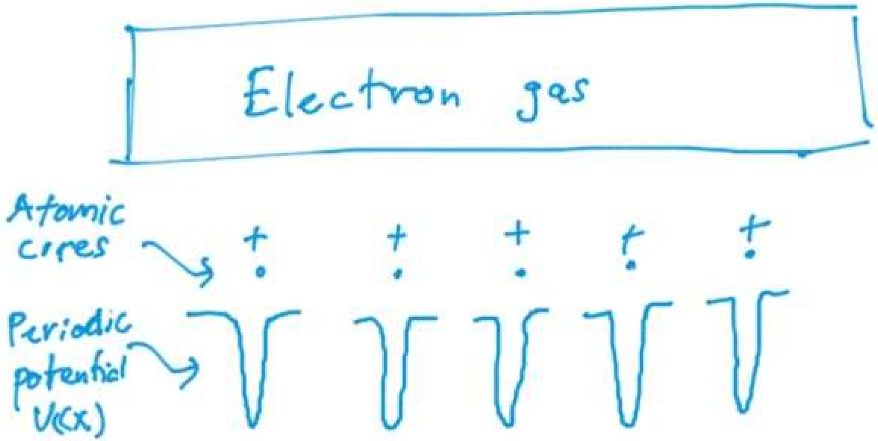
BAND STRUCTURE - BACKGROUND:

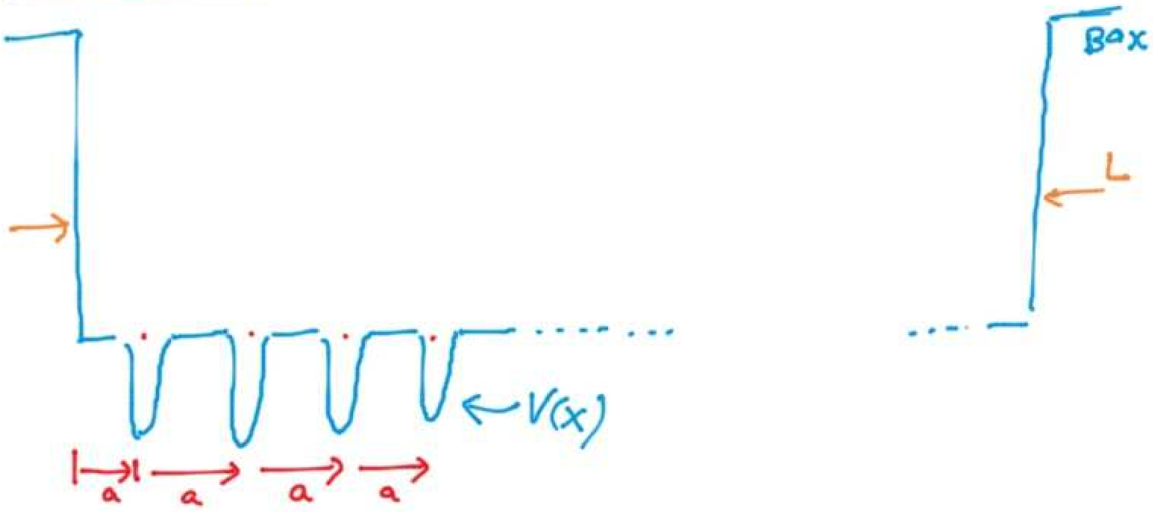


Schrödinger Equation

$$\left\{\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right\}\psi(x) = E_k\,\psi(x)$$

What happens to $\psi(x)$ and E when $V(x) \neq 0$.

MODEL



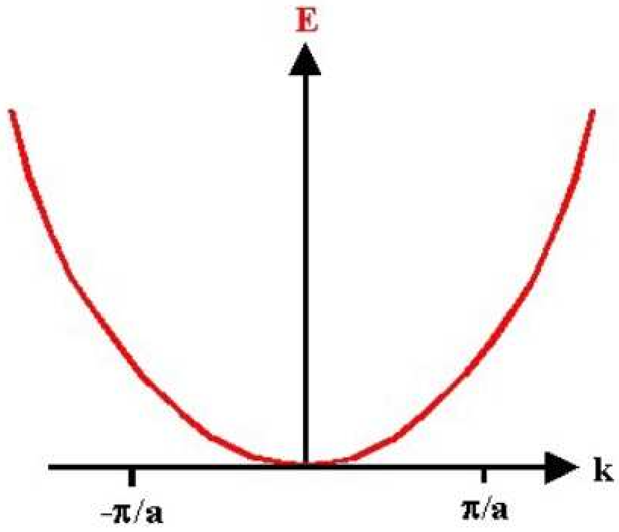
PERIODIC BOUNDARY CONDITIONS

$$\psi(0) = \psi(L) \Rightarrow k = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \ldots$$

