Bloch theorem :- States that the energy eigen States for an electron in a crystal can be written as bloch waves.

- If a wave is a bloch wave, its wave-function can be described as

$$\psi(r) = \underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\text{Plane wave}}\ \underbrace{u(r)}_{\text{periodic bloch cell function}}$$

~~Eigenstates (ψe)~~

~~one dimensional schrodinger wave eq. for a free $e^{\ominus}$ which is moving in a constant potential is~~

$$\frac{d^2\psi}{dx^2} + (2m/\hbar^2)(E-V_0)\psi = 0$$

~~solution of above differential eqn~~

$$\psi = \exp(\pm ikx)$$

~~K.E. of $e^{\ominus}$s~~ $E_{K.E} = \cancel{E-V_0} = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}$ [$p = \hbar k$]

=

~~To make the wave function~~

Thus, we will consider a periodic solid through Bloch's theorem.

→ Bloch's theorem is just a way to describe the wave function for periodic solids.

Postulates of Bloch's theorem :-

Bloch (1) As we have a solid that is periodic at the atomic scale, we get a traveling wave solution ($e^{i\vec{k}\cdot\vec{r}}$) for ψ that is modulated by

the translational symmetry of the lattice free
$(u_{\vec{k}})$
sim

$\rightarrow \quad \psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$ — (1)

where $u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}+\vec{T})$ — (2)

$\rightarrow$ wavefunction reflects the symmetry of the lattice
$u_{\vec{k}}$

Bloch-2) we can desribe the wavefunction

$$\psi_{\vec{k}}(\vec{r}+\vec{T}) = C\psi_{\vec{k}}(\vec{r})$$

$\Rightarrow$ wavefunction at $(\vec{r}+\vec{T})$ is very related to the wavefunction at $\vec{r}$.

where C = modulation term.

Derivation of Bloch-2 using Bloch-1 :-

We are going ~~to~~ with Bloch-1 postulate

In eqn (1), replace r with $r+T$ because $u_{\vec{k}}$ is Periodic in T [eqn (2)]

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

$$= e^{ik\cdot(\vec{r}+\vec{T})} \frac{\psi_{\vec{k}}(r)}{e^{i\vec{k}\cdot\vec{r}}}$$ [combining (1) & (2) expression]

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

Implementation of bloch: The vanishing potential :-

(1) If the potential is periodic but so weak that it is vanishing.

$\Rightarrow$ we can estimate our potential as a flat box & our dispersion will basically be parabollic like the free electron model. ⑯

→ Since we still have periodic conditions,

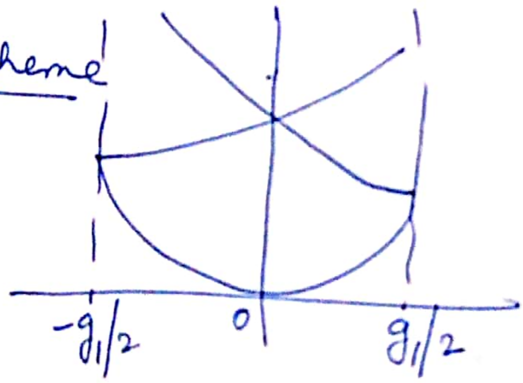
$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}+\vec{G}}(\vec{r})$$

⇒ we repeat our parabolas at $k+g$, $k-g$, $k+2g$ & so on for the dispersion [where k is shift to $+g$ or $-g$ (in 1-D crystal)]

→ Call one parabola centred at $k=0$ (the extended zone scheme)

→ & multiple parabolas (the periodic zone scheme)

→ <u>Reduced zone scheme</u>



1st Brillion zone is b/w the dotted lines.

<u>Physical Interpretation of bloch's Theorem :-</u>

wavefunction is periodic at two length scales:

- u is periodic in T (the atomic scale, lattice spacing)
- $e^{i\vec{k}\cdot\vec{r}}$ is periodic in L (sample scale)