Bloch Hamiltonian.

Recall $\hat{H}\,\Psi_{qn} = E_{qn}\,\Psi_{qn}$; $H = T + V(x)$

q: crystal momentum. n: band index. $V(x)$: cell periodic potential.

Recall Bloch theorem: $\Psi_{qn} = e^{iqx} u_{qn}$

$\therefore \hat{H}\,\Psi_{qn}$:

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[e^{iqx} u_{qn}\right] + V\Psi_{qn}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[\frac{\partial}{\partial x}\left[(iq)e^{iqx} u_{qn} + e^{iqx}\frac{\partial}{\partial x}u_{qn}\right]\right] + V\Psi_{qn}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[(iq)(iq)e^{iqx} u_{qn} + (iq)\,e^{iqx}\left(\frac{\partial u_{qn}}{\partial x}\right)\right.$$

$$+(iq)\,e^{iqx}\frac{\partial}{\partial x}u_{qn} + e^{iqx}\left(\frac{\partial^2 u_{qn}}{\partial x^2}\right)\Bigg] + V\,\Psi_{qn}$$

$$\Rightarrow \frac{e^{iqx}}{2m}\left[\hbar^2 q^2 u_{qn} + 2(q\hbar)\left(-i\hbar\frac{\partial}{\partial x}\right)u_{qn} - \hbar^2\frac{\partial^2 u_{qn}}{\partial x^2}\right] + V\Psi_{qn}$$

$$\Rightarrow \frac{e^{iqx}}{2m}\left[\hbar^2 q^2 + 2\hbar q\,\hat{p} + \hat{p}^2\right]u_{qn} \quad + V\Psi_{qn}$$

$$\Rightarrow e^{iqx}\left[\frac{(\hat{p}+\hbar q)^2}{2m} + V\right]u_{qn}$$

$$\hat{H}\Psi_{qn} = E_{qn}\Psi_{qn}$$

$$\therefore \Rightarrow e^{iqx}\hat{H}_q u_{qn} = E_{qn}\,e^{iqx}u_{qn}$$

$$\Rightarrow \boxed{\hat{H}_q u_{qn} = E_{qn} u_{qn}}$$

where $\hat{H}_q = \frac{(\hat{p}+\hbar q)^2}{2m} + V(x) \longrightarrow$ Bloch Hamiltonian

Recall, $u_{qn} = \sum_{G} C_{G}^{qn} e^{iGx}$

$\therefore$ In Fourier space: (G space):

$$\underline{\underline{H}}_q \, \underline{C}_G^{qn} = E_{qn} \, \underline{C}_G^{qn}$$

Elements of $\underline{\underline{H}}_q$:

$$H_{q,GG'} = \left\langle G \right| \frac{(\hat{p} + \hbar q)^2}{2m} + V \left| G' \right\rangle \quad ; \quad \langle x | G \rangle = e^{iGx}$$

$$= \frac{(\hbar G + \hbar q)^2}{2m} \delta_{GG'} + V_{G'-G}$$

$$\therefore \underline{\underline{H}}_q \, \underline{C}_G^{qn} = E_{qn} \, C_G^{qn}$$

$G' \rightarrow$, $G \downarrow$

$$\begin{bmatrix} \frac{(\hbar G_{-2}+\hbar q)^2}{2m} + V_{G_0} & V_{G_1} & V_{G_2} & V_{G_3} & V_{G_4} \\ V_{G_{-1}} & \frac{(\hbar G_{-1}+\hbar q)^2}{2m} + V_{G_0} & V_{G_1} & G_2 & G_3 \\ V_{G_{-2}} & V_{G_{-1}} & \frac{(\hbar G_0+\hbar q)^2}{2m} + V_{G_0} & V_{G_1} & V_{G_2} \\ V_{G_{-3}} & V_{G_{-2}} & V_{G_{-1}} & \frac{(\hbar G_1+\hbar q)^2}{2m} + V_{G_0} & V_{G_1} \\ \cdots & \cdots & \cdots & \cdots & \frac{(\hbar G_2+\hbar q)^2}{2m} + V_{G_0} \end{bmatrix} \begin{bmatrix} C_{G_{-2}}^{qn} \\ C_{G_{-1}}^{qn} \\ C_{G_0}^{qn} \\ C_{G_1}^{qn} \\ C^{qn} \end{bmatrix} = E^{qn} \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}$$

$V_{G_{-4}} \quad V_{G_{-3}} \quad V_{G_{-2}} \quad V_{G_{-1}} \quad \frac{\quad}{2m} + V_{G_0} \quad G_2$

$\underline{\underline{H_q}}$ same as $\underline{\underline{h_q}}$ we had in the note on Bloch formalism.