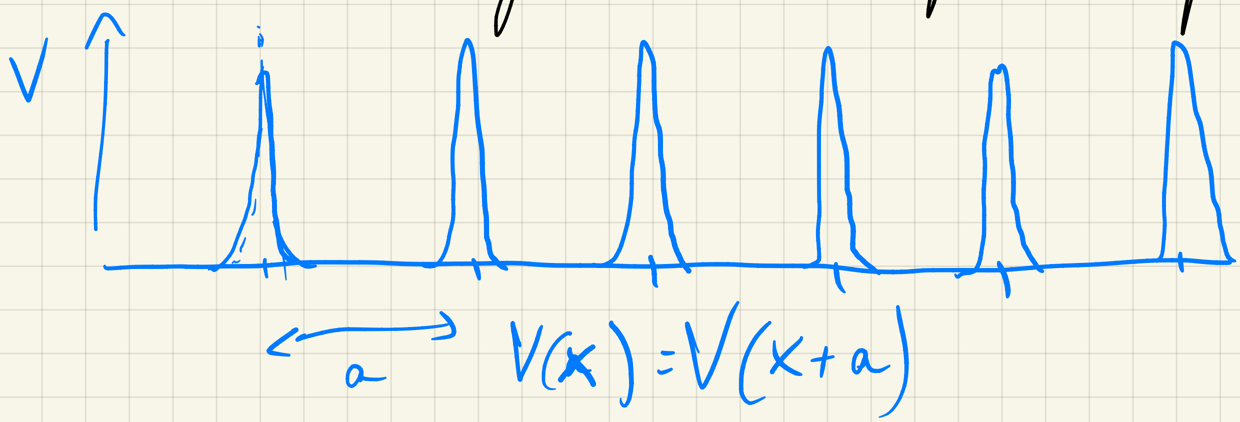
1.- Electrons in 1D Periodic Potentials

- Reductionist approach 3D → 1D
  (Not always works (!)), but a 1D crystal is the most simple model of a "solid". And here the theorems in 1D can be easily generalized to 3D.

- Key Feature: Periodicity
  - Translational symetry:
    → Atoms of the same element are identical and will form ordered structures.

- Consider a <u>single</u> e^- in a periodic potential:



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

Sch. eq

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

$V(x) = V(x + ma)$ — m → integer, a → period

* Take Fourier Transform of V:

$$V(x) = \sum_{n=-\infty}^{\infty} V_n\, e^{i h_n x}, \quad h_n = \frac{2\pi n}{a}$$

, wave # h_n

* What does Periodicity mean for ψ an E?
  - Consider $V(x) = 0$ (Trivially periodic)
    - Wavefunctions are plane waves (PW) $W_k(x) = \frac{1}{\sqrt{L}} e^^{ikx}$ — L = normalization length of crystal
    - Eigenvalues $E = \frac{\hbar^2 k^2}{2m}$
    - W_k are orthonormal, form a complete set
  - Now consider $V(x) \neq 0$. Apply H to W_k

since $V(x)\,W_k(x) = \frac{1}{\sqrt{L}} \sum_n V_n\, e^{i(h_n + k)x}$,

$$\langle x|H|W_k\rangle \in \underbrace{\{W_k(x), W_{k+h_1}(x), W_{k-h_1}(x), W_{k+h_2}(x) \dots\}}_{\text{subspace of PW with wave\# } k+h_n\text{, } S_k}$$

Also, $H|W_{k+h_n}\rangle \in S_k$ (closed)

$\Rightarrow$ Only need to diagonalize H in subspaces S_k

$\Rightarrow$ Eigenvectors of H labeled as $\psi_k(x)$

$\Rightarrow S_k \neq S_{k'}$ if $k \neq k' + \frac{2\pi n}{a}$ for $n \in \mathbb{Z}$

$\Rightarrow$ all different k labels reside in $-\frac{\pi}{a} < k < \frac{\pi}{a}$

First Brillouin zone

We can write $\psi_k(x) = \sum_n C_n(k) \frac{1}{\sqrt{L}} \exp(i(k+h_n)x)$

$$\boxed{\psi_k(x) = U_k(x)\, e^{ikx}}$$

$\rightarrow$ Travelling PW

Where $U_k(x) = \sum_n C_n(k) \frac{1}{\sqrt{L}} e^{ih_n x}$

$\uparrow$ Periodic function: $U_k(x+a) = U_k(x)$

(recall, $h_n = \frac{2\pi n}{a}$ and $e^{in2\pi} = 1$)

Bloch's Th: Any (physical) solution of S.E in a periodic potential can be written in the form of a travelling PW modulated by a microscopically periodic function

* Back To question: What does periodicity mean for ψ, ϵ?

