PHYS 563 HW5

Problem 1

The potential function $U(x)$ can be written as the following Fourier series:

$$U(x) = \sum_{n=1}^{\infty} V_n \cos\left(\frac{2\pi x}{a} n\right)$$

$$= \sum_{n=-\infty}^{\infty} \frac{V_n}{2} e^{i\frac{2\pi n x}{a}} \quad \left(\begin{matrix} V_n = V_{-n}, \ \forall n \in N \\ V_0 = 0 \end{matrix}\right)$$

Schrödinger equation is:

$$\left(\frac{\hbar^2}{2m} k^2 + U(x)\right)|\psi\rangle = \varepsilon |\psi\rangle$$

$$\Rightarrow \left(\frac{\hbar^2}{2m} k^2 - \varepsilon\right)|\psi\rangle + \sum_{n=-\infty}^{\infty} \frac{V_n}{2} e^{i\frac{2\pi n x}{a}} |\psi\rangle = 0$$

$$\Rightarrow \langle k | \left(\frac{\hbar^2}{2m} k^2 - \varepsilon\right)|\psi\rangle + \sum_{n=-\infty}^{\infty} \langle k | \frac{V_n}{2} e^{\frac{i2\pi n x}{a}} |\psi\rangle = 0$$

$$\Rightarrow (T_k - \varepsilon) \langle k|\psi\rangle + \sum_{n=-\infty}^{\infty} \langle k - G_n|\psi\rangle \frac{V_n}{2} = 0$$

$$\left(T_k := \frac{\hbar^2}{2m} k^2, \ G_n := \frac{2\pi n}{a}\right) \qquad (1.1)$$

We now want to calculate the perturbation of $|\psi\rangle$ with basis of $\{|k - G_n\rangle, n \forall Z\}$ from the 0-th order perturbation $|\psi\rangle^{(0)} = |k\rangle$, or equivalently:

$$|\psi\rangle = \sum_{n=-\infty}^{\infty} \langle k - G_n|\psi\rangle \, |k - G_n\rangle$$

and $|\langle k|\psi\rangle|^2 \gg |\langle k - G_n|\psi\rangle|^2, n \neq 0$

Then we define

$$T_0 := \frac{\hbar^2}{2m} k^2, \quad T_j := \frac{\hbar^2}{2m} |k - G_j|^2 \quad \forall j \in \mathbb{Z}$$

From (1.1), we know a more general equation:

$$(T_j - \varepsilon) \langle k - G_j | \psi \rangle + \sum_{n=-\infty}^{\infty} \frac{V_n}{2} \langle k - G_{j+n} | \psi \rangle = 0 \qquad (1.2)$$

We now want to solve $\langle k - G_j | \psi \rangle$ for $j \neq 0$.
In (1.2) we know since $|\langle k - G_{j+n} | \psi \rangle|^2 \ll |\langle k | \psi \rangle|^2$ for $j+n \neq 0$, thus the 1st order perturbation for $\langle k - G_j | \psi \rangle$ will be

$$(T_j - \varepsilon) \langle k - G_j | \psi \rangle + \frac{V_{-j}}{2} \langle k | \psi \rangle \approx 0$$

$$\Rightarrow \langle k - G_j | \psi \rangle = \frac{-V_{-j}}{2(T_j - \varepsilon)} \langle k | \psi \rangle \quad (1.3) \quad + O(V^2)$$

$$\therefore |\psi\rangle = |k\rangle + \sum_{j \neq 0} \frac{-V_{-j}}{2(T_j - \varepsilon)\langle k | \psi \rangle} |k - G_n\rangle + O(V^2) \qquad (1.3)$$

$$= |k\rangle + \sum_{j \neq 0} \frac{V_{-j}}{2(\varepsilon - T_j)\langle k | \psi \rangle} |k - G_n\rangle + O(V^2) \qquad (1.4)$$

To calculate the energy ε, we find from (1.1)

$$(T_0 - \varepsilon) \langle k | \psi \rangle + \sum_{n=-\infty}^{\infty} \langle k - G_n | \psi \rangle \frac{V_n}{2} = 0$$

$$\Rightarrow (T_0 - \varepsilon) \cdot 1 + \sum_{n=-\infty}^{\infty} \frac{V_n}{2} \cdot \frac{V_{-n}}{2(\varepsilon - T_n)} = 0 \quad (\because (1.3))$$

$$\Rightarrow \varepsilon = T_0 + \sum_{n=-\infty}^{\infty} \frac{|V_n|^2}{4(\varepsilon - T_n)} = T_0 + \sum_{n=-\infty}^{\infty} \frac{|V_n|^2}{4(T_0 - T_n)} + O(V^3)$$

