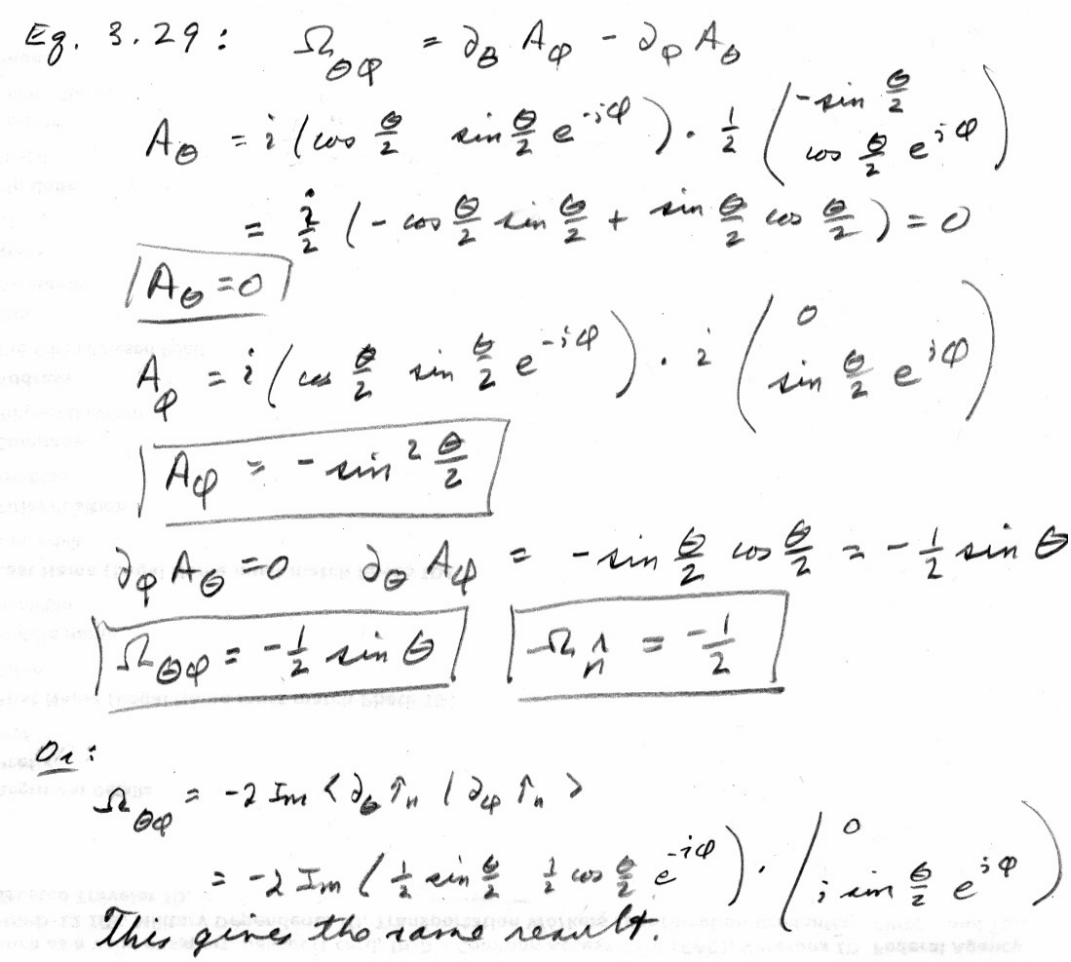
Output:

```
---------------------------------------
report of tight-binding model
---------------------------------------
k-space dimension           = 0
r-space dimension           = 2
number of spin components   = 1
periodic directions         = []
number of orbitals          = 3
number of electronic states = 3
lattice vectors:
 #  0  ===>  [     1.0 ,     0.0 ]
 #  1  ===>  [     0.0 ,     1.0 ]
positions of orbitals:
 #  0  ===>  [  -0.866 ,    -0.5 ]
 #  1  ===>  [   0.866 ,    -0.5 ]
 #  2  ===>  [     0.0 ,     1.0 ]
site energies:
 #  0  ===>       0.0
 #  1  ===>       0.0
 #  2  ===>       0.0
hoppings:
<  0 | H |  1 >     ===>  -1.3523 -  0.3623 i
<  1 | H |  2 >     ===>  -0.7727 -  0.2071 i
<  2 | H |  0 >     ===>  -0.7727 -  0.2071 i
hopping distances:
|  pos(  0 )  - pos(  1 ) |  =    1.7321
|  pos(  1 )  - pos(  2 ) |  =    1.7321
|  pos(  2 )  - pos(  0 ) |  =    1.7321

phi = 0.000 eval = -1.9705  evec = [-0.621 +0.j     -0.6164+0.0755j -0.4773+0.0291j]
phi = 0.524 eval = -1.9678  evec = [0.5856+0.j     0.6371-0.0732j 0.491 -0.0694j]
phi = 1.047 eval = -1.9651  evec = [0.5387+0.j     0.6454-0.0557j 0.5307-0.0923j]
phi = 1.571 eval = -1.9678  evec = [-0.4958+0.j     -0.6411+0.0167j -0.5798+0.0819j]
phi = 2.094 eval = -1.9705  evec = [-0.4782+0.j     -0.6199-0.0378j -0.6199+0.0378j]
phi = 2.618 eval = -1.9678  evec = [0.4958+0.j     0.5798+0.0819j 0.6411+0.0167j]
phi = 3.142 eval = -1.9651  evec = [-0.5387+0.j     -0.5307-0.0923j -0.6454-0.0557j]
phi = 3.665 eval = -1.9678  evec = [-0.5856+0.j     -0.491 -0.0694j -0.6371-0.0732j]
phi = 4.189 eval = -1.9705  evec = [0.621 +0.j     0.4773+0.0291j 0.6164+0.0755j]
phi = 4.712 eval = -1.9678  evec = [0.6413+0.j     0.4957-0.0129j 0.5817+0.0668j]
phi = 5.236 eval = -1.9651  evec = [-0.6478+0.j     -0.5367+0.0463j -0.5367-0.0463j]
phi = 5.760 eval = -1.9678  evec = [-0.6413+0.j     -0.5817+0.0668j -0.4957-0.0129j]
Berry phase calc by hand is     -0.0753
Berry phase using wf_array is   -0.0753
```