- $\psi(x+t_n) = e^{ik t_n} \psi(x)$ with $t_n = n \cdot a$

. Demonstrate This!

$\psi(x) = e^{ikx} U_n(x)$; $\psi(x+t_n) = e^{ik(x+t_n)} \underbrace{U_n(x+t_n)}_{U_n(x)}$

$\psi(x+t_n) = e^{ik t_n} \underbrace{e^{ikx} U_n(x)}_{\psi(x)}$. QED

- If the potential is not periodic we cannot write $\psi_k(x)$ as a linear combination of PW of Type $e^{i(k+h_n)x}$

i.e $\rightarrow$ Not discretized

$\underbrace{\psi(x) = \int_{-\infty}^{\infty} c(q) e^{iqx} dq}$ $\longrightarrow$ Not $\sum$ but continuous integral with any value of q

Nothing can be infered

- from This about The WF properties or spectral properties

- Periodicity →
  - itinerant WF (Bloch Th)
  - Allowed energy regions separated by energy gaps $E(k) = E(-k)$

- 1D
  - No degeneracy (bands cannot cross!)
  - Monotonic $0 \le k \le \pi/a$
  - Extremes at 0 & π/a

in 1D group Th. analysis prevents any degeneracy.
in 2D/3D yes!

- We consider $0 \le x \le \infty$, but a crystal is finite of size L ($L \sim 1\,cm$, $N \sim 10^8$ with $a = 1\,Å$)

So $0 \le x \le L$ $\qquad L = N \cdot a$

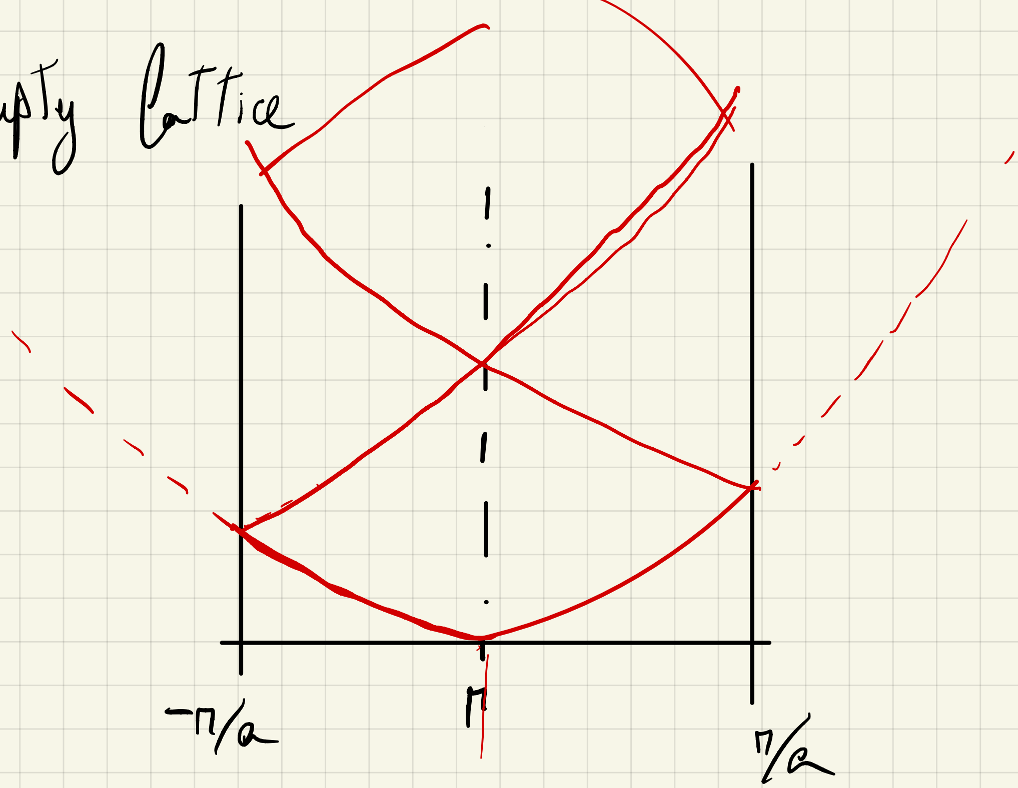
Use Born von Karman (PBC): $\psi(x + Na) = \psi(x)$

$$e^{ikNa} = 1 \implies k = \frac{2\pi}{Na} n \quad (n = 0, \pm 1, \pm 2 \dots)$$

