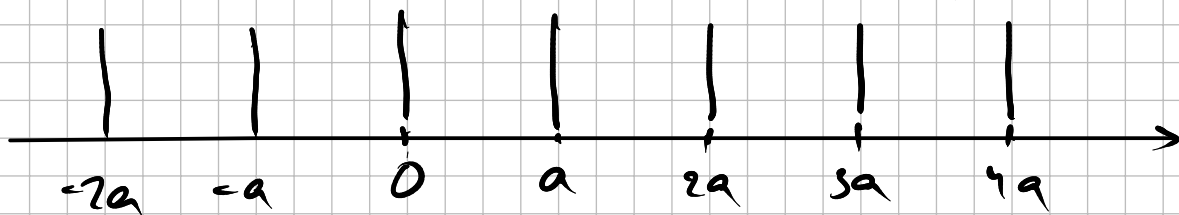


Band structure. Improvement of free electron gas model.

So far we treat solids as an empty box, confining the solid body, in which electrons are free of any potentials.

Now we add notion of nuclei which we treat as "frozen" in a periodic grid. We are not going to think about exact form of potential created by nuclei the most important is periodicity of the potential.

let's consider 1D space:



simplest form of such potential is delta function

$$V(x) = d \sum_{j=0}^{N-1} \delta(x - ja)$$

this comb takes $N \cdot a$ length, where N is humongous (avagadro number like) $\approx 10^{25}$

Notice that $\psi(x)$ should satisfy

$$\psi(x+a) = e^{-i\phi} \cdot \psi(x)$$

phase factor
is OK since
only $|\psi(x)|^2$ is important

if we slide by 1 slot
nothing should change
since potential still look
like the "same" comb.

Consequently, if we find

$\psi(x)$ where $0 < x < a$ we can find
in $a < x < 2a$ by simple $\psi(x+a)$
translation. Applying this idea to the next
"cell" (space in the grid) again and again we will
know $\psi(x)$ everywhere.

So we can focus only on the first cell
 $0 < x < a$. If we put origin in the middle
of the bulk, same translation
idea can be used with '-a' shift.

Between 0 and a we have empty space
i.e. free moving particle.

$$\text{So } \psi(x) = [A \sin(\kappa x) + B \cos(\kappa x)], \quad 0 < x < a$$

translating it to the side once and using

$$\psi(x+a) = \psi(x) e^{-i\phi}$$

$$\psi(x+a) = \underbrace{[A \sin(\kappa(x+a)) + B \cos(\kappa(x+a))]}_{\text{Literally } \psi(x+a)} = \psi(x) e^{-i\phi}$$

we get alternative way to express

$$\psi(x) = [A \sin(\kappa(x+a)) + B \cos(\kappa(x+a))] e^{i\phi}$$

$$\text{or } = [A \sin(\kappa x) + B \cos(\kappa x)]$$

Reminder: $\psi(x)$ is continuous, $\psi'(x)$ continuous except where $V(x)$ is infinite

1st form

alternative form

$$\psi(0) = B = (A \sin(ka) + B \cos(ka)) e^{iP} \quad (*)$$

Finding condition for ψ' is harder.
let's look back at Schrödinger eq.

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

$\epsilon \rightarrow 0$, i.e. we integrate around 0

$$-\frac{\hbar^2}{2m} \left. \frac{d\psi}{dx} \right|_{-\epsilon}^{\epsilon} + \underbrace{\int_{-\epsilon}^{\epsilon} V(x) \psi(x) dx}_{2\psi(0)} = \int_{-\epsilon}^{\epsilon} E \psi(x) dx \rightarrow 0 \text{ as } \epsilon \rightarrow 0$$

$$\psi'(0+) - \psi'(0-) = \frac{2m}{\hbar^2} \psi(0) \quad (**)$$

1st form $\rightarrow \psi'(x) = \kappa A \cos(\kappa x) - \kappa B \sin(\kappa x) \Rightarrow \psi'(0) = \kappa A$
 2nd form $\rightarrow \psi'(x) = [\kappa A \cos(\kappa(x+a)) - \kappa B \sin(\kappa(x+a))] e^{i\varphi}$
 $\Rightarrow \psi'(-0) = [\kappa A \cos(\kappa a) - \kappa B \sin(\kappa a)] e^{i\varphi}$

(~~xx~~) : $\kappa A - \kappa e^{i\varphi} [A \cos(\kappa a) - B \sin(\kappa a)] = \frac{2m\alpha}{\hbar^2} B$

(x) : $B = e^{i\varphi} [A \sin(\kappa a) + B \cos(\kappa a)]$

$A = B(e^{-i\varphi} - \cos(\kappa a)) \frac{1}{\sin(\kappa a)}$

~~$B(e^{-i\varphi} - \cos(\kappa a)) \frac{1}{\sin(\kappa a)} [1 - e^{i\varphi} \cos(\kappa a)] + e^{i\varphi} B \sin(\kappa a) = \frac{2m\alpha}{\hbar^2} B$~~

$(e^{-i\varphi} - \cos(\kappa a))^2 \cdot e^{i\varphi} + e^{i\varphi} \sin^2(\kappa a) = \frac{2m\alpha}{\hbar^2} \sin(\kappa a)$

$e^{-i\varphi} - 2\cos(\kappa a) + \underbrace{e^{i\varphi} \cos^2(\kappa a) + e^{i\varphi} \sin^2(\kappa a)}_{e^{i\varphi}} = \frac{2m\alpha}{\hbar^2} \sin(\kappa a)$

$\underbrace{e^{-i\varphi} + e^{i\varphi}}_{2 \cos(\varphi)} = 2 \cos(\kappa a) + \frac{2m\alpha}{\hbar^2} \sin(\kappa a)$

$\psi(0)$

$$\cos(\varphi) = \cos(ka) + \frac{m^2}{\hbar^2 k} \sin(ka)$$

$$z \equiv ka$$

$$\beta = \frac{m^2}{\hbar^2} a$$

$$\cos(\varphi) = \cos(z) + \beta \frac{\sin(z)}{z} = f(z)$$

if $|f(z)| > 1$ then there is no solution for ' φ ' ($\cos(\varphi) \leq 1$)

