e^- in a crystalline solid $\left(-\frac{\hbar^2}{2m}\nabla^2 + \underbrace{U(\underline{r})}\right)\psi(\underline{r}) = E\psi(\underline{r})$ (SE)

potential seen by electron (other electrons, atoms)

→ IT IS PERIODIC.

$U(\underline{r}+\underline{R}) = U(\underline{r})$

lattice vector.

Bloch's theorem – the solution to SE for a periodic potential $U(\underline{r})$ has the form

$$\psi_{\underline{k}}(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}\, u_{\underline{k}}(\underline{r})$$

where $u_{\underline{k}}(\underline{r}+\underline{R}) = u_{\underline{k}}(\underline{r})$ $\boxed{p = \hbar\underline{k} \rightarrow \text{momentum}}$

Simple "proof":

* A solution to the SE can always be written as

$$\psi(\underline{r}) = f(\underline{r})\, u(\underline{r})$$

this is the function to be determined! periodic

* Since $U(\underline{r})$ is periodic then all observable quantities must also be similarly periodic

ie $\underbrace{|\psi(\underline{r})|^2}_{\text{electron probability}}$ must have same periodicity as $U(\underline{r})$

$$\therefore \; |f(\underline{r}+\underline{R})|^2 = |f(\underline{r})|^2$$

→ The only function that satisfies this for all $\underline{R}$'s is $e^{i\underline{k}\cdot\underline{r}}$

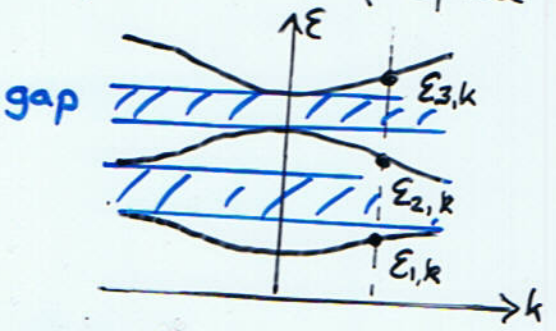
Bloch function, ψ_k

- it has the form of a travelling wave $(e^{ik\cdot r}) \rightarrow$ "free" particle
- $u_k(r)$ modulates wave spatially.

- since electron behaves as a wave with wave vector $\underline{k}$, it has deBroglie wavelength $\lambda = 2\pi/k$ and "crystal" momentum $\underline{p} = \hbar\underline{k}$

- Bloch function is a crystal orbital, delocalized throughout solid. Electron is shared by whole crystal. $|\psi_k|^2$ gives electron probability distribution.

Energy bands can be derived by solving the SE with ψ of the Bloch form, and by specifying $U(r)$



Dynamics of Bloch e's

→ filled electron bands → no current (no way to break symmetry)

→ partially filled bands, $-e\underline{E} = \underline{F} = \frac{\hbar d\underline{k}}{dt}$ → asymmetric distribution → current.