Converges to -0.079 after n_phi is increased to convergence

## Exercise 3.5




## Exercise 3.6

*No solution yet*

## Exercise 3.7

*No solution yet*

## Exercise 3.8

*No solution yet*

Exercise 3.9

$$0 = (i\hbar\partial_t - H)\, e^{i\phi_n} e^{-i\gamma_n} [|n\rangle + \dot\lambda |\delta n\rangle]$$

$i\hbar\partial_t e^{i\phi_n} \to -\hbar \partial_t \phi_n = -\hbar \dot\lambda \partial_\lambda \phi_n = -\hbar \dot\lambda A_n$

$i\hbar\partial_t e^{-i\gamma} \to E_n$

$E_n |n\rangle$ cancels against $H|n\rangle$

$E_n (\dot\lambda |\delta n\rangle) \to \dot\lambda (E_n |\delta n\rangle)$

$i\hbar \partial_t |n\rangle = i\hbar \dot\lambda \partial_\lambda |n\rangle$

$i\hbar \partial_t (\dot\lambda |\delta n\rangle) \to$ terms of order $(\dot\lambda)^2$ or $\ddot\lambda$; drop.

So

$$0 = \dot\lambda \left(-\hbar A_n |n\rangle + [E_n - H]|\delta n\rangle + i\hbar |\partial_\lambda n\rangle\right)$$

$$\boxed{(E_n - H)|\delta n\rangle = -i\hbar (\partial_\lambda + i A_n)|n\rangle}$$

$$Q_n \partial_\lambda |n\rangle = (1 - |n\rangle\langle n|)\partial_\lambda |n\rangle = |\partial_\lambda n\rangle + i A_n |n\rangle \qquad \downarrow A_n = i\langle n|\partial_\lambda n\rangle$$

$$\boxed{(E_n - H)|\delta n\rangle = -i\hbar Q_n |\partial_\lambda n\rangle}$$

## Exercise 3.10

a) $|\psi(t)\rangle = e^{i\alpha}\left(|n\rangle + \lambda^* |\delta n\rangle\right)$

$\langle \hat{O} \rangle = \langle n|\hat{O}|n\rangle + \lambda^*\{\langle n|\hat{O}|\delta n\rangle + c.c.\} + \lambda^{*2}\langle \delta n|\delta n\rangle$

FIRST ORDER:

$$\delta\langle \hat{O}\rangle = \lambda^* 2\,\mathrm{Re}\langle n|\hat{O}|\delta n\rangle$$

b) $\langle \underline{I}\rangle = -2e\lambda^* \mathrm{Re}\langle n|\underline{v}|\delta n\rangle$

$$|\delta n\rangle = -i\hbar\, T_n |\partial_\lambda n\rangle$$

$$\langle \underline{I}\rangle = 2e\hbar\lambda^* \mathrm{Re}\left[i\langle n|\underline{v}\, T_n|\partial_\lambda n\rangle\right]$$

$$= -2e\hbar\lambda^* \mathrm{Im}\langle n|\underline{v}\, T_n|\partial_\lambda n\rangle$$

c) $\underline{v} = -\frac{i}{\hbar}[\underline{r}, H]$

$$\langle \underline{I}\rangle = 2e\lambda^* \mathrm{Re}\langle n|[\underline{r}, H]\, T_n|\partial_\lambda n\rangle$$

$$= 2e\lambda^* \mathrm{Re}\sum_{m\neq n} \frac{\langle n|[\underline{r}, H]|m\rangle\langle m|\partial_\lambda n\rangle}{E_n - E_m}$$

$$= 2e\lambda^* \mathrm{Re}\sum_{m\neq n} \frac{(E_m - E_n)\langle n|\underline{r}|m\rangle\langle m|\partial_\lambda n\rangle}{E_n - E_m}$$

$$= -2e\lambda^* \mathrm{Re}\sum_{m\neq n}\langle n|\underline{r}|m\rangle\langle m|\partial_\lambda n\rangle$$

$$= -2e\lambda^* \mathrm{Re}\left\{\langle n|\underline{r}\left(\sum_m |m\rangle\langle m|\right)|\partial_\lambda n\rangle - \underbrace{\langle n|\underline{r}|n\rangle}_{\text{Real}}\underbrace{\langle n|\partial_\lambda n\rangle}_{\text{Pure imag}}\right\}$$

$$= -2e\lambda^* \mathrm{Re}\langle n|\underline{r}|\partial_\lambda n\rangle$$

so

$$\partial_\lambda \underline{d} = (\partial_* \underline{d})/\lambda^* = -2e\,\mathrm{Re}\langle n|\underline{r}|\partial_\lambda n\rangle$$

