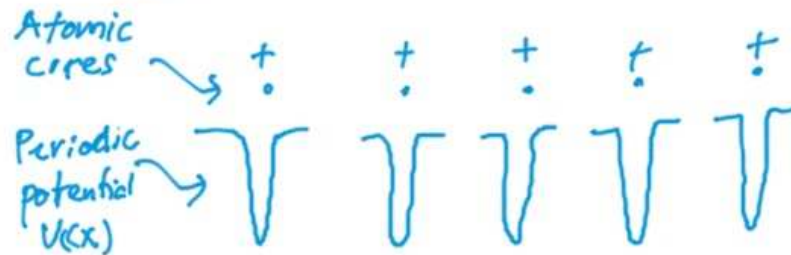


BAND STRUCTURE - BACKGROUND:

Electron gas



Schrödinger Equation

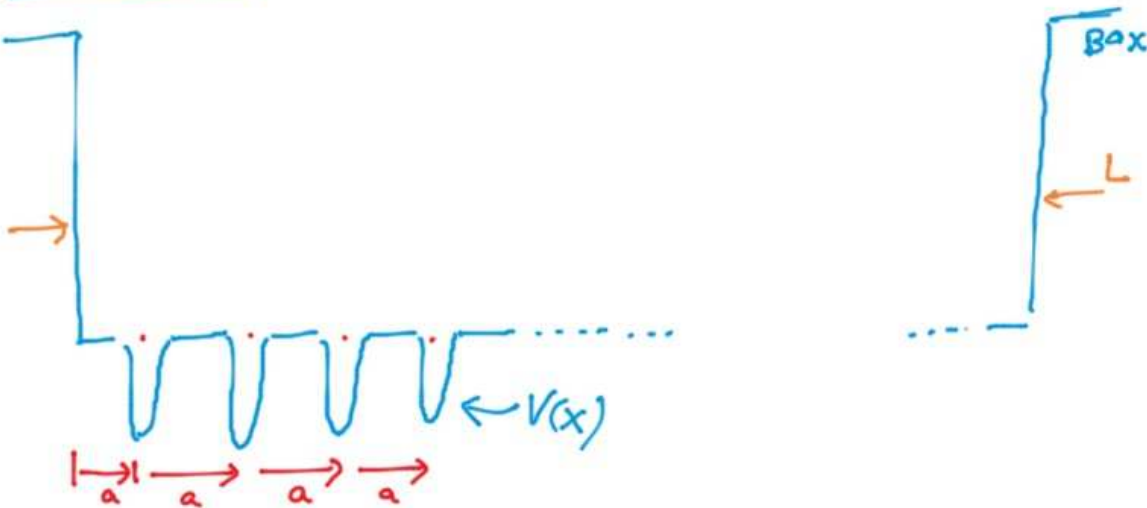
$$\left\{ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right\} \Psi(x) = E_k \Psi(x)$$

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

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MODEL




PERIODIC BOUNDARY CONDITIONS

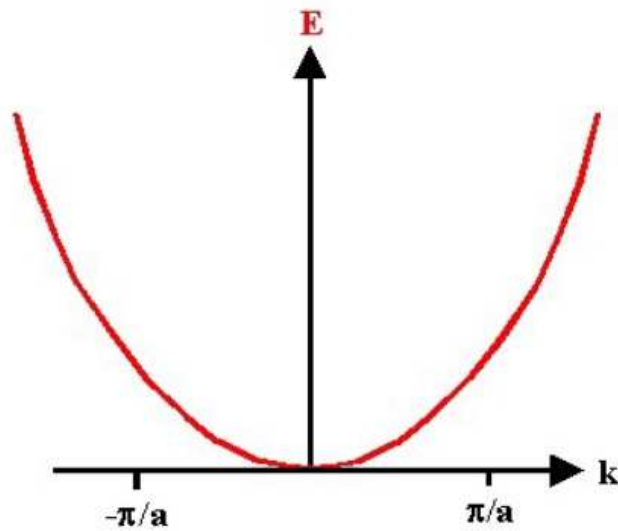
$$\Psi(0) = \Psi(L) \Rightarrow k = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots$$