(1.5)

We can see the last approximation in (1.5) holds for $|T_0 - T_n| \ll |V_n|$

(a) From (1.5), we can see that

$\varepsilon \approx T_0$ to the 1st order approximation of V which is the free electron approximation, and the condition is that

$$|T_0 - T_n| >> |V_n| \quad \forall\, n \neq 0,\ n \in \mathbb{Z}$$

(b) ① Near the gap at $k = \frac{\pi}{a}$, (1st & 2nd band)

$T_0 \approx T_1 \approx \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$, and to the 1-st order approximation, the determinant for eigen-energy is:

$$\begin{vmatrix} T_0 - \varepsilon & \frac{V_1}{2} \\ \frac{V_1}{2} & T_1 - \varepsilon \end{vmatrix} = 0 \quad \text{Similar to A\&M (9.24)}$$

$$\Rightarrow \varepsilon = \left(\frac{T_0 + T_1}{2}\right) \pm \sqrt{\left(\frac{T_0 - T_1}{2}\right)^2 + \left(\frac{V_1}{2}\right)^2}$$

And at $k = \frac{\pi}{a}$, $T_0 = T_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$

$$\therefore \varepsilon = T_0 \pm \left|\frac{V_1}{2}\right|, \quad \text{Gap} = V_1 = \varepsilon_+ - \varepsilon_-$$

② Near the gap at $k=0$ or $k = \frac{2\pi}{a}$ equivalently for extended zone (2nd & 3rd band gap)(reduced zone)

$$T_0 \approx \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = \frac{\hbar^2}{2m}\left|\frac{2\pi}{a} - \frac{4\pi}{a}\right|^2 \approx T_2$$

$$\begin{vmatrix} T_0 - \varepsilon & \frac{V_2}{2} \\ \frac{V_2}{2} & T_2 - \varepsilon \end{vmatrix} = 0 \Rightarrow \varepsilon = \left(\frac{T_0 + T_2}{2}\right) \pm \sqrt{\left(\frac{T_0 - T_2}{2}\right)^2 + \left(\frac{V_2}{2}\right)^2}$$

At the band edge, $\varepsilon = T_2 \pm \left|\frac{V_2}{2}\right|$

$T_0 = T_2 \quad \Rightarrow \text{Gap} = |V_2| = \varepsilon_+ - \varepsilon_-$

Problem 2

From (1.5), we know

$$\varepsilon = T_0 + \sum_{n=-\infty}^{\infty} \frac{|V_n|^2}{T_0 - T_n} + O(V^3)$$

For the lowest band, $T_0 < T_n$ for $n \neq 0, n \in \mathbb{Z}$

And $\left|\sum_{n=-\infty}^{\infty} \frac{|V_n|^2}{T_0 - T_n}\right| >> O(V^3)$

$$\therefore \varepsilon = T_0 + \sum_{n=-\infty}^{\infty} \frac{|V_n|^2}{T_0 - T_n} < \underset{\text{Free electron approximation}}{T_0} \quad \left(\because \frac{1}{T_0 - T_n} < 0\right)$$

for the lowest band

Problem 3.

$$U(x,y) = -V\cos(2\pi x/a)\cos(2\pi y/a)$$

$$= -\frac{V}{4}\left(e^{iGx}+e^{-iGx}\right)\left(e^{iGy}+e^{-iGy}\right)$$

$$= -\frac{V}{4}\sum_{m,n} e^{iG_m x + iG_n y}$$

$$(m,n) = (\pm 1, \pm 1)\ ,\ G_m := \frac{2\pi}{a}m$$

Following the philosophy of Problem 1,

$$T_{0,0} \simeq \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2+\left(\frac{\pi}{a}\right)^2\right]$$

$$= \frac{\hbar^2}{2m}\left(\left|\frac{\pi}{a}-\frac{2\pi}{a}\right|^2+\left|\frac{\pi}{a}-\frac{2\pi}{a}\right|^2\right)$$

$$\approx T_{1,1} \quad \left(T_{m,n} := \frac{\hbar^2}{2m}\left|\vec{k}-\vec{G}_{m,n}\right|^2\right)$$

$$\vec{G}_{m,n} := (G_m, G_n)$$

$\therefore$ We need to only consider the effect of $U_{1,1}$ perturbation :