Density of k states in k space: $DOS = \frac{L}{2\pi}$

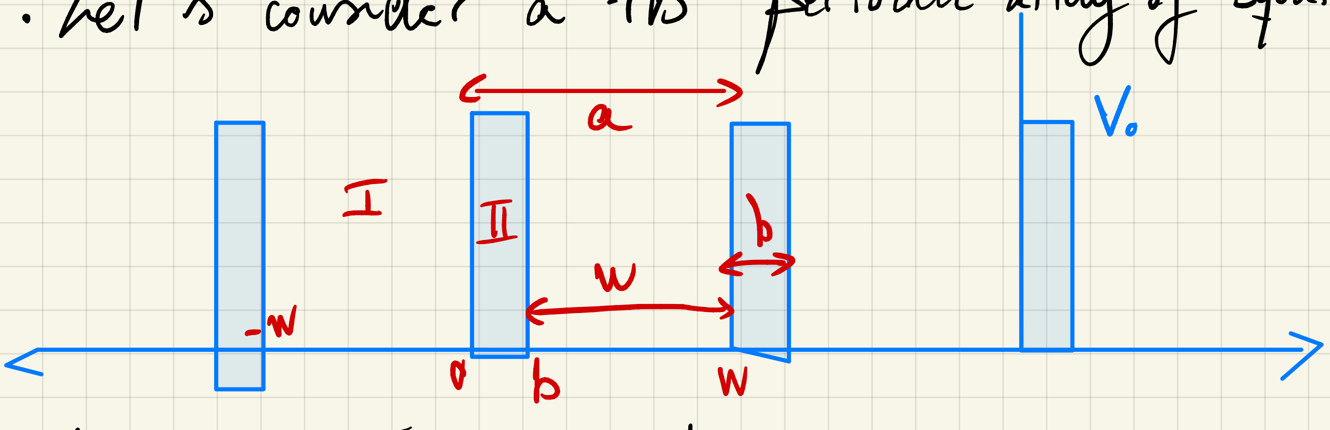
Example: empty lattice

$V(x) = 0$



Kronig-Penney Model

- Let's consider a 1D periodic array of square wells



- Lattice constant: $a = w + b$
- in unit cell $0 < x < b$

$$\begin{cases} \text{I} & -w < x < 0 \quad \text{is well} \\ \text{II} & 0 < x < b \quad \text{is barrier} \end{cases}$$

• Recall S.E in finite Well $0 < E < V_0$

$$\psi_I(x) = Ae^{iqx} + Be^{-iqx} \quad , \; q = \sqrt{2mE/\hbar^2}$$

$$\psi_{II}(x) = Ce^{\beta x} + De^{-\beta x} \quad , \; \beta = \sqrt{2m(V_0 - E)/\hbar^2}$$

Constants A-D from boundary Conditions

$$\psi_I(0) = \psi_{II}(0) \qquad \left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0}$$

$$\psi_{II}(b) = e^{ika}\,\psi_I(-w) \qquad \left.\frac{d\psi_{II}}{dx}\right|_{x=b} = e^{ika}\left.\frac{d\psi_I}{dx}\right|_{x=-w}$$

as $\psi(b) = \psi(-w+a)$ and the potential is periodic we apply B.T ($\psi(x+a) = e^{ika}\psi(x)$)

$$\begin{cases} A + B = C + D \\ Aiq - Biq = C\beta - D\beta \\ Ce^{\beta b} + De^{-\beta b} = e^{ika}\left[Ae^{-iqw} + Be^{iqw}\right] \\ C\beta e^{\beta d} - D\beta e^{-\beta b} = e^{ika}\left[Aiqe^{-iqw} - Biqe^{iqw}\right] \end{cases}$$

- Solving Analytically and graphically ;

- Analytically :

$$0 = \begin{vmatrix} 1 & 1 & -1 & -1 \\ iq & -iq & -\beta & \beta \\ -e^{ika-iqw} & -e^{ika+iqw} & e^{\beta b} & e^{-\beta b} \\ -iq\,e^{ika-iqw} & iq\,e^{ika+iqw} & \beta e^{\beta b} & -\beta e^{-\beta b} \end{vmatrix}$$

$$\frac{\beta^2 - q^2}{2q\beta} \sinh \beta \sin qw + \cosh \beta b \cos qw = \cos ka$$