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

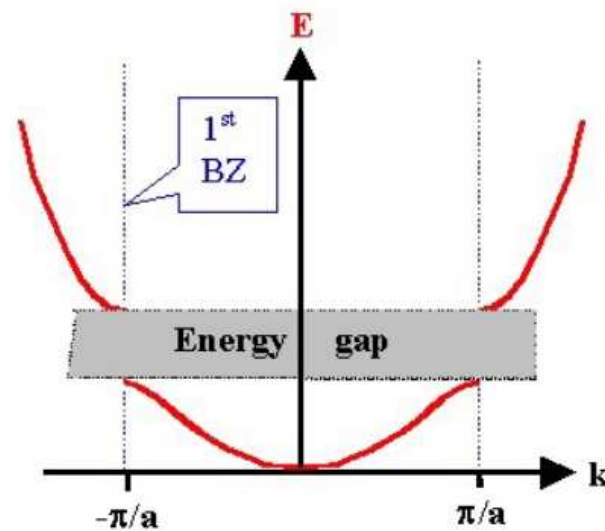
$$\Rightarrow e^{iGa} = 1 \Rightarrow G = 0, \pm \frac{2\pi}{a}, \pm \frac{4\pi}{a}, \dots$$

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BANDS & BAND GAPS



Free electron gas



Free electron gas and diffraction at Brillouin zones

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REDUCED ZONE SCHEME

Multiple Bands

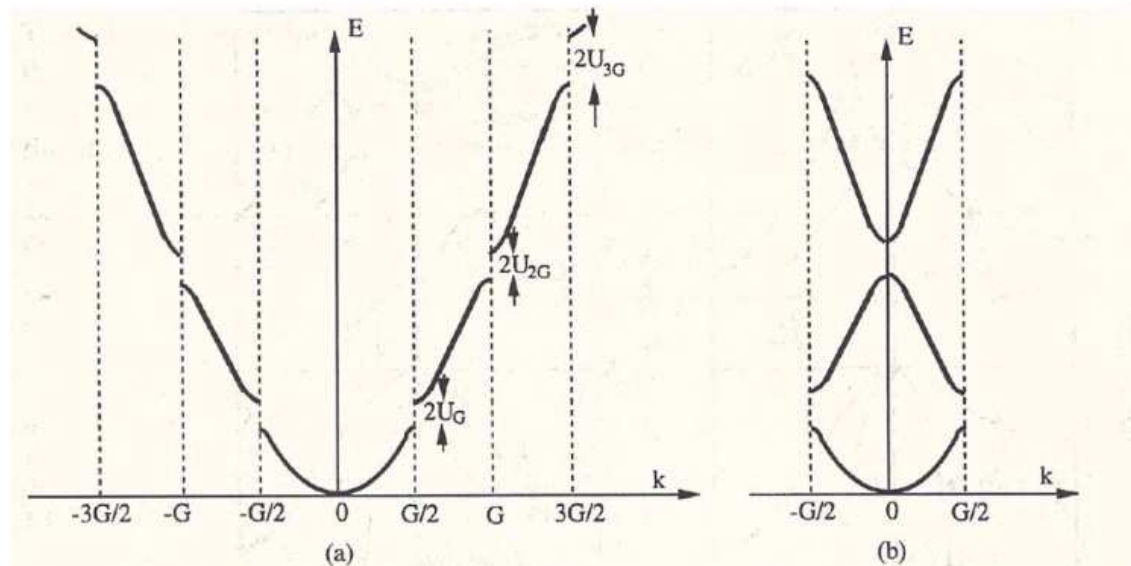
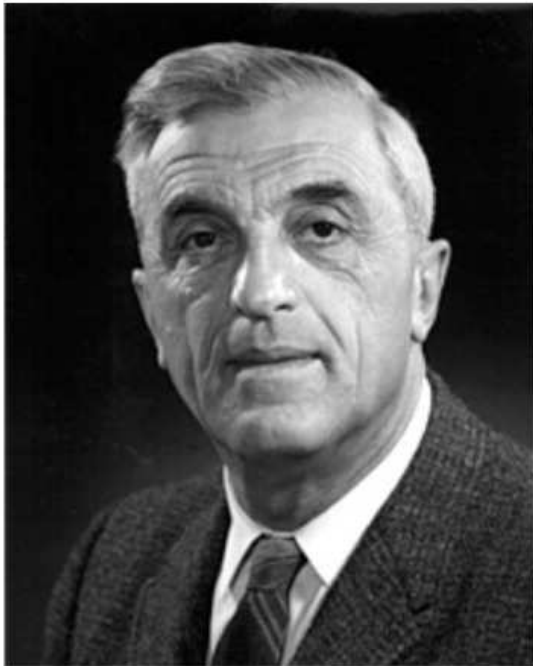