$$\begin{vmatrix} T_{0,0}-\varepsilon & U_{1,1} \\ U_{1,1} & T_{1,1}-\varepsilon \end{vmatrix} = 0$$

$$\Rightarrow \quad \varepsilon = \frac{T_{0,0}+T_{1,1}}{2} \pm \sqrt{\left(\frac{T_{0,0}-T_{1,1}}{2}\right)^2+|U_{1,1}|^2}$$

$$\therefore \quad \text{Gap} = \varepsilon_+\left(T_{0,0}=T_{1,1}=\frac{\hbar^2}{2m}\cdot 2\left(\frac{\pi}{a}\right)^2\right) - \varepsilon_-(\text{same cond.})$$

$$= 2|U_{1,1}| = 2\cdot\frac{|V|}{4} = \frac{|V|}{2}$$

Problem 4.

A&M Problem 9.3

(a)

At around W point, there are four bands and four Brillouin zones approaching together to the W point, and their centers are

$$\vec{G}_{000} = \frac{2\pi}{a}(0,0,0) := \vec{G}_1$$

$$\vec{G}_{111} = \frac{2\pi}{a}(1,1,1) := \vec{G}_2$$

$$\vec{G}_{11\bar{1}} = \frac{2\pi}{a}(1,1,-1) := \vec{G}_3$$

$$\vec{G}_{200} = \frac{2\pi}{a}(2,0,0) := \vec{G}_4$$

Which means we need to solve the following eq. $\left(T_{klm} := \frac{\hbar}{2m}|\vec{k} - \vec{G}_{klm}|^2\right)$

$$(T_{000} - \varepsilon)\langle \vec{k} | \psi \rangle + \sum_{ijk} U_{ijk} \langle \vec{k} - \vec{G}_{ijk} | \psi \rangle = 0$$

or 111 $\quad \langle \vec{k} - \vec{G}_{111} | \psi \rangle \qquad \langle \vec{k} - \vec{G}_{i+1\, j+1\, k+1} | \psi \rangle$

or $11\bar{1}$ $\quad \langle \vec{k} - \vec{G}_{11\bar{1}} | \psi \rangle \qquad \langle \vec{k} - \vec{G}_{i+1\, j+1\, k-1} | \psi \rangle$

or 200 $\quad \langle \vec{k} - \vec{G}_{200} | \psi \rangle \qquad \langle \vec{k} - \vec{G}_{i+2\, j\, k} | \psi \rangle$

Where we only need to consider (i,j,k) so that (4.1)

$$\begin{aligned}
(i,j,k) + (0,0,0) &= (0,0,0) \text{ or} \\
(1,1,1) &\quad (1,1,1) \text{ or} \\
(1,1,-1) &\quad (1,1,-1) \text{ or} \\
(2,0,0) &\quad (2,0,0)
\end{aligned}$$

because only $\langle \vec{k} - \vec{G}_{000} | \psi \rangle$ are prominent.

$\quad 111$

$\quad 11\bar{1}$

$\quad 200$

We will list the (i,j,k) for the four cases:

V_{ijk} terms

① For $\langle \vec{k} - \vec{G}_{000} | \psi \rangle$,

$$(i,j,k) = (0,0,0) \Rightarrow U_{000} = 0$$
$$(1,1,1) \Rightarrow U_{111} = U_1$$
$$(1,1,-1) \Rightarrow U_{11\bar{1}} = U_1$$
$$(2,0,0) \Rightarrow U_{200} = U_2$$

② For $\langle \vec{k} - \vec{G}_{111} | \psi \rangle$,

$$(i,j,k) = (-1,-1,-1) \rightarrow U_{\bar{1}\bar{1}\bar{1}} = U_1$$
$$(0,0,0) \rightarrow U_{000} = 0$$
$$(0,0,-2) \rightarrow U_{00\bar{2}} = U_2$$
$$(1,-1,-1) \rightarrow U_{1\bar{1}\bar{1}} = U_1$$

③ For $\langle \vec{k} - \vec{G}_{11\bar{1}} | \psi \rangle$,

$$(i,j,k) = (-1,-1,1) \rightarrow U_{\bar{1}\bar{1}1} = U_1$$
$$(0,0,2) \rightarrow U_{002} = U_2$$
$$(0,0,0) \rightarrow U_{000} = 0$$
$$(1,-1,1) \rightarrow U_{1\bar{1}1} = U_1$$

