Ph135 - Problem Set 6

November 28, 2018

Problem 1

We first diagonalize M using plane wave ansatz. Let

$$\vec{v}(p) = (\dots, e^{2ipa}, e^{ipa}, 1, e^{-ipa}, e^{-2ipa}, \dots)^T, \tag{1}$$

then

$$\begin{aligned}
\sum_{n=-\infty}^{\infty} M_{mn} v_n(p) &= \sum_{n=-\infty}^{\infty} \left(\delta_{nm} + e^{-\lambda a} \left(1 + \frac{\lambda a}{2}\right) \delta_{|n-m|,1} \right) e^{-inpa} \\
&= e^{-impa} + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right)\left(e^{-i(m+1)pa} + e^{-i(m-1)pa}\right) \\
&= e^{-impa} + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right) 2\cos(pa) e^{-impa} \\
&= \left\{1 + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right) 2\cos(pa)\right\} e^{-impa},
\end{aligned} \tag{2}$$

Hence, $\vec{v}(p)$ is an eigenvector of M with eigenvalue

$$\lambda(p) = 1 + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right) 2\cos(pa). \tag{3}$$

Hence

$$M = UDU^\dagger, \tag{4}$$

where the columns of U are $\vec{v}(p)$, and D is diagonal with entries $\lambda(p)$.

Next, we observe that

$$\begin{aligned}
h_{nm} &= -|\epsilon| M_{nm} + \frac{mV_0^2}{2\hbar^2} e^{-\lambda a} \delta_{|n-m|,1} \\
&= \epsilon\left(\delta_{nm} + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right)\delta_{|n-m|,1}\right) - \epsilon e^{-\lambda a} \delta_{|n-m|,1} \\
&= \epsilon\left(\delta_{nm} + e^{-\lambda a}\frac{\lambda a}{2}\delta_{|n-m|,1}\right),
\end{aligned} \tag{5}$$

which has the same form as

$$M_{nm} = \delta_{nm} + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right)\delta_{|n-m|,1}, \tag{6}$$

so the plane wave basis also diagonalizes h_{nm}, with eigenvalues

$$\mu(p) = \epsilon\Big(1 + e^{-\lambda a}\lambda a \cos(pa)\Big). \tag{7}$$

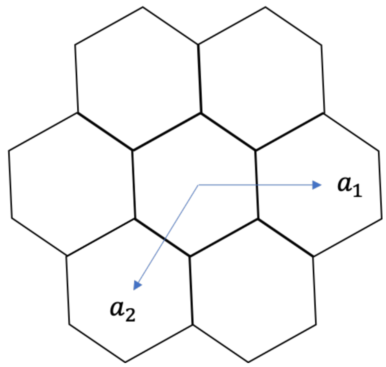

Figure 1: Illustration of the lattice and basis vectors.

The tight-binding energy eigenvalues, which are the eigenvalues of the matrix

$$h_{\text{eff}} = M^{-1/2} h M^{-1/2}, \tag{8}$$

is therefore given by

$$\begin{aligned} E(p) &= \frac{\mu(p)}{\lambda(p)} \\ &= \epsilon - \frac{2\epsilon e^{-\lambda a}\cos(pa)}{1 + e^{-\lambda a}(2+\lambda a)\cos(pa)}, \end{aligned} \tag{9}$$

and

$$E(p) \approx \epsilon - 2\epsilon e^{-\lambda a}\cos(pa) \tag{10}$$

in the strongly bound limit ($\lambda a \gg 1$).

Problem 2

(a) The basis vector are given by

$$\vec{a}_1 = (\sqrt{3}a, 0), \quad \vec{a}_2 = (-\frac{\sqrt{3}a}{2}, -\frac{3a}{2}), \tag{11}$$

illustrated in Figure 1.

(b) The time-independent Schrödinger equation reads

$$\begin{cases} H\psi^A_{\vec{r}} = -t\psi^B_{\vec{r}} - t\psi^B_{\vec{r}-\vec{a}_1} - t\psi^B_{\vec{r}+\vec{a}_2} = E\psi^A_{\vec{r}} \\ H\psi^B_{\vec{r}} = -t\psi^A_{\vec{r}} - t\psi^A_{\vec{r}+\vec{a}_1} - t\psi^B_{\vec{r}-\vec{a}_2} = E\psi^B_{\vec{r}}. \end{cases} \tag{12}$$

(c) To solve the Schrödinger equation above, we use the plane wave ansatz

$$\begin{pmatrix} \psi^A_{\vec{r}} \\ \psi^B_{\vec{r}} \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} e^{i\vec{p}\cdot\vec{r}}, \tag{13}$$

and (12) reads

$$\begin{aligned} H\begin{pmatrix} u \\ v \end{pmatrix} e^{i\vec{p}\cdot\vec{r}} &= -t\begin{pmatrix} (1+e^{-i\vec{p}\cdot\vec{a}_1} + e^{i\vec{p}\cdot\vec{a}_2})v \\ (1+e^{i\vec{p}\cdot\vec{a}_1} + e^{-i\vec{p}\cdot\vec{a}_2})u \end{pmatrix} \\ &= \begin{pmatrix} 0 & -t(1+e^{-i\vec{p}\cdot\vec{a}_1} + e^{i\vec{p}\cdot\vec{a}_2}) \\ -t(1+e^{i\vec{p}\cdot\vec{a}_1} + e^{-i\vec{p}\cdot\vec{a}_2}) & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \end{aligned} \tag{14}$$