Figure 1-26 (a) Effect of periodic potential on the structure of a single free-electron parabolic band, E_k . When $k = nG/2$ ($n = 1, 2, 3, \dots$), the interaction of the electron wavefunction and the periodic potential creates a forbidden energy gap. (b) The band structure within the first Brillouin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

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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

$$U(x+a) = U(x)$$

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MODEL

PERIODIC BOUNDARY CONDITIONS

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

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

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

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CENTRAL EQUATION

Schrödinger Equation

$$\left\{ \frac{\hbar^2 k^2}{2m} + V(x) \right\} \Psi(x) = \epsilon_k \Psi(x)$$

Discrete FOURIER TRANS.
 $\Psi(x) = \sum_k c_k e^{ikx}$

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

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

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


$k' = k + G$
 $k = k' - G$

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

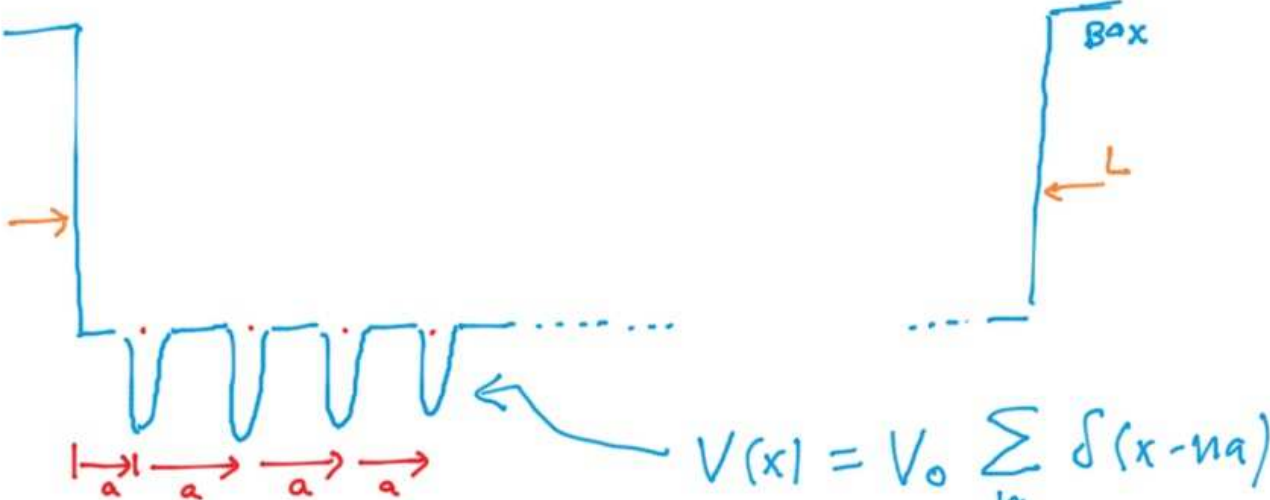
⇓

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

CENTRAL EQUATION

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KRONIG PENNEY MODEL




The diagram illustrates the Kronig-Penney model. On the left, a periodic potential is shown as a series of rectangular wells of height V_0 and width a , separated by regions of zero potential. The period of the potential is a . An orange arrow points to the right, indicating the direction of wave propagation. On the right, a single rectangular potential well is shown with height V_0 and width L , labeled "Box". An orange arrow points to the left, indicating the direction of wave propagation. The potential is defined by the equation:

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

where $V_G = \text{CONSTANT}$.

$$V(x) = \sum_G V_G \exp(iGx) = V_0 + V_0 \left\{ \exp\left(i\frac{2\pi x}{a}\right) + \exp\left(-i\frac{2\pi x}{a}\right) \right\} + \dots$$

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

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$$\Downarrow \left[(\lambda_k - \epsilon_k) \cdot C_k + \sum_G V_G C_{k-G} = 0 \right] \quad \text{CENTRAL EQUATION}$$

