BLOCH'S THEOREM

$$\psi(\vec{r}) = \sum_{q} c_q \, e^{i \vec{q} \cdot \vec{r}}$$

$$\underset{\text{PERIODIC}}{U(\vec{r})} = \sum_{\underset{\vec{K} \in RL}{\vec{K}}} U_K \, e^{i \vec{K} \cdot \vec{r}} \qquad U_0 = \frac{1}{V} \int_{\text{CELL}} d^3\vec{r} \; U(\vec{r}) = 0$$

$U(\vec{r})$ IS REAL $\Rightarrow U_K^* = U_{-K}$

INVERSION SYMMETRIC $U(\vec{r}) = U(-\vec{r}) \Rightarrow U_{-K} = U_K = U_K^*$

S.E.:

$$-\frac{\hbar^2\nabla^2}{2m}\varphi + U(\vec{r})\,\varphi(\vec{r}) = \varepsilon\,\varphi(\vec{r})$$

$$\nabla^2 \longrightarrow -q^2$$

$$-\frac{\hbar^2\nabla^2}{2m}\varphi \longrightarrow \sum_{q} \frac{\hbar^2 q^2}{2m} c_q\, e^{i\vec{q}\cdot\vec{r}}$$

$$U(\vec{r})\,\varphi(\vec{r}) = \sum_{\vec{k},\vec{q}} U_k\, e^{i\vec{k}\cdot\vec{r}}\, c_q\, e^{i\vec{q}\cdot\vec{r}}$$

$$= \sum_{\vec{k},\vec{q}} U_k c_q\, e^{i(\vec{k}+\vec{q})\cdot\vec{r}} = \sum_{\vec{k},q'} U_{\vec{k}}\, c_{\vec{q}'-\vec{k}}\, e^{i\vec{q}'\cdot\vec{r}}$$

$$\vec{q}\,' = \vec{K} + \vec{q}$$

$$\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \underbrace{\left[\left(\frac{\hbar^2 q^2}{2m} - \varepsilon \right) C_{\vec{q}} + \sum_{\vec{K}'} U_{\vec{K}'} C_{\vec{q}-\vec{K}'} \right]}_{=0} = 0$$

S.E. IN FOURIER SPACE

$$\left(\frac{\hbar^2 q^2}{2m} - \varepsilon \right) C_{\vec{q}} + \underbrace{\sum_{\vec{K}'} U_{\vec{K}'} C_{\vec{q}-\vec{K}'}}_{\text{CONVOLUTION}} = 0$$

$$\vec{q} = \vec{k} - \vec{K} \qquad \vec{K} \in \text{R.L.} \qquad \vec{k} \in \text{B.Z.}$$

$$\left(\frac{\hbar^2}{2m}(\vec{k}-\vec{K})^2-\varepsilon\right)C_{\vec{k}-\vec{K}}+\sum_{\vec{K}'}U_{K'}\,C_{\underbrace{\vec{k}-\vec{K}-\vec{K}'}_{-\vec{K}''}} \qquad \vec{K}''=\vec{K}'+\vec{K}$$

$$\left(\frac{\hbar^2}{2m}(\vec{k}-\vec{K})^2-\varepsilon\right)C_{\vec{k}-\vec{K}}+\sum_{\vec{K}''}U_{\vec{K}''-\vec{K}}\,C_{\vec{k}-\vec{K}''}=0$$

S.E. IN FOURIER SPACE FOR $\vec{k} \in$ B.Z.

$$\varphi_{\vec{k}}(\vec{r}+\vec{L})=\varphi_{\vec{k}}(\vec{r}) \Rightarrow e^{ikL}=1 \qquad k=\frac{2\pi}{L}j \qquad j\in\mathbb{Z}$$

LENGTH OF SAMPLE

$(L = Na)$

(BORN - VON KARMEN)

$\vec{k} \in$ B.Z. FOURIER COMPONENTS $e^{i(\vec{k}-\vec{K})\cdot\vec{r}}$

$$\boxed{\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{K}} C_{\vec{k}-\vec{K}}\, e^{i(\vec{k}-\vec{K})\cdot\vec{r}}}$$

FORM OF S.E. WAVE FUNCTION FOR PERIODIC POTENTIAL

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \underbrace{\left(\sum_{\vec{K}} C_{\vec{k}-\vec{K}}\, e^{-i\vec{K}\cdot\vec{r}}\right)}_{u_{\vec{k}}(\vec{r})}$$

$$u_{\vec{k}}(\vec{r}+\vec{R}) = u_{\vec{k}}(\vec{r})$$

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \underbrace{u_{\vec{k}}(\vec{r})}_{\text{PERIODIC}} \equiv \text{BLOCH'S THM.}$$