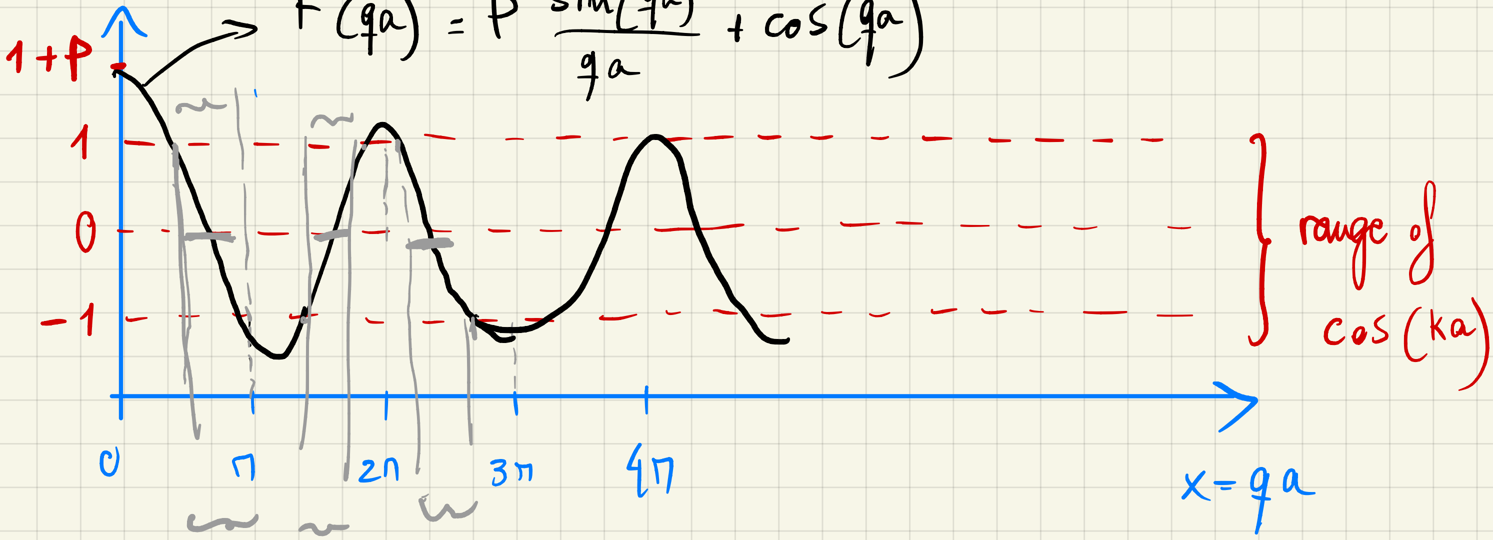
- Additional simplification : $b \to 0$, $V_0 \to \infty$ but with $V_0 \cdot b = \text{constant}$ (area of potential is conserved)

