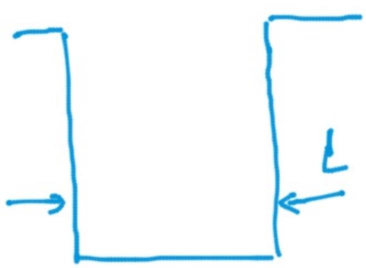
FREE ELECTRON GAS MODEL: N electrons in BOX



Schrödinger Eq.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = \varepsilon\psi$$

$\psi \sim e^{ikx}$ and $\varepsilon = \frac{(\hbar k)^2}{2m}$

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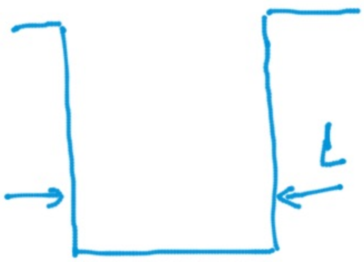


PERIODIC BOUNDARY COND.

$$\psi(0) = \psi(L)$$

$$\Downarrow$$

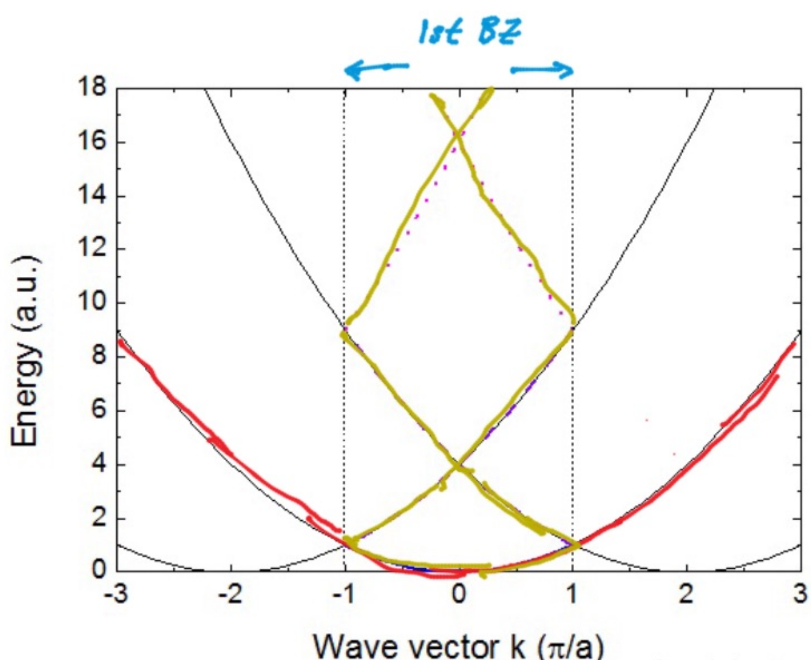
$$k = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \ldots$$

Schrödinger Eq.

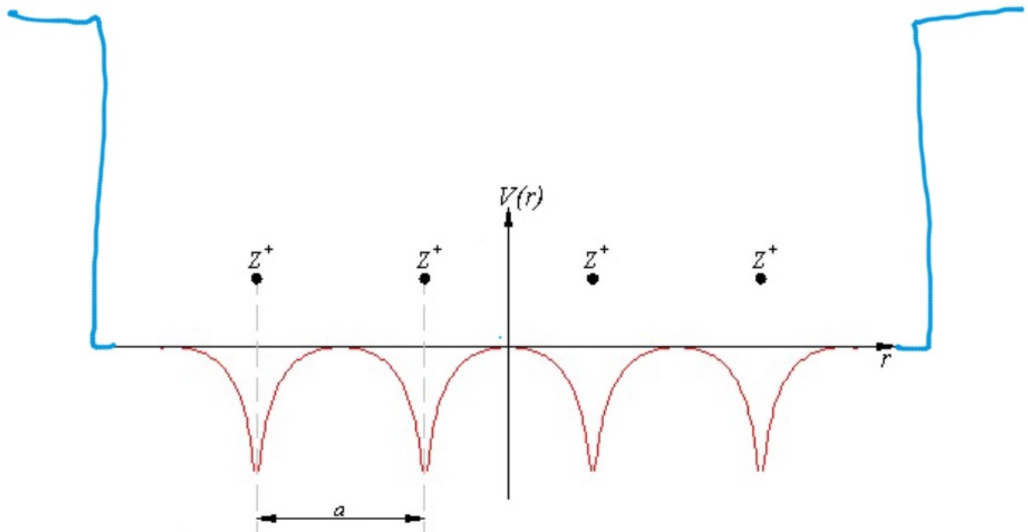
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = \varepsilon\psi$$