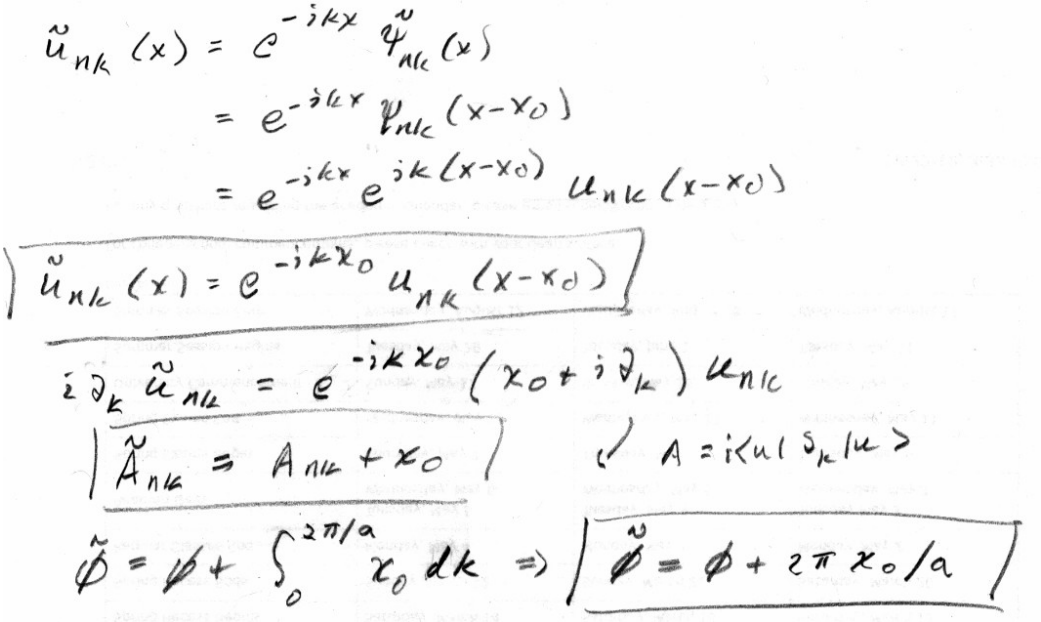
But

$$\partial_\lambda\langle \underline{d}\rangle = -e\,\partial_\lambda\langle n|\underline{r}|n\rangle$$

$$= -e\left(\langle n|\underline{r}|\partial_\lambda n\rangle + \langle \partial_\lambda n|\underline{r}|n\rangle\right)$$

$$= -2e\,\mathrm{Re}\langle n|\underline{r}|\partial_\lambda n\rangle$$

Exercise 3.11




Exercise 3.12

*No solution yet*

Exercise 3.13

*No solution yet*

Exercise 3.14

*No solution yet*

Exercise 3.15

*No solution yet*

Exercise 3.16

*No solution yet*

## Exercise 3.17

(a) $x|w_n\rangle = \frac{a}{2\pi} i \int dk\, e^{ikx} |\partial_k u_{nk}\rangle$

$\langle w_n | x = \frac{a}{2\pi}(-i) \int dk' e^{ik'x} |\partial_{k'} u_{nk'}\rangle$

Inner product $\Rightarrow \frac{2\pi}{a}\delta(k-k')$

$\therefore \langle w_n | x^2 | w_n\rangle = \frac{a}{2\pi}\int dk \langle \partial_k u_{nk} | \partial_k u_{nk}\rangle$

(b) $\langle \partial_k u_{nk} | \partial_k u_{nk}\rangle = \langle \partial_k u_{nk} | \left(Q_k + |u_{nk}\rangle\langle u_{nk}|\right) |\partial_k u_{nk}\rangle$

Term involving $Q_k \Rightarrow \tilde{\Omega}_n$

Other term $\Rightarrow \frac{a}{2\pi}\int dk \underbrace{\langle \partial_k u_{nk} | u_{nk}\rangle}_{= -\langle u_{nk}|\partial_k u_{nk}\rangle} \langle u_{nk}|\partial_k u_{nk}\rangle$

$= \frac{a}{2\pi}\int dk\, A_{nk}^2$ ✓

(c) $\bar{x}_n = \frac{a}{2\pi}\int dk\, A_{nk} = \bar{A}_n$

$\frac{a}{2\pi}\int dk (A_{nk} - \bar{A}_n)^2 = \frac{a}{2\pi}\int dk\, A_{nk}^2 - 2\bar{A}_n \underbrace{\frac{a}{2\pi}\int dk\, A_{nk}}_{\bar{A}_n} + \bar{A}_n^2 \underbrace{\frac{a}{2\pi}\int dk}_{1}$