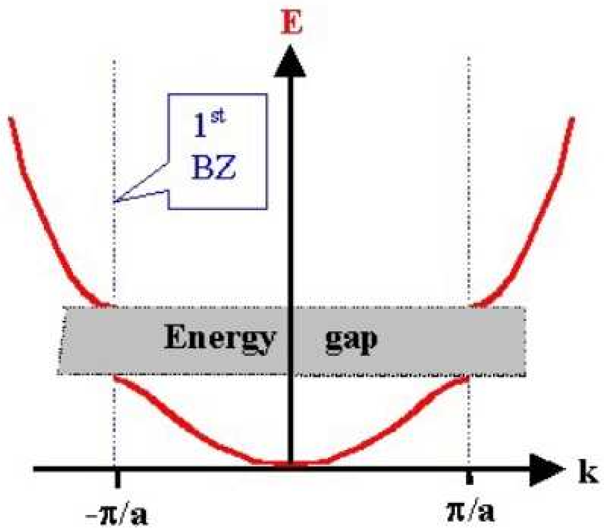
$$V(x) = V(x+a) \Rightarrow V(x) = \sum_G V_G \cdot e^{iGx} = \sum_G V_G \cdot e^{iG(x+a)} = \sum_G V_G \cdot e^{iGx} e^{iGa}$$

$$\Rightarrow e^{iGa} = 1 \Rightarrow G = 0, \pm\frac{2\pi}{a}, \pm\frac{4\pi}{a}, \ldots$$

BANDS & BAND GAPS



Free electron gas



Free electron gas and
diffraction at Brillouin zones

REDUCED ZONE SCHEME

Multiple Bands

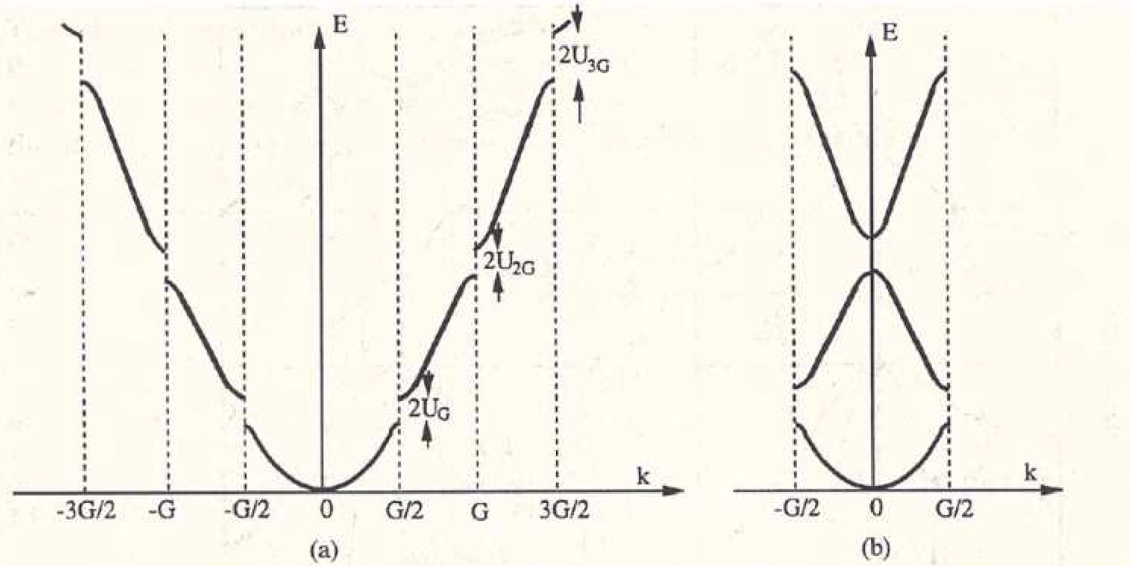
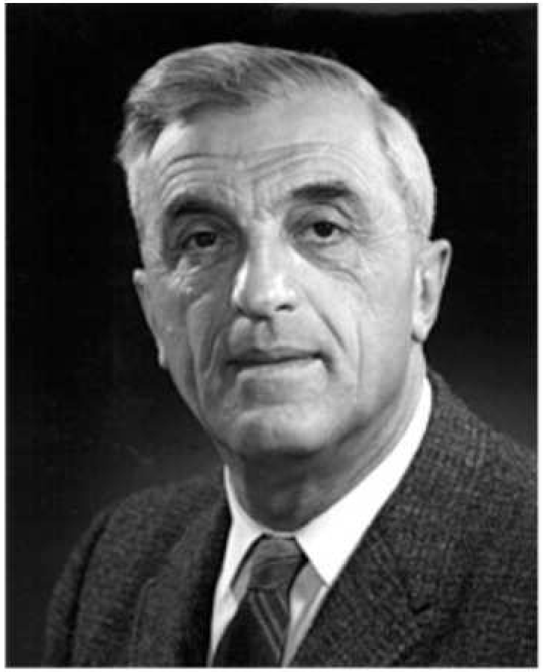


