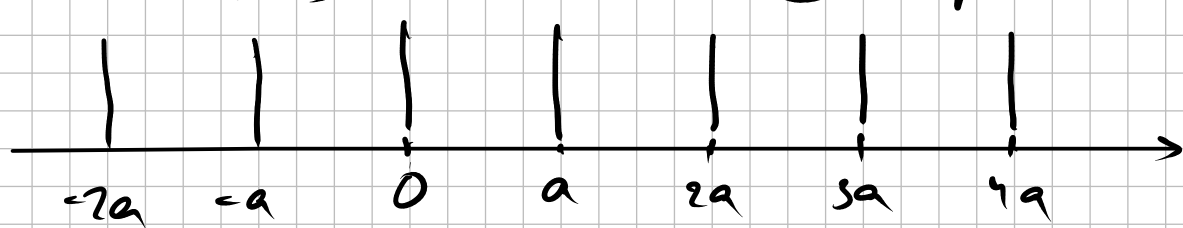
Band structure. Imrovement of free electron gas model.

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

let's consider 1D space:



simplest form of such potential is delta function

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

this comb takes $N \cdot a$ length, where N is humongous (avagadro number like) $\gtrsim 10^{23}$

Notice that $\psi(x)$ should satisfy

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

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

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

Consequently, if we find $\psi(x)$ where $0<x<a$ we can find in 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 midle 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.

So $\psi(x) = \left[A\sin(\kappa x) + B\cos(\kappa x)\right]$, $0 < x < a$

translating it to the side once and using

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

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

we get alternative way to express

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

or $= \left[A\sin(\kappa x) + B\cos(\kappa x)\right]$

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

1st form

alternative form

$$\psi(0) = \boxed{B = \left(A\sin(\kappa a) + B\cos(\kappa a)\right)e^{i\varphi} \qquad (*)}$$

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

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

$\varepsilon \to 0$, i.e. we integrate around 0

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\varepsilon}^{\varepsilon} + \underbrace{\int_{-\varepsilon}^{\varepsilon}\alpha\delta(x)\psi(x)}_{\alpha\psi(0)} = \underbrace{E\int_{-\varepsilon}^{\varepsilon}\psi(x)dx}_{0 \text{ as } \varepsilon\to 0}$$

$$\boxed{\psi'(+0) - \psi'(-0) = \frac{2m}{\hbar^2}\alpha\,\psi(0) \qquad (**)}$$

1st form $\rightarrow \psi'(x) = \kappa A\cos(\kappa x) - \kappa B\sin(\kappa x) \Rightarrow \psi'(+0) = \kappa A$

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

$$\Rightarrow \psi'(-0) = [\kappa A\cos(\kappa a) - \kappa B\sin(\kappa a)]\, e^{i\varphi}$$

$\psi(0)$

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

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

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

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

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

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

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

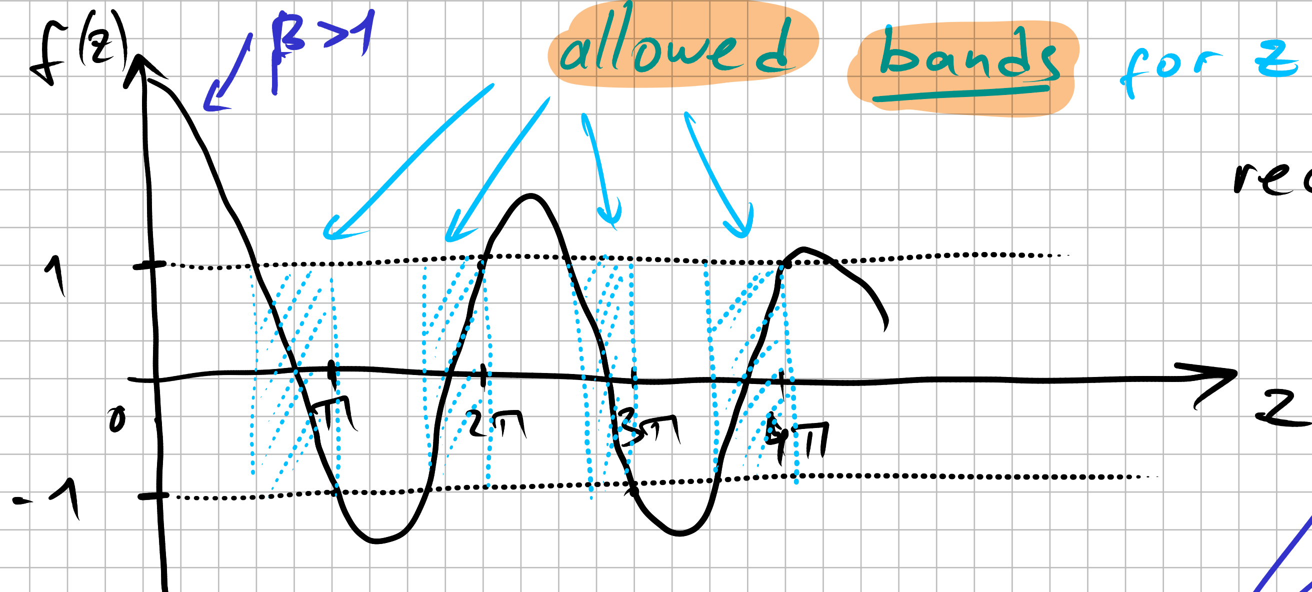
$$\cos(\varphi) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)$$

$$z \equiv ka \qquad \beta = \frac{m\alpha}{\hbar^2}a$$

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

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

allowed bands for $z \Rightarrow ka$



recall that

$$E = \frac{\hbar^2}{2m}k^2$$