$= \left(\frac{a}{2\pi}\int dk\, A_{nk}^2\right) - \bar{A}_n^2$

$\bar{A}_n^2 \hookleftarrow \bar{x}_n^2$

(d) $|\tilde{u}_{nk}\rangle = e^{i\beta(k)}|u_{nk}\rangle \Rightarrow |\partial_k \tilde{u}_{nk}\rangle = |\partial_k u_{nk}\rangle + i\partial_k\beta |u_{nk}\rangle$

$\langle \partial_k \tilde{u}_{nk} | Q_k | \partial_k \tilde{u}_{nk}\rangle$

$\hookleftarrow\hookrightarrow$ $Q_k$ kills $(i\partial_k\beta)|u_{nk}\rangle$ pieces

So $\tilde{\Omega}_n$ is gauge-invariant.

(e) $\Omega_n = \tilde{\Omega}_n + \frac{a}{2\pi}\int dk (A_{nk} - \bar{A}_n)^2$

$\tilde{\Omega}_n$ is gauge-invariant, as is $\bar{A}_n$.

The second term cannot be negative, so if we can make it zero, we have minimized $\Omega_n$.

But we can choose $A_{nk} = \bar{A}_n$ indep. of $k$, so this does it.

Exercise 3.18

*No solution yet*

Exercise 3.19

See sample solution program ex-3.19.py

(a) The band gap closes at a critical value of *t* around 0.86eV

(b) For small *t*, the Wannier center sits on the atomic site, while for large *t*, it sits at a mid-bond position

(c) Strong *t*: weakly interacting dimers. Weak *t*: Wannier function is *s*-like.

Exercise 3.20

*No solution yet*

Exercise 3.21

*No solution yet*

## Exercise 3.22

See sample solution program ex-3.22.py

Output:

```
Unmodified at chain end

Finite-chain Wannier centers associated with band 0:
 0.3329 1.3193 2.3188 3.3188 4.3188 5.3188 6.3188 7.3188 8.3184 9.3073

Finite-chain Wannier centers associated with band 1:
 0.0697 0.9225 1.9106 2.9093 3.9092 4.9092 5.9093 6.9100 7.9155 8.9548

First 10 finite-chain Wannier centers for both bands:
 0.0195 0.3627 0.8962 1.3436 1.8871 2.3421 2.8861 3.3419 3.8860 4.3419

Modified site energies at chain end

Finite-chain Wannier centers associated with band 0:
 0.2787 1.3175 2.3187 3.3188 4.3188 5.3188 6.3188 7.3188 8.3184 9.3073

Finite-chain Wannier centers associated with band 1:
 0.1148 0.9246 1.9107 2.9093 3.9092 4.9092 5.9093 6.9100 7.9155 8.9548

First 10 finite-chain Wannier centers for both bands:
 0.0078 0.3646 0.8971 1.3437 1.8871 2.3421 2.8861 3.3419 3.8860 4.3419

Also modified hopping at chain end

Finite-chain Wannier centers associated with band 0:
 0.3648 1.3211 2.3189 3.3188 4.3188 5.3188 6.3188 7.3188 8.3184 9.3073

Finite-chain Wannier centers associated with band 1:
 0.0358 0.8976 1.9089 2.9092 3.9092 4.9092 5.9093 6.9100 7.9155 8.9548

First 10 finite-chain Wannier centers for both bands:
 0.0010 0.3586 0.8930 1.3429 1.8867 2.3420 2.8861 3.3419 3.8860 4.3419
```

Exercise 3.23

(a) $\tilde{A}_{\mu,mn} = (U^+ A U)_{mn} + (U^+ i\partial_\mu U)_{mn}$

$\mathrm{Tr}[\tilde{A}_\mu] = \underbrace{\mathrm{Tr}[U^+ A U]}_{\mathrm{Tr}[A]\ (\text{use cyclic property})} + \mathrm{Tr}[U^+ i\partial_\mu U]$

(b) $U = V B V^+ \quad (B \text{ diagonal}, B_{mn} = e^{-i\beta_n}\delta_{mn})$

$\Delta \mathrm{Tr}[A_\mu] = i\mathrm{Tr}[V B^+ V^+ \partial_\mu (V B V^+)]$

$\partial_\mu$ acts on $V$: $\Rightarrow i\mathrm{Tr}[V B^+ V^+ (\partial_\mu V) B V^+]$

$= i\mathrm{Tr}[V^+ (\partial_\mu V)]$

$\partial_\mu$ acts on $V^+$: $\Rightarrow i\mathrm{Tr}[(\partial_\mu V^+) V]$

These add to $i\mathrm{Tr}[\partial_\mu (V^+ V)] = i\mathrm{Tr}[\partial_\mu \mathbb{1}] = 0$

so $\Delta \mathrm{Tr}[A_\mu] = i\mathrm{Tr}[B^+ (\partial_\mu B)] \to -i\begin{pmatrix} (\partial_\mu \beta_1) e^{-i\beta_1} & & \\ & \ddots & \\ & & (\partial_\mu \beta_n) e^{-i\beta_n} \end{pmatrix}$