Figure 1-26 (a) Effect of periodic potential on the structure of a single free-electron parabolic band, $E_{\mathbf{k}}$. When $\mathbf{k} = n\mathbf{G}/2$ $(n = 1, 2, 3, \ldots)$, the interaction of the electron wavefunction and the periodic potential creates a forbidden energy gap. (b) The band structure within the first Brillouin zone contains all the information of the total band structure, if all the other bands $E_{\mathbf{k}}$, $E_{\mathbf{k+G}}$, $E_{\mathbf{k-G}}$, ... are considered.

BLOCH - THEOREM



Felix Bloch

Er erhielt 1952 den Nobelpreis für Physik
Born in Zurich (1905)
First Director of CERN

'When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal.... By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation'

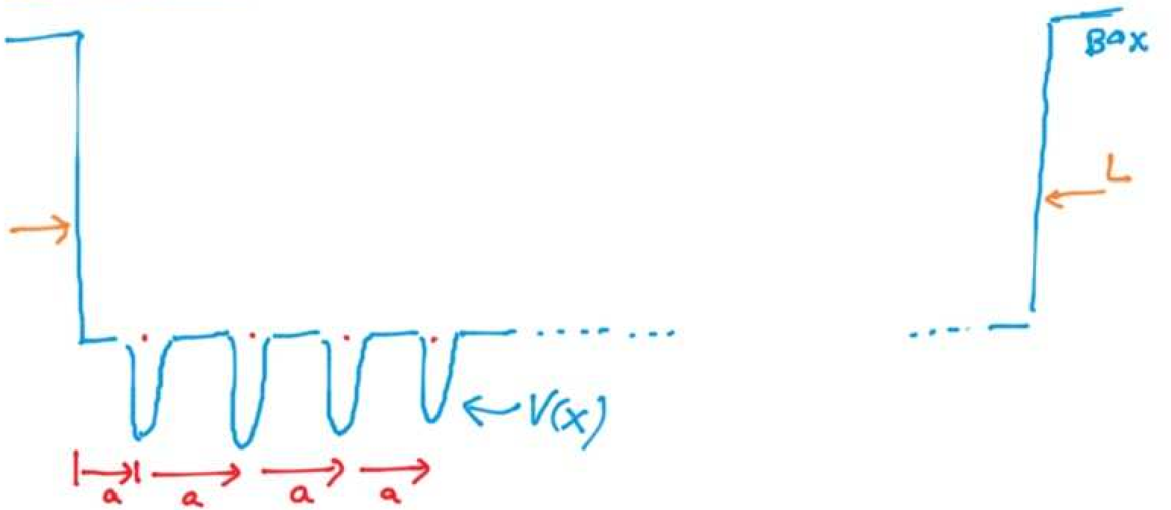
F. BLOCH

$$\psi(x) = u(x) \cdot e^{ikx}$$

with

$$u(x+a) = u(x)$$

MODEL



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CENTRAL EQUATION

Schrödinger Equation

$$\left\{\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right\}\psi(x) = \varepsilon_k \psi(x)$$

