HW #5 Solution

Problem I

Let's try $\phi = \phi_0 e^{ikna}$.

$$\begin{bmatrix} a & ib & -ib \\ -ib & a & ib \\ ib & -ib & a \end{bmatrix} \{\phi\} = E \{\phi\}$$

Each line identically gives the following equation.

$$E = a + ib e^{ika} - ib e^{-ika}$$
$$= a - 2b \sin ka$$

According to the Hamiltonian given, we have periodic boundary condition. Which means,

$$e^{i3ka} = 1 \Rightarrow ka = \frac{2\pi n}{3} \quad (n : \text{integer})$$

ka E Eigenvectors

$$\begin{pmatrix} -\frac{2\pi}{3} \\ 0 \\ \frac{2\pi}{3} \end{pmatrix} \begin{matrix} \longrightarrow \\ \longrightarrow \\ \longrightarrow \end{matrix} \begin{pmatrix} a+\sqrt{3}\,b \\ a \\ a-\sqrt{3}\,b \end{pmatrix} \begin{matrix} ① \\ ② \\ ③ \end{matrix} \qquad \overset{①}{\begin{pmatrix} e^{i2\pi/3} \\ 1 \\ e^{-i2\pi/3} \end{pmatrix}}, \overset{②}{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}}, \overset{③}{\begin{pmatrix} e^{-i2\pi/3} \\ 1 \\ e^{i\frac{2\pi}{3}} \end{pmatrix}}$$

Problem 2

$$
H = \begin{array}{c} \begin{array}{cccccc} 1 & & & & & 6\text{th} \end{array} \\ \begin{bmatrix} \varepsilon & t & & & & t \\ t & \varepsilon & t & & & \\ & t & \varepsilon & t & & \\ & & t & \varepsilon & t & \\ & & & t & \varepsilon & t \\ t & & & & t & \varepsilon \end{bmatrix} \end{array} \qquad (H^{+} = H)
$$

$$H\psi = E\psi$$

$$\psi = \psi_0 e^{ikna} \qquad n = 1, 2, 3, 4, 5, 6 \quad \text{(atom index)}$$

Each line will give the following equation.

$$E = \varepsilon + t e^{ika} + t e^{-ika} = \varepsilon + 2t\cos ka$$

PBC $\quad e^{ik\cancel{n}a\,6} = e^{ik\cancel{n}a} \Rightarrow e^{ik6a} = 1 \Rightarrow ka = \dfrac{\nu\pi}{3}$; ν: integer

$$\left(k = \frac{\nu\pi}{3a}\right)$$

$$ka \Rightarrow \left\{0, \frac{\pi}{3}, \frac{2\pi}{3}, \pi, \frac{4}{3}\pi, \frac{5}{3}\pi\right\}$$

$$E \Rightarrow \{\varepsilon+2t, \varepsilon+t, \varepsilon-t, \varepsilon-2t, \varepsilon-t, \varepsilon+t\}$$

eigen vector

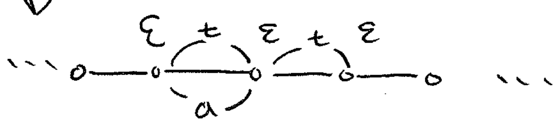
$$
\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}
\begin{pmatrix} e^{i\pi/3} \\ e^{i2\pi/3} \\ e^{i\pi} = -1 \\ e^{i\frac{4}{3}\pi} \\ e^{i5/3\pi} \\ 1 \end{pmatrix}
\begin{pmatrix} e^{i2\pi/3} \\ e^{i4\pi/3} \\ 1 \\ e^{i8\pi/3} \\ e^{i10\pi/3} \\ 1 \end{pmatrix}
\begin{pmatrix} e^{i\pi} = -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}
\begin{pmatrix} e^{i4\pi/3} \\ e^{i8\pi/3} \\ 1 \\ e^{i16\pi/3} \\ e^{i20\pi/3} \\ 1 \end{pmatrix}
\begin{pmatrix} e^{i5\pi/3} \\ e^{i10\pi/3} \\ -1 \\ e^{i20\pi/3} \\ e^{i25\pi/3} \\ 1 \end{pmatrix}
$$