$= \sum_n (\partial_\mu \beta_n) = \partial_\mu \beta$

Check: $\beta = -\mathrm{Im}\ln\det U = -\mathrm{Im}\ln\det B = \sum_n \beta_n$ ✓

(c) $\bar{x}_n = \frac{V}{(2\pi)^3}\int_{BZ} d^3k\, A_{n,x}(\underline{k})$

$\bar{x}_{tot} = \sum_n \bar{x}_n = \frac{V}{(2\pi)^3}\int_{BZ} d^3k\, \mathrm{Tr}[A_x]$

$\Delta$ from gauge change $= \frac{V}{(2\pi)^3}\int_{BZ} d^3k\, (\partial_x \beta)$

$= \frac{bc}{(2\pi)^2}\int dk_y \int dk_z \frac{a}{2\pi}\underbrace{\int_0^{2\pi/a} (\partial_{k_x}\beta)\, dk_x}_{\beta(\frac{2\pi}{a}) = \beta(0) \Rightarrow 0}$

(d) Now $\int_0^{2\pi/a} (\partial_{k_x}\beta)\, dk_x = 2\pi m$ (Const!), $\frac{b}{2\pi}\int dk_y = 1$ etc.

$\Delta \bar{x}_{tot} = ma$ ✓

# Chapter 4

Exercise 4.1

*No solution yet*

Exercise 4.2

*No solution yet*

Exercise 4.3

Start from (4.25) (see Errata : "$i$" does not belong):

$$\langle \mathcal{O} \rangle_{n\underline{k}} / \dot{\lambda} = 2\hbar \, \mathrm{Im} \langle \partial_\lambda u_{n\underline{k}} | T_{n\underline{k}} \mathcal{O} | u_{n\underline{k}} \rangle$$

$$= 2\hbar \, \mathrm{Im} \langle u_{n\underline{k}} | (\partial_\lambda H_{\underline{k}}) T_{n\underline{k}}^2 \mathcal{O} | u_{n\underline{k}} \rangle$$

Here $H_{\underline{k}} = \frac{1}{2m} (\hat{p} + \hbar \underline{k} - e\underline{\lambda})^2$, $\underline{\lambda} = -\frac{1}{c}\underline{A} = \underline{\varepsilon} t$ $(\dot{\underline{\lambda}} = \underline{\mathcal{E}})$

$$\partial_{\lambda_\nu} H_{\underline{k}} = \frac{1}{m} (\hat{p} + \hbar \underline{k} - e\underline{\lambda})_\nu (-e) = -e v_{\underline{k},\nu}$$

Note $\langle \mathcal{O} \rangle_{n\underline{k}} / \dot{\lambda} = \partial_{\mathcal{E}_\nu} \langle \mathcal{O} \rangle_{n\underline{k}}$

$\therefore$ We call this $\partial_\nu \langle \mathcal{O} \rangle_{n\underline{k}}$

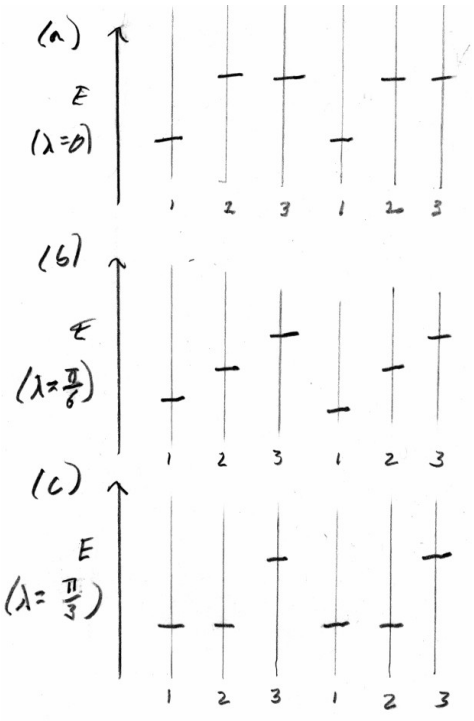
So $\partial_\nu \langle \mathcal{O} \rangle_{n\underline{k}} = -2e\hbar \, \mathrm{Im} \langle u_{n\underline{k}} | v_{\underline{k},\nu} T_{n\underline{k}}^2 \mathcal{O} | u_{n\underline{k}} \rangle$

After integrating over the BZ, we get Eq. (4.22), from which formulas such as (4.23) follow.

Exercise 4.4

*No solution yet*

## Exercise 4.5




The three sketches show the site energies of the model for three sequential values of the cyclic parameter covering 1/6 of a cycle.

(a)

- The WF of band 1 (lowest in energy) will "fall to the bottom" near 1.0, 1.1, and 1.5 in frames (a-c) respectively.
- The WF of band 3 will "bubble to the top" near 2.5, 2.9, and 3.0 respectively (referring to the horizontal axis).
- The WF of band 2 is harder to guess, since site 1 is taken, it is also shared between sites 2 and 3 in (a), i.e., at 2.5. Then it moves to 2 and then 1.5 in (b) and (c).
- So WF 1 and 3 move to the right by 3 sites in a full cycle, while WF 2 moves left by 6 sites. This is consistent with Chern numbers 1, -2, and 1 for bands 1, 2, and 3, respectively.