Discrete FOURIER TRANS.

$$\psi(x) = \sum_k c_k e^{ikx}$$

$$\sum_k \frac{(\hbar k)^2}{2m} c_k e^{ikx} + \sum_G V_G e^{iGx} \cdot \sum_k c_k e^{ikx} = \varepsilon_k \sum c_k e^{ikx}$$

$$\lambda_k \equiv \frac{(\hbar k)^2}{2m}$$

$$\sum_k (\lambda_k - \varepsilon_k) c_k e^{ikx} + \sum_k \sum_G V_G c_k e^{i(G+k)x} = 0$$

$k' = k + G$

$k = k' - G$

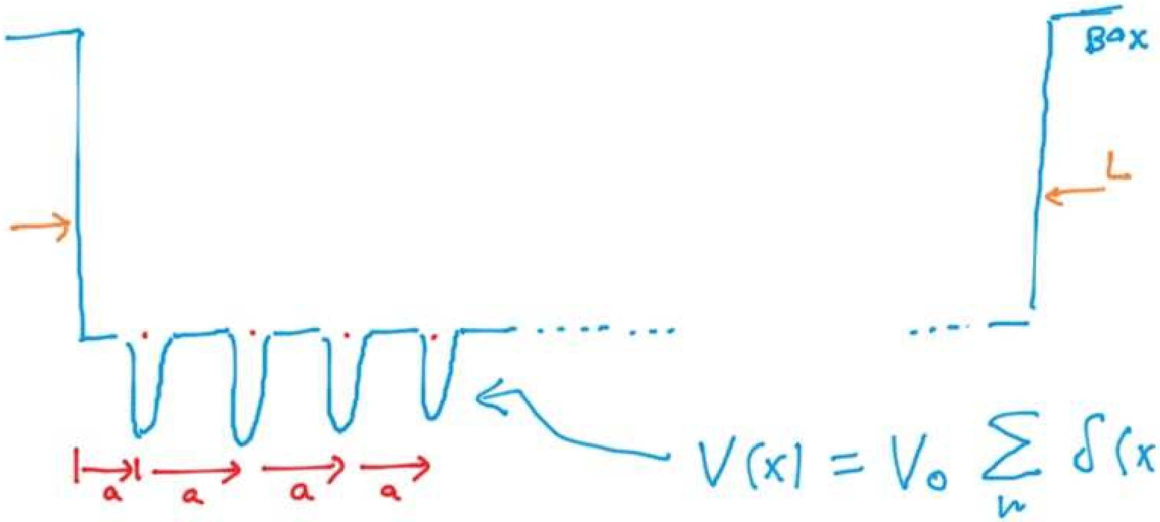
$$\sum_{k'} (\lambda_{k'} - \varepsilon_{k'}) c_{k'} e^{ik'x} + \sum_{k'} \sum_G V_G c_{k'-G} e^{ik'x} = 0$$

$$\Downarrow$$

$$\boxed{(\lambda_{k'} - \varepsilon_{k'}) \cdot c_{k'} + \sum_G V_G c_{k'-G} = 0}$$

CENTRAL Equation

KRONIG - PENNEY MODEL



$$V(x) = V_0 \sum_n \delta(x-na)$$

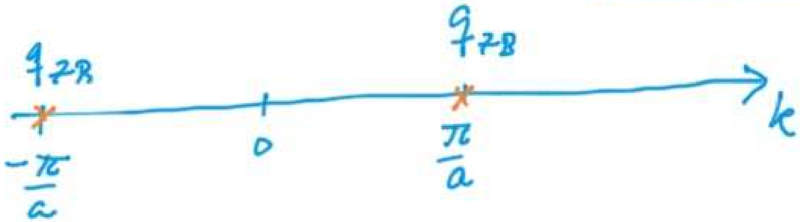
$$V_G = \text{CONSTANT}$$

$$V(x) = \sum_G V_G \exp(iGx) = V_0 + V_0\left\{\exp\left(i2\pi\frac{x}{a}\right) + \exp\left(-i2\pi\frac{x}{a}\right)\right\} + \dots$$

$$G = 0, \pm\frac{2\pi}{a}; \pm\frac{4\pi}{a}; \dots$$

$$\Downarrow \quad \boxed{(\lambda_{k'} - \mathcal{E}_{k'}) \cdot C_{k'} + \sum_G V_G \, C_{k'-G} = 0}$$