$$\frac{1}{\sqrt{6}}\left[\begin{Bmatrix}1\\1\\1\\1\\1\\1\end{Bmatrix},\begin{Bmatrix}e^{i\pi/3}\\e^{i2\pi/3}\\-1\\e^{i4\pi/3}\\e^{i5\pi/3}\\1\end{Bmatrix},\begin{Bmatrix}e^{i2\pi/3}\\e^{i4\pi/3}\\1\\e^{i2\pi/3}\\e^{i4\pi/3}\\1\end{Bmatrix},\begin{Bmatrix}-1\\1\\-1\\1\\-1\\1\end{Bmatrix},\begin{Bmatrix}e^{i4\pi/3}\\e^{i2\pi/3}\\1\\e^{i4\pi/3}\\e^{i2\pi/3}\\1\end{Bmatrix},\begin{Bmatrix}e^{i5\pi/3}\\e^{i4\pi/3}\\-1\\e^{i2\pi/3}\\e^{i\pi/3}\\1\end{Bmatrix}\right]$$

problem 3

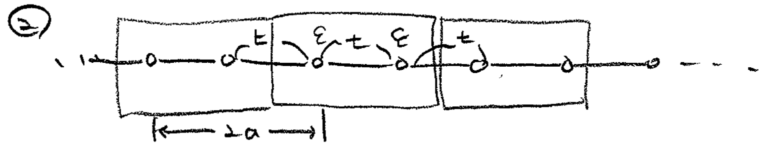
Two approaches equivalent

①



$$\Rightarrow \quad E = \varepsilon + te^{ika} + te^{-ika} = \varepsilon + 2t\cos ka \quad (-\pi \le ka \le \pi)$$

②



$$\det\left[E\, I_{2\times 2} - \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{2ika} - \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} e^{-2ika} - \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}\right]$$

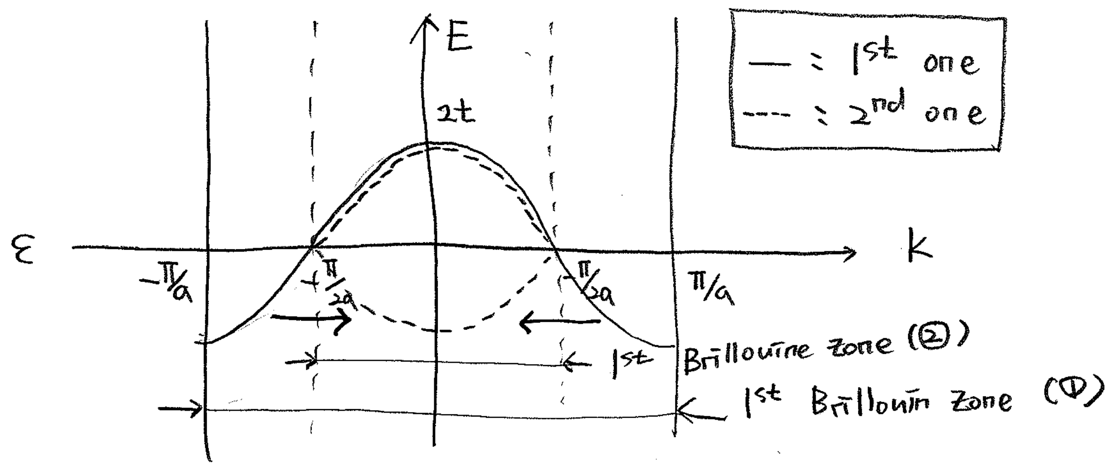
$$= \det \begin{bmatrix} E-\varepsilon & -(t+te^{-2ika}) \\ -(t+te^{2ika}) & E-\varepsilon \end{bmatrix} = 0$$

$$\Rightarrow \quad E = \varepsilon \pm \sqrt{(t+te^{-2ika})(t+te^{2ika})}$$

$$= \varepsilon \pm t\sqrt{(e^{ika}+e^{-ika})(e^{-ika}+e^{ika})}$$

$$= \varepsilon \pm t\,(2\cos ka)$$

$$= \varepsilon \pm 2t\cos ka \quad (-\pi \le k\cdot(2a) \le \pi)$$



$E > \varepsilon$ parts are equivalent (① & ②)

$E < \varepsilon$, ② Eigenvalues corresponding to $\frac{\pi}{2a} \le |k| \le \frac{\pi}{a}$

Folded into the $0 \le |k| \le \frac{\pi}{2a}$ region ① with same

eigenvalues & eigenvectors.

These are two approaches to solve the same problem.