TRY TO FIGURE-OUT $\epsilon_{q_{2B}}$

$$(\lambda_{q_{2B}} - \epsilon_{q_{2B}}) \cdot C_{q_{2B}} + V_0 \cdot C_{q_{2B}} + V_0 \cdot C_{-q_{2B}} = 0$$

$$(\lambda_{-q_{2B}} - \epsilon_{-q_{2B}}) C_{-q_{2B}} + V_0 C_{-q_{2B}} + V_0 C_{q_{2B}} = 0$$

$$\Downarrow \left[\begin{array}{cc|c} \lambda_{q_{2B}} - \epsilon_{q_{2B}} + V_0 & V_0 & C_{q_{2B}} \\ V_0 & \lambda_{q_{2B}} - \epsilon_{q_{2B}} + V_0 & C_{-q_{2B}} \end{array} \right] = 0$$

$$(\lambda_{q_{2B}} - \epsilon_{q_{2B}} + V_0)^2 - V_0^2 = 0 \Rightarrow \epsilon_{q_{2B}} = \begin{cases} \lambda_{q_{2B}} \\ \lambda_{q_{2B}} - 2V_0 \end{cases}$$

$$E_{qzB} = \begin{cases} \lambda_{qzB} \\ \lambda_{qzB} - 2V_0 \end{cases} = \begin{cases} \frac{\hbar^2 q_{zB}^2}{2m} \\ \frac{\hbar^2 q_{zB}^2}{2m} - 2V_0 \end{cases}$$

Multiple Bands

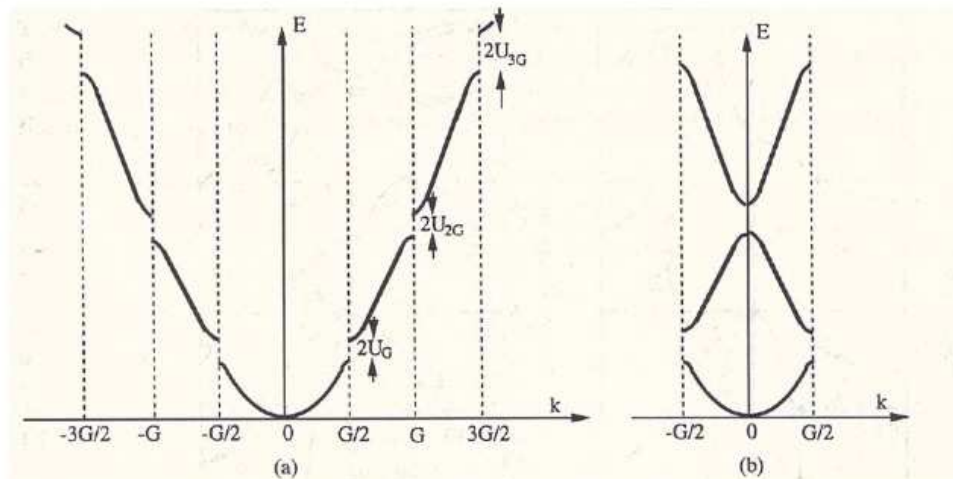


Figure 1-26 (a) Effect of periodic potential on the structure of a single free-electron parabolic band, E_k . When $k = nG/2$ ($n = 1, 2, 3, \dots$), the interaction of the electron wavefunction and the periodic potential creates a forbidden energy gap. (b) The band structure within the first Brillouin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

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BLOCH'S THEOREM

$$\psi_{q_{2B}} = \sum_G c_{q_{2B}-G} \exp(i[q_{2B}-G] \cdot x)$$

$$= \sum_G \left\{ c_{q_{2B}-G} e^{-iGx} \right\} e^{iq_{2B} \cdot x}$$

$$= u(x) \cdot e^{iq_{2B} \cdot x}$$

where

$$u(x) = \sum_G c_{q_{2B}-G} e^{-iGx}$$

$$u(x+a) = \sum_G c_{q_{2B}-G} e^{-iG(x+a)} = \sum_G c_{q_{2B}-G} e^{-iGx} \cdot e^{-iGa} = u(x) \cdot \overbrace{e^{-iGa}}^{=1}$$

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