④ For $\langle \vec{k} - \vec{G}_{200} | \psi \rangle$,

$$(i,j,k) = (-2,0,0) \rightarrow U_{\bar{2}00} = U_2$$
$$(-1,1,1) \rightarrow U_{\bar{1}11} = U_1$$
$$(-1,1,-1) \rightarrow U_{\bar{1}1\bar{1}} = U_1$$
$$(0,0,0) \rightarrow U_{000} = 0$$

We can rewrite (4.1) into a matrix to solve $\langle \vec{k} - \vec{G}_i | \psi \rangle$ $i = 1, 2, 3, 4$ and the eigen energy

$$\begin{vmatrix} T_1 - \varepsilon & U_1 & U_1 & U_2 \\ U_1 & T_2 - \varepsilon & U_2 & U_1 \\ U_1 & U_2 & T_3 - \varepsilon & U_1 \\ U_2 & U_1 & U_1 & T_4 - \varepsilon \end{vmatrix} = 0$$

$T_1 := T_{000}$, $T_2 := T_{111}$, $T_3 := T_{1\bar{1}\bar{1}}$, $T_4 := T_{200}$

At W point, $T_1 = T_2 = T_3 = T_4 = T$,

and the determinant value becomes

$$(T - \varepsilon - U_2)^2 \left[(T - \varepsilon + U_2)^2 - 4 U_1^2 \right] = 0$$

$\Rightarrow$ $T - \varepsilon = U_2$ (double root)

or $T - \varepsilon = -U_2 \pm 2U_1$

$$\Rightarrow \varepsilon = T - U_2$$
$$\text{or} = T + U_2 \pm 2U_1$$

$$T = \frac{\hbar^2}{2m} |\vec{k}_W|^2 = \frac{\hbar^2}{2m} \cdot \left(\frac{2\pi}{a}\right)^2 \cdot \left(1 + \frac{1}{4}\right)$$
$$= \frac{5\pi^2}{2} \frac{\hbar^2}{ma^2}$$

(b) At $U = \frac{2\pi}{a}(1, \frac{1}{4}, \frac{1}{4})$, we only need to consider the bands from

$\vec{G}_1 := \frac{2\pi}{a}(0, 0, 0)$,

$\vec{G}_2 := \frac{2\pi}{a}(1,1,1)$

$\vec{G}_3 := \frac{2\pi}{a}(2, 0, 0)$

$\therefore$

$$\begin{vmatrix} T_1 - \varepsilon & U_{\bar{1}\bar{1}\bar{1}} & U_{\bar{2}00} \\ U_{111} & T_2 - \varepsilon & U_{\bar{1}11} \\ U_{200} & U_{1\bar{1}\bar{1}} & T_3 - \varepsilon \end{vmatrix} = 0$$

$$\Rightarrow \begin{vmatrix} T_1 - \varepsilon & U_1 & U_2 \\ U_1 & T_2 - \varepsilon & U_1 \\ U_2 & U_1 & T_3 - \varepsilon \end{vmatrix} = 0$$

At U, $T_1 = T_2 = T_3 := T$

$$\Rightarrow \begin{vmatrix} T - \varepsilon & U_1 & U_2 \\ U_1 & T - \varepsilon & U_1 \\ U_2 & U_1 & T - \varepsilon \end{vmatrix} = 0$$

$\Rightarrow (T-\varepsilon)\left[(T-\varepsilon)^2 - U_1^2\right] - U_1^2(T-\varepsilon-U_2) + U_2\left[U_1^2 - U_2(T-\varepsilon)\right] = 0$

$\Rightarrow (T-\varepsilon)\left[(T-\varepsilon)^2 - U_2^2\right] - 2U_1^2(T-\varepsilon-U_2) = 0$

$\Rightarrow (T-\varepsilon-U_2)\left[(T-\varepsilon+U_2)(T-\varepsilon) - 2U_1^2\right] = 0$

$\Rightarrow (T-\varepsilon-U_2)\left[(T-\varepsilon)^2 + U_2(T-\varepsilon) - 2U_1^2\right] = 0$

$\Rightarrow T - \varepsilon = U_2$ or $-\frac{U_2}{2} \pm \sqrt{U_2^2 + 8U_1^2}\,/2$

$\therefore \varepsilon = T - U_2$ or $T + \frac{U_2}{2} \pm \sqrt{\left(\frac{U_2}{2}\right)^2 + 2U_1^2}$