Ch. X : Supplement 2

- An alternative way in getting Eq. (a) on p. X-Ⓐ.

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = E\psi$$

Bloch's theorem: $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})$ with $u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}+\vec{R})$

Eq. of $u_{\vec{k}}(\vec{r})$: (See Ch. IX)

$$\underbrace{-\frac{\hbar^2}{2m}\left(\nabla^2 + 2i\vec{k}\cdot\vec{\nabla} - k^2\right)u_{\vec{k}}(\vec{r}) + V(\vec{r})\,u_{\vec{k}}(\vec{r}) = \mathcal{E}(\vec{k})\,u_{\vec{k}}(\vec{r})}_{\text{This is of the form}} \quad (a)$$

$$\hat{\mathcal{H}}_{\vec{k}}\, u_{\vec{k}}(\vec{r}) = \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{r})$$

From Ch. IV (reciprocal lattice):

$$V(\vec{r}) = \sum_{\vec{G}} V(\vec{G})\, e^{i\vec{G}\cdot\vec{r}} \qquad (\because V(\vec{r}) = V(\vec{r}+\vec{R}))$$

$$V(\vec{G}) = \frac{1}{\Omega_c}\int_{\Omega_c} V(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, d^3r$$

Now, we turn (a) into a matrix problem.

- Expand $u_{\vec{k}}(\vec{r})$ in terms of a complete set.

Since $u_{\vec{k}}(\vec{r})$ is periodic, there is a natural choice of the set of functions.

$$u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}+\vec{R})$$ ← so as to satisfy Bloch's theorem

<u>One can write:</u>

$$\underbrace{u_{\vec{k}}(\vec{r})}_{\text{unknown}} = \sum_{\vec{G}} \underbrace{u_{\vec{k}}(\vec{G})}_{\text{unknowns}} \underbrace{e^{i\vec{G}\cdot\vec{r}}}_{\text{known set of functions}}$$

known set of functions $\{e^{i\vec{G}\cdot\vec{r}}\}$ infinite many $\vec{G}$'s

1st term of (a):

$$\sum_{\vec{G}} -\frac{\hbar^2}{2m}\left(\nabla^2 + 2i\vec{k}\cdot\vec{\nabla} - k^2\right) u_{\vec{k}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

$$= \sum_{\vec{G}} -\frac{\hbar^2}{2m}\left(-G^2 - 2\vec{k}\cdot\vec{G} - k^2\right) u_{\vec{k}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

$$= \sum_{\vec{G}} \frac{\hbar^2}{2m} |\vec{k}+\vec{G}|^2 u_{\vec{k}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

<u>Eq. (a) becomes:</u>

$$\sum_{\vec{G}} \frac{\hbar^2}{2m} |\vec{k}+\vec{G}|^2 u_{\vec{k}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}} + \sum_{\vec{G}} V(\vec{r})\, u_{\vec{k}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}} = \sum_{\vec{G}} \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

- Multiply by $e^{-i\vec{G}'\cdot\vec{r}}$
- Integrate $\frac{1}{\Omega_c}\int_{\Omega_c} d^3r$ over a unit cell

$$\sum_{\vec{G}} \frac{\hbar^2}{2m}|\vec{k}+\vec{G}|^2 u_{\vec{k}}(\vec{G}) \frac{1}{\Omega_c}\int_{\Omega_c} e^{i(\vec{G}-\vec{G}')\cdot\vec{r}}\, d^3r$$

$$+ \sum_{\vec{G}} \frac{u_{\vec{k}}(\vec{G})}{\Omega_c}\int_{\Omega_c} V(\vec{r})\, e^{-i(\vec{G}'-\vec{G})\cdot\vec{r}}\, d^3r = \sum_{\vec{G}} \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{G}) \frac{1}{\Omega_c}\int_{\Omega_c} e^{i(\vec{G}-\vec{G}')\cdot\vec{r}}\, d^3r$$

$$\Rightarrow \boxed{\frac{\hbar^2}{2m}|\vec{k}+\vec{G}'|^2 u_{\vec{k}}(\vec{G}') + \sum_{\vec{G}} V(\vec{G}'-\vec{G})\, u_{\vec{k}}(\vec{G}) = \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{G}')} \quad (b)$$

$$\sum_{\vec{G}} \frac{\hbar^2}{2m}|\vec{k}+\vec{G}|^2 u_{\vec{k}}(\vec{G})\, \delta_{\vec{G},\vec{G}'} + \sum_{\vec{G}} V(\vec{G}'-\vec{G})\, u_{\vec{k}}(\vec{G}) = \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{G}')$$

$$\Rightarrow \sum_{\vec{G}} \left[\frac{\hbar^2}{2m}|\vec{k}+\vec{G}|^2 \delta_{\vec{G},\vec{G}'} + V(\vec{G}'-\vec{G})\right] u_{\vec{k}}(\vec{G}) = \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{G}')$$

$$\Rightarrow \sum_{\vec{G}} \mathcal{H}_{\vec{k}}(\vec{G}',\vec{G})\, u_{\vec{k}}(\vec{G}) = \mathcal{E}(\vec{k})\, u_{\vec{k}}(\vec{G}')$$