$$\psi \sim e^{ikx} \quad \text{and} \quad \varepsilon = \frac{(\hbar k)^2}{2m}$$

ELECTRON DISPERSION:



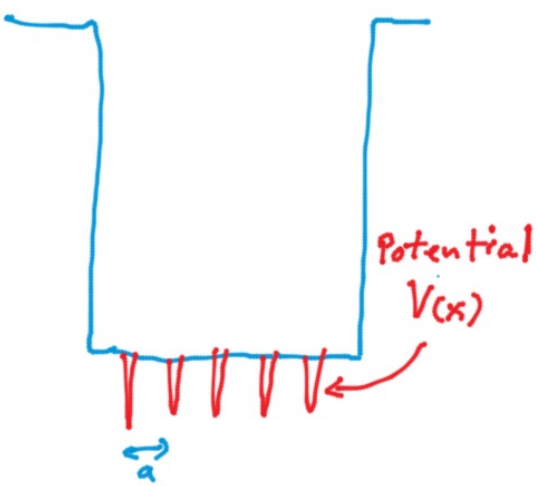
PERIODIC POTENTIAL:



Scrödinger Eq.

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = \varepsilon\psi$$

PERIODIC POTENTIAL:



Scrödinger Eq. (SE)

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = \varepsilon\psi$$

PERIODICITY IMPLIES

$$V(x) = V(x+a)$$

FOURIER TRANSFORM

$$V(x) = \sum_G V_G\, e^{iGx}$$

$$= \sum_G V_G\, e^{iG(x+a)}$$

$$= \sum_G V_G\, e^{iGx} \cdot e^{iGa}$$

THEREFORE

$$e^{iGa} = 1$$

$$\Downarrow$$

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

HARMONIC OSCILLATOR:

$$\ddot{x}(t) + \gamma\dot{x}(t) + \omega_0^2 x(t) = f(t)$$

$$\Downarrow$$

$$-\omega^2 x(\omega) + i\gamma\omega x(\omega) + \omega_0 x(\omega) = f(\omega)$$

$$\Downarrow$$

$$x(\omega) = \frac{f(\omega)}{\omega_0^2 - \omega^2 + i\gamma\omega}$$

Response function

$$\chi(\omega) \equiv \frac{x(\omega)}{f(\omega)} = \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

FOURIER TRANSFORMS

$$x(t) = \int x(\omega)\, e^{i\omega t}\, d\omega$$

$$\dot{x}(t) = \int i\omega x(\omega) e^{i\omega t} d\omega$$

$$\ddot{x}(t) = \int -\omega^2 x(\omega) e^{i\omega t} d\omega$$

$$f(t) = \int f(\omega)\, e^{i\omega t} d\omega$$

REFORMULATION OF SE

FOURIER TRANSFORM

$$\psi = \sum_k c_k\, e^{ikx}$$

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = \varepsilon\psi$$

$$\Downarrow$$

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

$$\Downarrow$$

$$(\lambda - \varepsilon)\sum_k c_k e^{ikx} + \sum_k\sum_G V_G\, c_k\, e^{i(G+k)x} = 0 \quad \text{where } \lambda = \frac{(\hbar k)^2}{2m}$$

$$\Downarrow$$

$$(\lambda - \varepsilon)\sum_{k'} c_{k'} e^{ik'x} + \sum_{k'}\sum_G V_G\, c_{k'-G}\, e^{ik'x} = 0 \quad \text{with } \begin{array}{l} k' = k + G \\ k = k' - G \end{array}$$