CENTRAL EQUATION



TRY TO FIGURE-OUT $\mathcal{E}_{q_{ZB}}$

$$(\lambda_{q_{ZB}} - \mathcal{E}_{q_{ZB}}) \cdot C_{q_{ZB}} + V_0 \cdot C_{q_{ZB}} + V_0 \, C_{-q_{ZB}} = 0$$

$$(\lambda_{-q_{ZB}} - \mathcal{E}_{-q_{ZB}}) \, C_{-q_{ZB}} + V_0 \, C_{-q_{ZB}} + V_0 \, C_{q_{ZB}} = 0$$

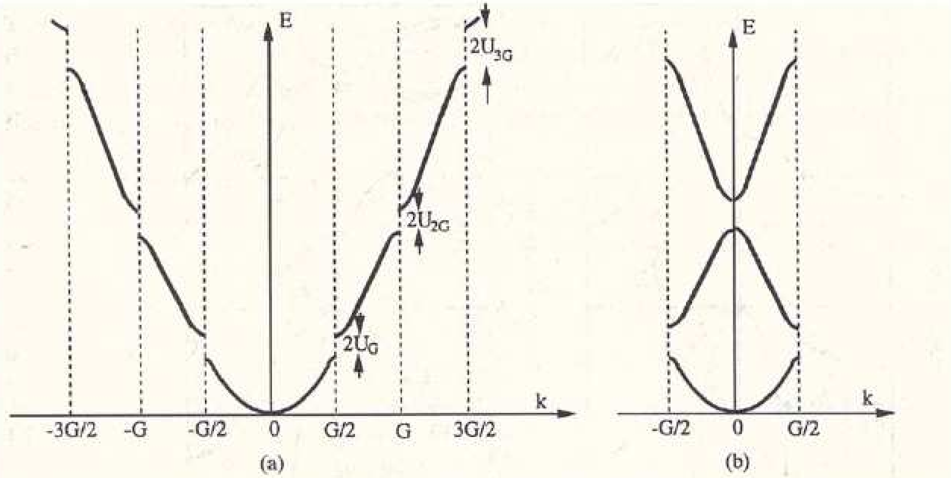
$$\Downarrow$$

$$\begin{bmatrix} \lambda_{q_{ZB}} - \mathcal{E}_{q_{ZB}} + V_0 & V_0 \\ V_0 & \lambda_{q_{ZB}} - \mathcal{E}_{q_{ZB}} + V_0 \end{bmatrix} \begin{bmatrix} C_{q_{ZB}} \\ C_{-q_{ZB}} \end{bmatrix} = 0$$

$$(\lambda_{q_{ZB}} - \mathcal{E}_{q_{ZB}} + V_0)^2 - V_0^2 = 0 \quad \Rightarrow \quad \mathcal{E}_{q_{ZB}} = \begin{cases} \lambda_{q_{ZB}} \\ \lambda_{q_{ZB}} - 2V_0 \end{cases}$$

$$\varepsilon_{q_{ZB}} = \begin{cases} \lambda_{q_{ZB}} \\ \lambda_{q_{ZB}} - 2V_0 \end{cases} = \begin{cases} \frac{\hbar^2 q_{ZB}^2}{2m} \\ \frac{\hbar^2 q_{ZB}^2}{2m} - 2V_0 \end{cases}$$

Multiple Bands



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BLOCH'S THEOREM

$$\psi_{q_{ZB}} = \sum_G C_{q_{ZB}-G} \exp(i[q_{ZB}-G]\cdot x)$$

$$= \sum_G \left\{ C_{q_{ZB}-G}\, e^{-iGx} \right\} e^{i q_{ZB}\cdot x}$$

$$= u(x)\cdot e^{i q_{ZB}\cdot x}$$

where

$$u(x) = \sum_G C_{q_{ZB}-G}\, e^{-iGx}$$

$$u(x+a) = \sum_G C_{q_{ZB}-G}\, e^{-iG(x+a)} = \sum_G C_{q_{ZB}-G}\, e^{-iGx}\cdot \underbrace{e^{-iGa}}_{=1}$$

$$= u(x)$$