- $(\vec{G}',\vec{G})$ matrix element
- a matrix problem for each $\vec{k}$

c.f. $\sum_{i} H_{ji}\, a_i = E\, a_j$

- Look at diagonal elements of $\hat{\mathcal{H}}_{\vec{k}}$

  i.e. $\vec{G} = \vec{G}'$

$$\frac{\hbar^2}{2m}|\vec{k}+\vec{G}'|^2 + \overbrace{V(\vec{0})}^{\text{a constant}} \equiv \mathcal{E}^0(\vec{k}+\vec{G}') + \overline{V}$$

- Off-diagonal elements $\vec{G} \neq \vec{G}'$

$$V(\vec{G}' - \vec{G})$$

$$\begin{array}{c|ccccc}
 & 1 & e^{i\vec{G}_1\cdot\vec{r}} & e^{i\vec{G}_2\cdot\vec{r}} & e^{i\vec{G}_3\cdot\vec{r}} & \cdots \\
\hline
1 & \mathcal{E}^0(\vec{k})+\overline{V} & V(-\vec{G}_1) & V(-\vec{G}_2) & V(-\vec{G}_3) & \cdots \\
e^{i\vec{G}_1\cdot\vec{r}} & V(\vec{G}_1) & \mathcal{E}^0(\vec{k}+\vec{G}_1)+\overline{V} & V(\vec{G}_1-\vec{G}_2) & V(\vec{G}_1-\vec{G}_3) & \cdots \\
e^{i\vec{G}_2\cdot\vec{r}} & V(\vec{G}_2) & V(\vec{G}_2-\vec{G}_1) & \mathcal{E}^0(\vec{k}+\vec{G}_2)+\overline{V} & V(\vec{G}_2-\vec{G}_3) & \cdots \\
e^{i\vec{G}_3\cdot\vec{r}} & V(\vec{G}_3) & V(\vec{G}_3-\vec{G}_1) & V(\vec{G}_3-\vec{G}_2) & \mathcal{E}^0(\vec{k}+\vec{G}_3)+\overline{V} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots &
\end{array}$$

$$\begin{pmatrix} & & \\ & & \\ & & \end{pmatrix}
\begin{pmatrix} u_{\vec{k}}(\vec{0}) \\ u_{\vec{k}}(\vec{G}_1) \\ u_{\vec{k}}(\vec{G}_2) \\ u_{\vec{k}}(\vec{G}_3) \\ \vdots \end{pmatrix}
= \mathcal{E}(\vec{k})
\begin{pmatrix} u_{\vec{k}}(\vec{0}) \\ u_{\vec{k}}(\vec{G}_1) \\ u_{\vec{k}}(\vec{G}_2) \\ u_{\vec{k}}(\vec{G}_3) \\ \vdots \end{pmatrix} \qquad (C)$$

Same as Eq.(b)

- Start again from Eq.(b):

$$\frac{\hbar^2}{2m}|\vec{k}+\vec{G}'|^2 u_{\vec{k}}(\vec{G}') + V(\vec{0})u_{\vec{k}}(\vec{G}') + \sum_{\vec{G}\neq\vec{G}'} V(\vec{G}'-\vec{G})u_{\vec{k}}(\vec{G}) = \mathcal{E}(\vec{k})u_{\vec{k}}(\vec{G}')$$

$$\Rightarrow \left(\mathcal{E}(\vec{k}) - V(\vec{0}) - \frac{\hbar^2}{2m}|\vec{k}+\vec{G}'|^2\right)u_{\vec{k}}(\vec{G}') = \sum_{\substack{\vec{G} \\ (\vec{G}\neq\vec{G}')}} V(\vec{G}'-\vec{G})u_{\vec{k}}(\vec{G})$$

$$= \sum_{\substack{\vec{G}'' \\ (\vec{G}''\neq 0)}} V(\vec{G}'')u_{\vec{k}}(\vec{G}'-\vec{G}'') \qquad (d)$$

which is the equation (Eq.(a)) on page X-④.