(b) See PythTB solution program. I intended for you to plot the individual Wannier center positions of bands 1+2, not just their sum. Since the total Chern number is -1, there is an overall downward flow of one unit, shared between the two Wannier bands.

## Exercise 4.6

*No solution yet*

## Exercise 4.7

*No solution yet*

## Exercise 4.8

There were errors of prefactors in the problem statement. Below (4.61) I defined $\rho_j = -e\bar{\phi}_j/2\pi$ so the equation at the bottom of p. 172 should have been

$$\rho_j = \frac{-e}{2\pi}\bar{\phi}^{(n_j)}$$

and near the end of the problem statement I should have written

$$\rho_j = \frac{e}{2\pi}\,\mathrm{Im}\,\ln\det M$$

The k-point string only connects $\underline{k}=\underline{0}$ and $\underline{k}=\underline{b}_j$. So there is only one inner product

$$M^{\underline{0},\underline{b}_j}_{mn} = \langle u_{m\underline{0}} | u_{m\underline{b}_j}\rangle$$

$$= \langle u_{m\underline{0}} | e^{-i\underline{b}_j\cdot\underline{r}} | u_{m\underline{0}}\rangle = M_{mn}$$

Call this $M_{mn}$.

$\phi = -\mathrm{Im}\ln\det M$ for this string.

But there is only one string, so $\bar{\phi}=\phi$, and

$$\rho_j = \frac{-e}{2\pi}\bar{\phi}_n = \frac{e}{2\pi}\,\mathrm{Im}\ln\det(M)$$

Exercise 4.9

The problem statement is misleading since I neglected to specify that ionic contributions should be ignored for the purposes of this argument.

(a) There are N bands and N Wannier functions. Each shifts by $\frac{a}{2}$ along x, so

$$\Delta P_x^{elec} = \underbrace{(-Ne)}_{\Delta \text{ dipole}}\underbrace{\left(\frac{a}{2}\right)}\underbrace{\frac{1}{ab}}_{1/\text{area}} = \frac{-Ne}{2b}$$

(b) The polarization lattice is defined modulo $\frac{ea}{ab} = \frac{e}{b}$, so N must be even.

Exercise 4.10

*No solution yet*

Exercise 4.11

*No solution yet*

Exercise 4.12

See modified chain_alt_surf.py.

For the last part, note that the model has ionic charges of +1 at $x=0$ and $x=\frac{1}{2}$ as well as the Wannier center at $\bar{x}$ (charge -2). $\Delta Q$ is obtained first by counting how many ionic charges and how many Wannier centers are left over at the surface after the tiling is finished — or, if you like, the charge in the "last tile" (like in Fig. 4.15 (b), dotted tile).

# Chapter 5

## Exercise 5.1

Let's label the bands so that the group below the lower gap is group A, then the isolated group is B, and all higher bands form C, and let the total Chern number of each group be $C_A$, $C_B$, and $C_C$. If the Fermi energy lies between groups A and B, then a cycle drives $C_A$ electrons to the top edge, requiring a net number $C_A$ of downgoing (vs. upgoing) edge channels. A similar argument applies to the gap between B and C, where the number of edge channels is $(C_A + C_B)$. Thus, the Chern number $C_B$ of group B is equal to the difference between the number of downdoing edge channels in the gaps above and below the group.

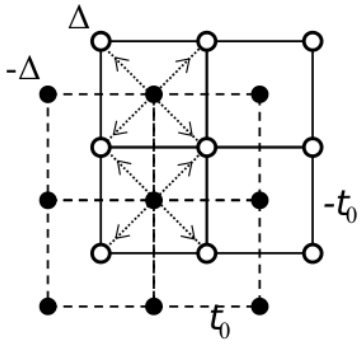
Note that I asked here about the Chern number of the group of bands B; this is by definition the BZ integral of the Berry curvature of these bands. It is also possible to assign a Chern number to a gap; this is by definition the total Chern number of all bands under that gap. The latter is only related to the edge channels crossing the gap in question, but this is not the kind of Chern number I asked about.

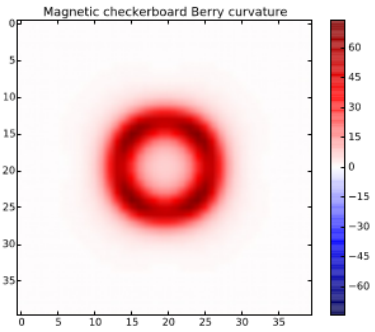
## Exercise 5.2

*No solution yet*

## Exercise 5.3

(a) A sketch of the model is shown below. The hoppings shown by dotted arrows pointing up-right, up-left, down-left and down-right are respectively *t'*, *it'*, *-t'* and *-it'*.

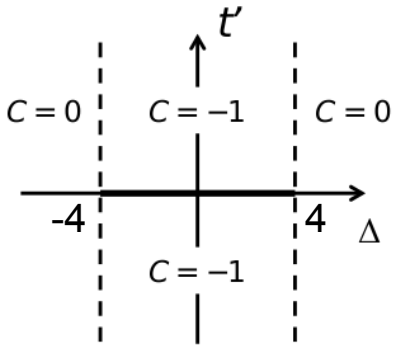



In what follows I take $t_0$=+1 unless otherwise specified.