$\to$ δ-like potential barriers

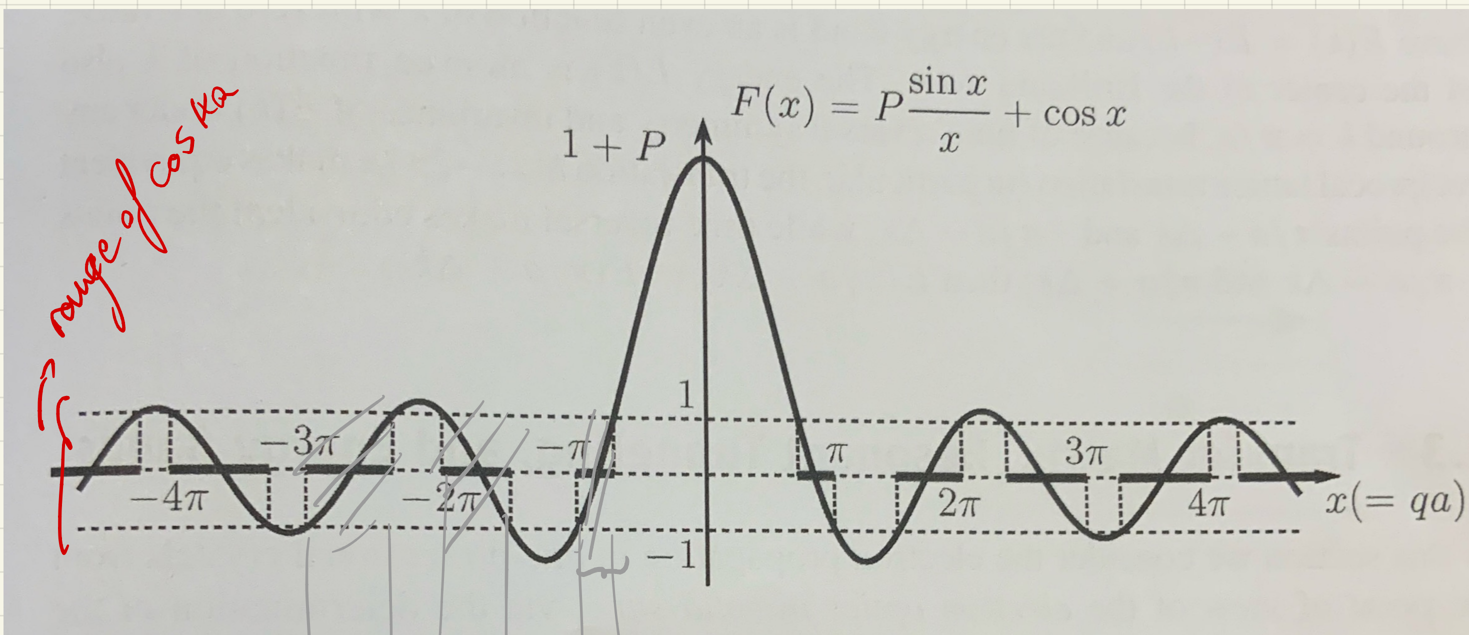
$$\underbrace{\frac{m V_0 b a}{\hbar^2}}_{\text{unitless} \equiv P} \frac{\sin qa}{qa} + \cos qa = \underbrace{\cos ka}_{\text{ranges from } -1 \text{ to } 1}$$

- Solve graphically

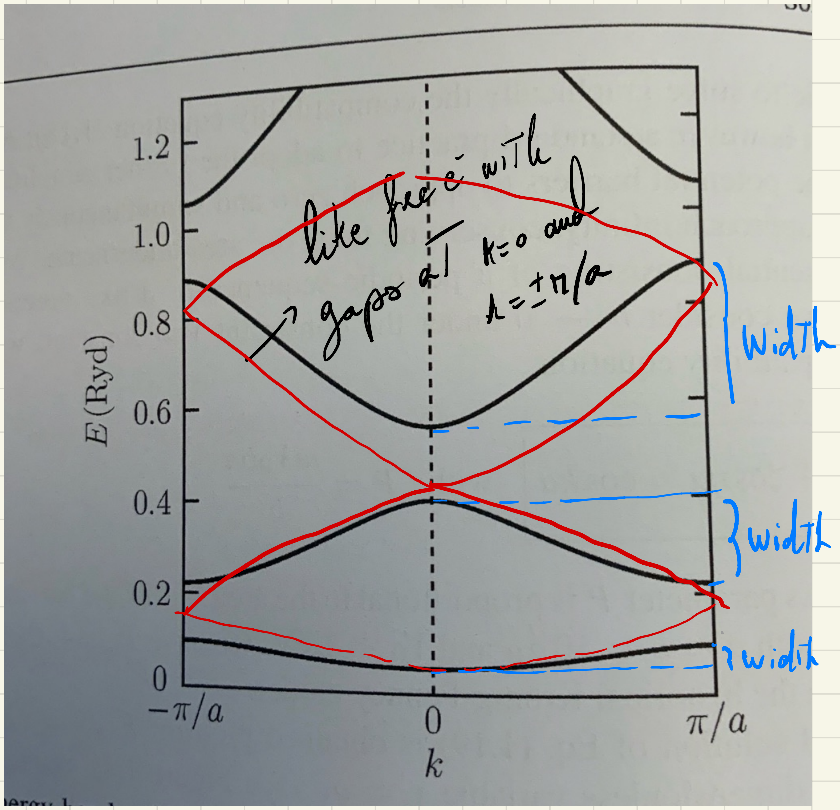
$$F(qa) = P\,\frac{\sin(qa)}{qa} + \cos(qa)$$



allowed energy regions $E = \dfrac{q^2\hbar^2}{2m}$ $\Rightarrow$ Note they increase as E increases



allowed energy regions. The width increases with x (so energy increases also)



Width increases as E increases

Note we have folded back the energies in the 1st BZ!