The energy eigenvalues are therefore given by

$$E(\vec{p}) = \pm t\sqrt{(1+e^{-i\vec{p}\cdot\vec{a}_1}+e^{i\vec{p}\cdot\vec{a}_2})(1+e^{i\vec{p}\cdot\vec{a}_1}+e^{-i\vec{p}\cdot\vec{a}_2})}$$
$$= \pm t\sqrt{3+2\cos(\vec{p}\cdot\vec{a}_1)+2\cos(\vec{p}\cdot\vec{a}_2)+2\cos(\vec{p}\cdot\vec{a}_1+\vec{p}\cdot\vec{a}_2)}, \tag{15}$$

with corresponding eigenstates

$$\begin{pmatrix} u \\ v \end{pmatrix} = \frac{1}{\sqrt{3+2\cos(\vec{p}\cdot\vec{a}_1)+2\cos(\vec{p}\cdot\vec{a}_2)+2\cos(\vec{p}\cdot\vec{a}_1+\vec{p}\cdot\vec{a}_2)}} \begin{pmatrix} \sqrt{1+e^{i\vec{p}\cdot\vec{a}_1}+e^{-i\vec{p}\cdot\vec{a}_2}} \\ \mp\sqrt{1+e^{-i\vec{p}\cdot\vec{a}_1}+e^{i\vec{p}\cdot\vec{a}_2}} \end{pmatrix}. \tag{16}$$

(d) We first find the reciprocal lattice vectors

$$\vec{k}_1 = (\frac{2\pi}{\sqrt{3}a}, -\frac{2\pi}{3a}), \quad \vec{k}_2 = (0, -\frac{4\pi}{3a}). \tag{17}$$

We want to find $\vec{p} = p_1\vec{k}_1 + p_2\vec{k}_2$, such that $E(\vec{p}) = 0$, which by (15) is equivalent to

$$1+e^{-i\vec{p}\cdot\vec{a}_1}+e^{i\vec{p}\cdot\vec{a}_2} = 0, \tag{18}$$

so the real and imaginary part are both equal to 0, from which we get the two solutions

$$\vec{p}_K = \frac{1}{3}\vec{k}_1 - \frac{2}{3}\vec{k}_2$$
$$= \left(\frac{2\pi}{3\sqrt{3}a}, \frac{2\pi}{3a}\right), \tag{19}$$

and

$$\vec{p}_{K'} = \frac{1}{3}\vec{k}_1 + \frac{1}{3}\vec{k}_2$$
$$= \left(\frac{2\pi}{3\sqrt{3}a}, -\frac{2\pi}{3a}\right). \tag{20}$$

For $\vec{p}$ close to $\vec{p}_K$, we expand

$$\vec{p} = \vec{p}_K + \delta\vec{p}$$
$$= \left(\frac{2\pi}{3\sqrt{3}a} + \delta p_x, \frac{2\pi}{3a} + \delta p_y\right) \tag{21}$$

then

$$E = \pm t\sqrt{3+2\cos(\vec{p}\cdot\vec{a}_1)+2\cos(\vec{p}\cdot\vec{a}_2)+2\cos(\vec{p}\cdot\vec{a}_1+\vec{p}\cdot\vec{a}_2)}$$
$$= \pm t\sqrt{3+2\cos\left(\sqrt{3}p_x a\right)+2\cos\left(\frac{\sqrt{3}}{2}p_x a+\frac{3}{2}p_y a\right)+2\cos\left(\frac{\sqrt{3}}{2}p_x a-\frac{3}{2}p_y a\right)}$$
$$= \pm t\sqrt{3+2\cos\left(\sqrt{3}p_x a\right)+4\cos\left(\frac{\sqrt{3}}{2}p_x a\right)\cos\left(\frac{3}{2}p_y a\right)}$$
$$\approx \pm t\sqrt{3+2\left(-\frac{1}{2}+\sqrt{3}a\delta p_x-\frac{1}{4}3a^2\delta p_x^2\right)+4\left(-\frac{1}{2}-\frac{3a}{4}\delta p_x+\frac{3}{16}a^2\delta p_x^2\right)\left(1-\frac{9}{8}a^2\delta p_y^2\right)}$$
$$\approx \pm t\sqrt{\frac{9}{4}a^2\delta p_x^2+\frac{9}{4}a^2\delta p_y^2}$$
$$= \pm\frac{3}{2}ta|\delta\vec{p}|$$
$$= \pm\frac{3}{2}ta|\vec{p}-\vec{p}_K|. \tag{22}$$

Therefore, $E(\vec{p}) \propto |\vec{p}-\vec{p}_K|$. Similarly, $E(\vec{p}) \propto |\vec{p}-\vec{p}_{K'}|$.