(b) When $t'$ = 0, the two sublattices are decoupled and intersect on a curve when $-4 < \Delta < 4$. For $\Delta$ a bit less than +4 this is a loop around the Γ point (0,0) (shown above right); for $\Delta$ a bit greater than −4 this is a loop around the M point (π, π); and for $\Delta$ near zero it looks close to a diamond shape. When $t'$ is turned on, the system is gapped all along this curve, becoming an insulator.

(c) The system is a normal insulator if $|\Delta| > 4$, and a QAH insulator with $C$ = Chern number = −1 if $|\Delta| < 4$ as long as $t'$ is not zero. A sketch of the phase diagram for fixed $t_0$ = +1 is shown at right (vertical dashed lines are at $\Delta = \pm 4$; system has gap closures there and on heavy horizontal line segment). It may seem strange that flipping the sign of $t'$ does not reverse the Chern number, but actually that is equivalent to a simple redefinition of the sign of the TB orbitals on one sublattice but not the other, which should not change the physics. On the other hand, reversing the sign of $t_0$ does flip the sign of the Chern number, basically because it interchanges the lower (valence) and upper (conduction) bands.




(d) See ex-5.3.py.

## Exercise 5.4

*No solution yet*

## Exercise 5.5

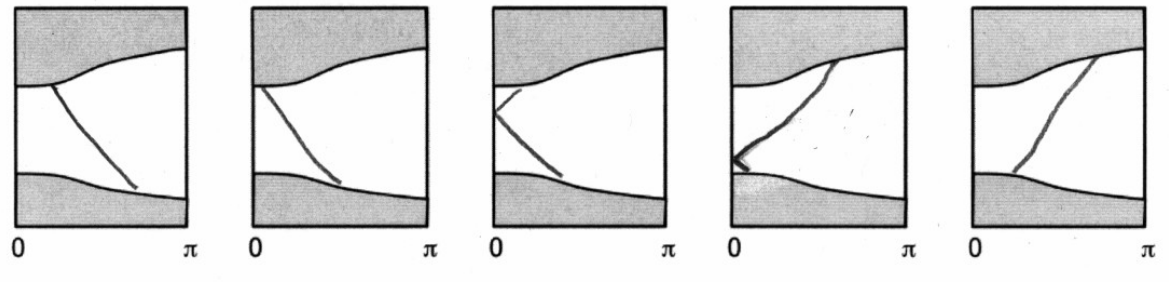
*No solution yet*

## Exercise 5.6

*No solution yet*

Exercise 5.7

Here is one possible scenario:




Exercise 5.8

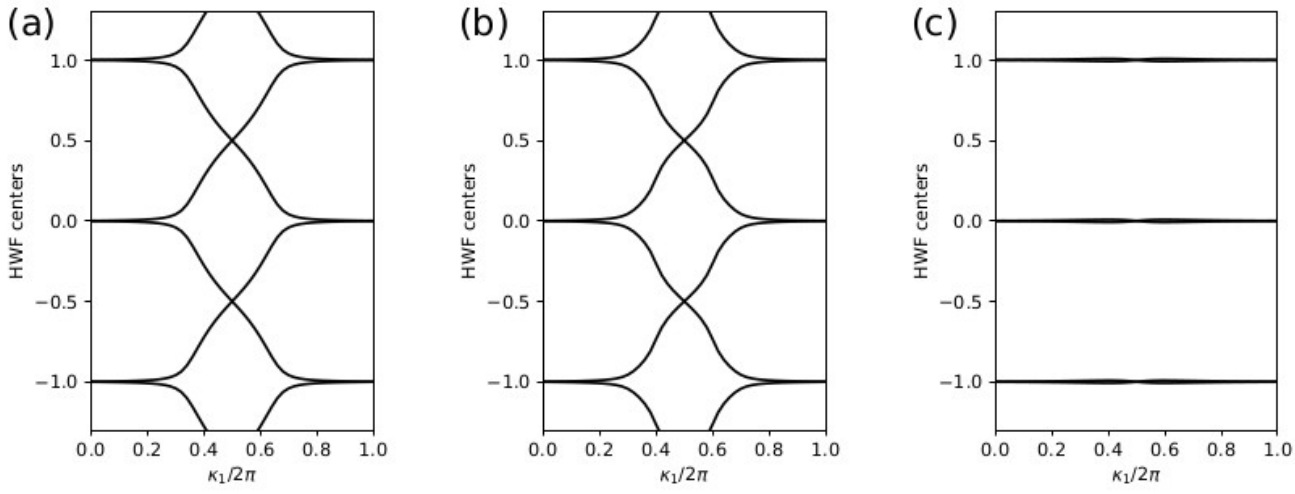
*No solution yet*

Exercise 5.9

*No solution yet*

Exercise 5.10

See sample solution program ex-5.10.py, which generated the figure below:
(a) Only sigma_z coupling (topo phase); (b) With Rashba (topo phase); (c) with Rashba (trivial phase).
You may need to be a bit careful to avoid a metallic bulk band structure.