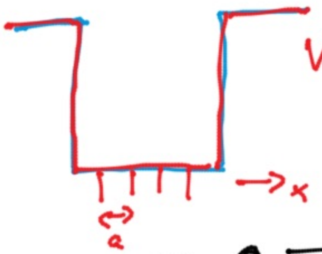
$$\Downarrow$$

$$\sum_{k'} e^{ik'x}\left\{(\lambda - \varepsilon)c_{k'} + \sum_G V_G\, c_{k'-G}\right\} = 0$$

We now have that:

$$\boxed{(\lambda_{k'} - \varepsilon)c_{k'} + \sum_G V_G\, c_{k'-G} = 0 \quad \text{CENTRAL EQUATION (CE)}}$$

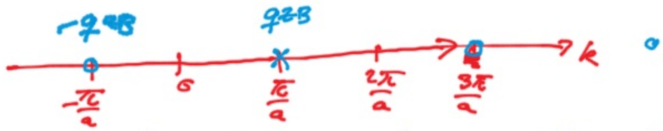
Example: KRONIG-PENNEY MODEL



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

$$V_G = V_0$$ → REMEMBER FOURIER TRANSFORM OF δ = constant

IN THE FOLLOWING WE CONSIDER AN ELECTRON WITH $k = q_{ZB}$



FOR $V_0 = 0$, WE KNOW THE SOLUTION:

$$\psi \sim e^{i q_{ZB} x} \quad \& \quad \mathcal{E} = \frac{(\hbar q_{ZB})^2}{2m}$$

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CONSIDER $V_0 \to 0$ LIMIT

Example: KRONIG-PENNEY MODEL

WE CONSIDER
→ $V_0 \to 0$ LIMIT
&
→ ELECTRON WITH $q_{ZB} = \frac{\pi}{a}$

WE APPLY CENTRAL EQUATION

$$(\lambda_{k'} - \varepsilon) C_{k'} + \sum_G V_G C_{k'-G} = 0$$

↓

$$(\lambda - \varepsilon + V_0) C_{q_{ZB}} + V_0 C_{-q_{ZB}} = 0$$
$$(\lambda - \varepsilon + V_0) C_{-q_{ZB}} + V_0 C_{q_{ZB}} = 0$$

↓

2 EQUATION & 2 UNKNOWNS

EASY

Since $V_0 \to 0$ the solution should be close to $V_0 = 0$ case. THEREFORE WE ONLY SUM OVER q_{ZB} & $-q_{ZB}$

$$(\lambda-\varepsilon+V_0)\,C_{qzB} + V_0\,C_{-qzB} = 0$$
$$(\lambda-\varepsilon+V_0)\,C_{-qzB} + V_0\,C_{qzB} = 0$$

2 EQUATION & 2 UNKNOWNS

EASY

$$\left(\begin{array}{cc|c} \lambda-\varepsilon+V_0 & V_0 & 0 \\ V_0 & \lambda-\varepsilon+V_0 & 0 \end{array}\right)$$

The determinant gives:

$$(\lambda-\varepsilon+V_0)^2 = V_0^2$$

$$\Downarrow$$

$$\varepsilon = \begin{cases} \lambda \\ \lambda-2V_0 \end{cases}$$

Where

$$\lambda = \frac{(\hbar q_{zB})^2}{2m}$$

THE DISPERSION HAS TWO SOLUTION AT q_{zB}!!

$$(\lambda-\varepsilon+V_0)\,C_{qzB} + V_0\,C_{-qzB} = 0$$
$$(\lambda-\varepsilon+V_0)\,C_{-qzB} + V_0\,C_{qzB} = 0$$

2 EQUATION & 2 UNKNOWNS

EASY

YOU CAN ALSO SOLVE FOR C_{qzB} & C_{-qzB}.