CRYSTAL MOMENTUM

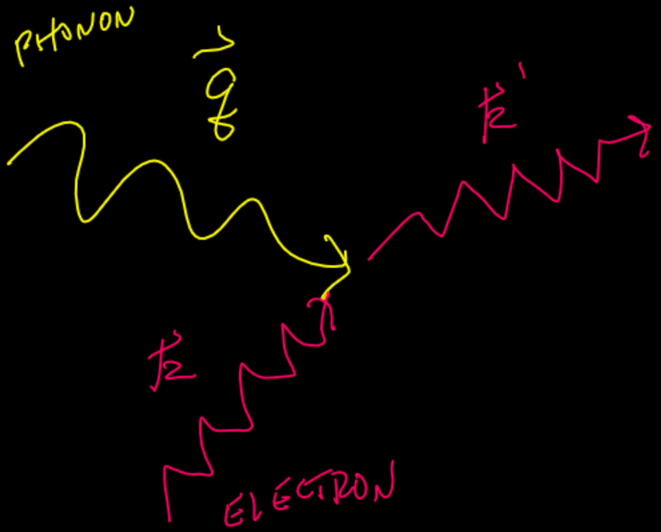
$$\psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\,\psi_{\vec{k}}(\vec{r})$$

$\hbar\vec{k} \neq$ MOMENTUM $\quad \frac{\hbar\nabla}{i}\psi_{\vec{k}} \neq \hbar k\,\psi_{\vec{k}}$

$$\boxed{\hbar\vec{k} \equiv \text{CRYSTAL MOMENTUM}}$$

SELECTION RULES IN SCATTERING

CRYSTAL MOMENTUM IS CONSERVED!



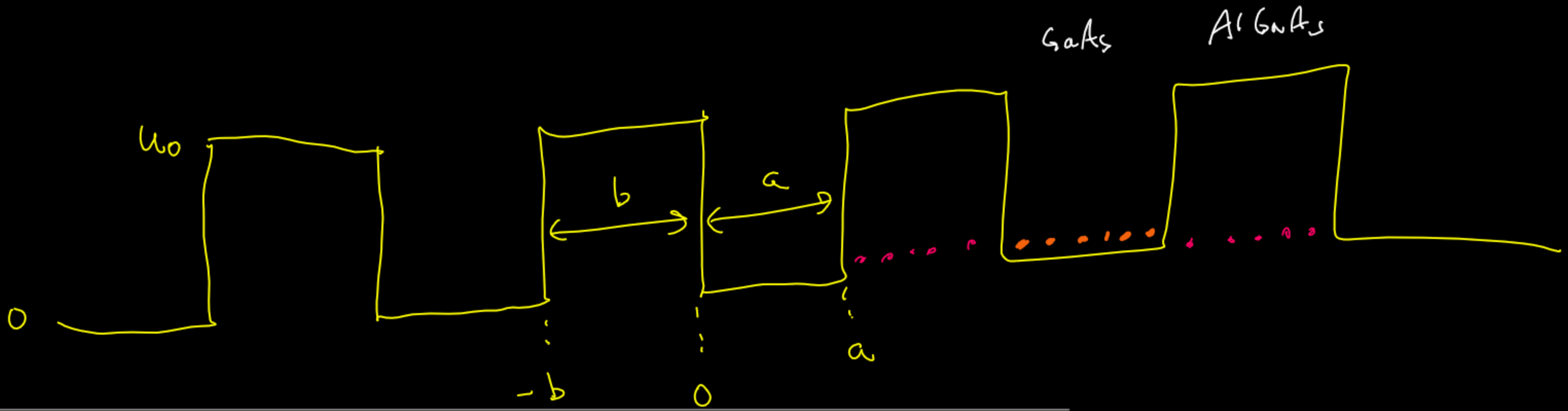
$$\vec{q} + \vec{k} = \vec{k}' + \vec{K} \qquad \vec{K} \in \text{R.L.}$$

CONSERVATION OF X'TAL MOMENTUM

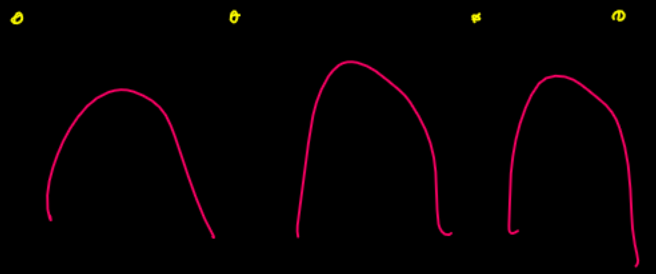
$\vec{K} = 0$ NORMAL

$\vec{K} \neq 0$ UMKLAPP

KRONIG - PENNEY MODEL (ELECTRONS IN PERIODIC POTENTIAL)



1-D, PERIODIC, SQUARE WELL POTENTIAL



"SUPER LATTICE"

$$\boxed{U(x) = \underbrace{\underset{\text{CONSTANT (AREA)}}{A}\;\underset{\text{SEPARATION}}{a}} \sum_s \delta(x - sa)}$$

WORK IN UNITS

$L = Na = 1$

$\Rightarrow S = 0 \rightarrow \frac{1}{a}$