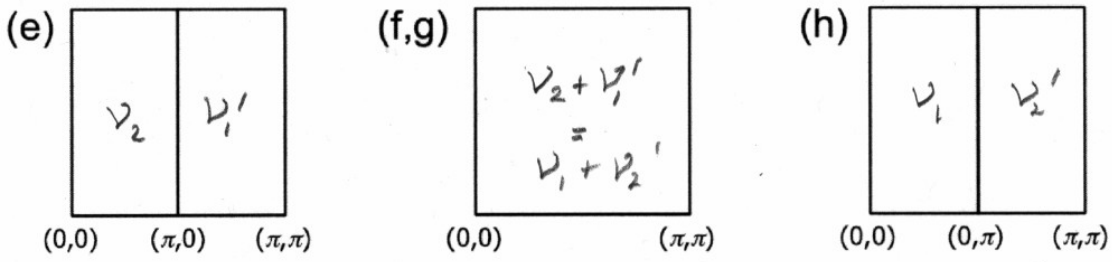



Exercise 5.11

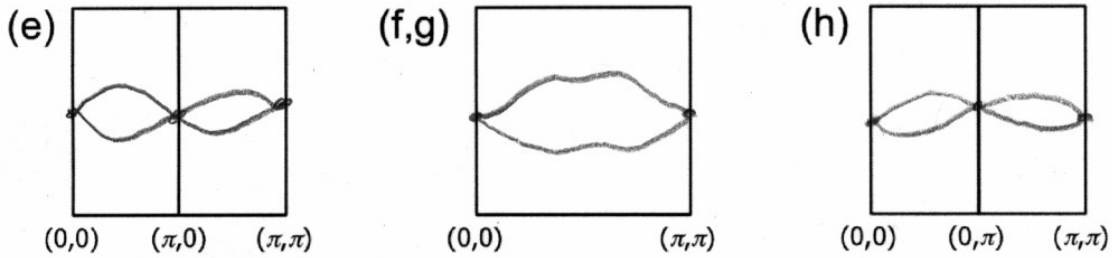
*No solution yet*

Exercise 5.12

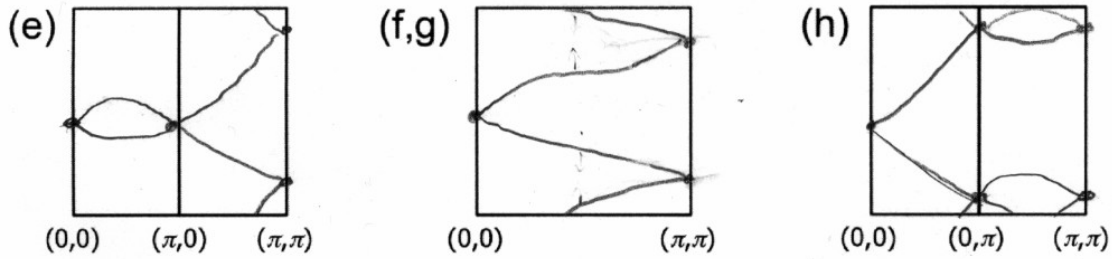
Indices:



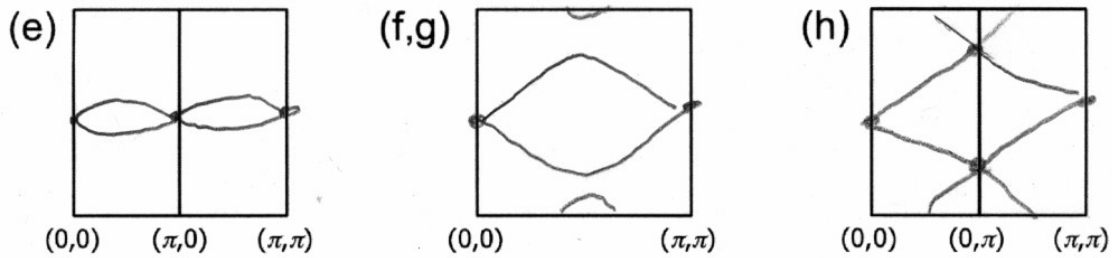

From Fig. 5.16(a): $\nu_1 = \nu_2' = \nu_2 = \nu_2' = 0$




From Fig. 5.16(b): $\nu_1 = \nu_1' = 1$, $\nu_2 = \nu_2' = 0$




From Fig. 5.16(c): $\nu_1 = \nu_2' = 1$, $\nu_1' = \nu_2 = 0$



Exercise 5.13

| | $\nu_2$ | $\nu_2'$ | $\nu_3$ | $\nu_3'$ |
|---|---|---|---|---|
| (a) | 0 | 0 | 1 | 1 |
| (b) | 0 | 0 | 1 | 1 |
| (c) | 1 | 1 | 1 | 1 |
| (d) | 1 | 0 | 1 | 0 |
| (e) | 0 | 1 | 1 | 0 |
| (f) | 1 | 0 | 1 | 0 |

Last column:
Deduce from
$\nu_2 \nu_2' = \nu_3 \nu_3'$ $(= \nu_0)$