THIS WILL GIVE YOU THE WAVE-FUNC.

You should find

$$\psi = e^{iq_{zB}} \pm e^{-iq_{zB}}$$

If we had included all terms in $\sum_G$ sum of the central equation, we would have

$$\psi = \sum_G C_{qZB-G}\, e^{i(qZB-G)x}$$

This result is valid for all k's hence

$$\begin{aligned}\psi &= \sum_G C_{k-G}\, e^{i(k-G)x}\\ &= \left(\sum_G C_{k-G}\, e^{-iGx}\right)\cdot e^{ikx}\\ &= u(x)\cdot e^{ikx}\end{aligned}$$

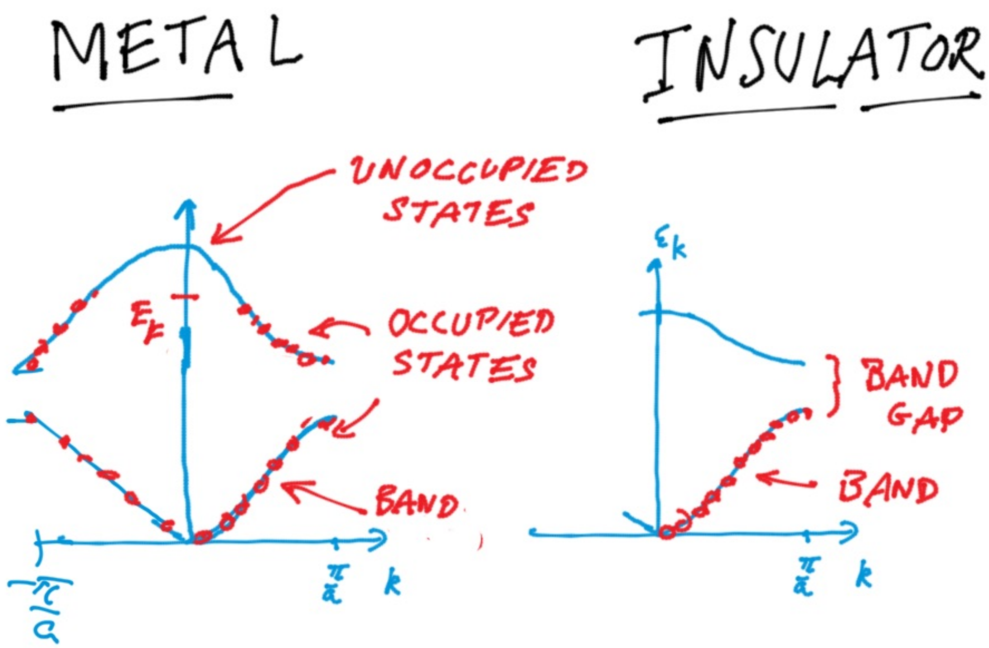
$$\left.\begin{aligned}\psi &= \sum_G C_{k-G}\, e^{i(k-G)x}\\ &= \left(\sum_G C_{k-G}\, e^{-iGx}\right)\cdot e^{ikx}\end{aligned}\right\}\ \text{WAVE FUNCTION}$$

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

Notice that:

$$\begin{aligned}u(x+a) &= \sum_G C_{k-G}\, e^{-iG(x+a)}\\ &= \sum_G C_{k-G}\, e^{-iGx}\, e^{-iGa}\\ &= \sum_G C_{k-G}\, e^{-iGx}\\ &= u(x)\end{aligned}$$

$$\boxed{\text{THEREFORE: } \psi = (\text{PERIODIC FUNCTION}) \times (\text{PLANE WAVE})}$$


METAL
INSULATOR
UNOCCUPIED STATES
OCCUPIED STATES
BAND
E_F
$-\frac{\pi}{a}$
$\frac{\pi}{a}$
k
ε_k
BAND GAP
BAND
$\frac{\pi}{a}$
k