Quantum Solids

Free electron gas – each electron occupies a "volume" in a momentum space

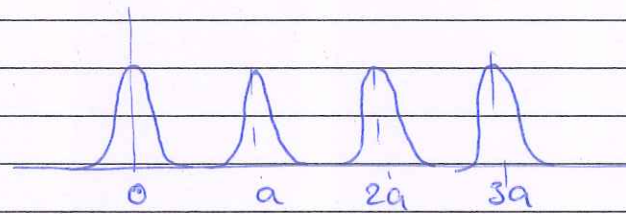
$d^3\vec{k} = dk_x\, dk_y\, dk_z = \pi^3/V$

Free electrons occupy all available kinetic energies from zero to the Fermi energy E_f (highest single-particle energy in the ensemble ground state)

$$E_f = \frac{\hbar^2 k_f^2}{2m} \qquad k_f = \sqrt[3]{2\pi^2 \frac{N}{V}} = \sqrt[3]{2\pi^2 \rho}$$

Periodic potential $\longrightarrow$ more realistic solids

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



In such potential we expect same periodicity in the measurable quantities

$$|\psi(x)|^2 = |\psi(x+a)|^2$$

Bloch theorem : $\psi(x+a) = e^{iKa}\psi(x)$

$$\psi(x+2a) = e^{i2Ka}\psi(x)$$

To account for the finite (but very large) size of the sample we impose cyclic boundary conditions $\psi(0) = \psi(L = Na)$ and in general $\psi(x) = \psi(x + Na)$

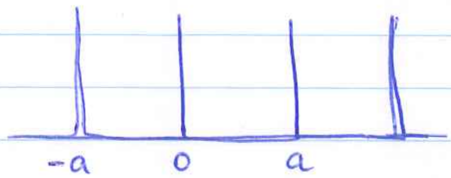
$$\psi(x) = e^{iNKa}\psi(x) \implies K = \frac{2\pi n}{Na}$$

(same quantization as we did for free electrons)

Since $N \gg 1$ it is almost continuous spectrum

To simplify the calculations, we will model a 1D crystal as an array of N periodik δ- functions, separated by the distance a

$$U(x) = \alpha \sum_{j=0}^{N-1} \delta(x - j\cdot a)$$



Let's first check inside the first "cell" $0<x<a$

Since the particle is free, its wave function is

$$\psi(x) = A\cos kx + B\sin kx$$

The wave function in all consecutive "cells" must be similar, but include an extra phase as per Block theorem $\psi(x+a) = e^{iKa}\psi(x)$

The wave function also must be continuous at $x = j\cdot a$, thus "stitching" the wave functions at different "cells"

$\underline{x=0}$ $$\lim_{\varepsilon\to 0}\psi(\cancel{a+}\varepsilon) = \lim_{\varepsilon\to 0}\psi(-\varepsilon) = \lim_{\varepsilon\to 0} e^{-iKa}\psi(a-\varepsilon)$$

$$A = e^{-iKa}(A\cos ka + B\sin ka)$$

or

$\underline{x=a}$ $$\lim_{\varepsilon\to 0}\psi(a-\varepsilon) = \lim_{\varepsilon\to 0}\psi(a+\varepsilon) = \lim_{\varepsilon\to 0} e^{iKa}\psi(\varepsilon)$$

$$A\cos ka + B\sin ka = e^{iKa}\cdot A$$

Also, $\cancel{\psi'}$ the change in the derivative is $\frac{2m\alpha}{\hbar^2}\cdot A$

$\underline{x=0}$ $$\lim_{\varepsilon\to 0}\psi'(\varepsilon) - \lim_{\varepsilon\to 0}\psi'(-\varepsilon) = \lim_{\varepsilon\to 0}\psi'(\varepsilon) - e^{-iKa}\lim_{\varepsilon\to 0}\psi'(a-\varepsilon) = \frac{2m\alpha}{\hbar^2}A$$

$$kB - k e^{-iKa}(-A\sin ka + B\cos ka) = \frac{2m\alpha}{\hbar^2}A$$

$$B\sin ka = (e^{iKa} - \cos ka)A$$

$$k\cdot(1 - e^{-iKa}\cos ka)B = \left(\frac{2m\alpha}{\hbar^2} - k e^{-iKa}\sin ka\right)A$$

$$k(1-e^{-iKa}\cos ka)(e^{iKa}-\cos ka) = \frac{2m\alpha}{\hbar^2}\sin ka - k e^{-iKa}\sin^2 ka$$

$$e^{iKa} - \cos ka - \cos ka + \underbrace{e^{-iKa}\cos^2 ka + e^{-iKa}\sin^2 ka}_{e^{-iKa}} = \frac{2m\alpha}{\hbar^2 k}\sin ka$$

$$e^{iKa} + e^{-iKa} = 2\cos Ka$$

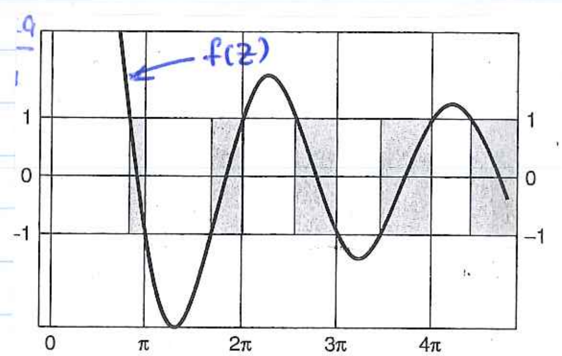
$$2\cos Ka - 2\cos ka = \frac{2m\alpha}{\hbar^2 k}\sin ka$$

or $$\cos Ka = \cos ka + \frac{m\alpha}{\hbar^2 k}\sin ka$$

using $\beta = \frac{m\alpha a}{\hbar^2}$ and $z = ka$

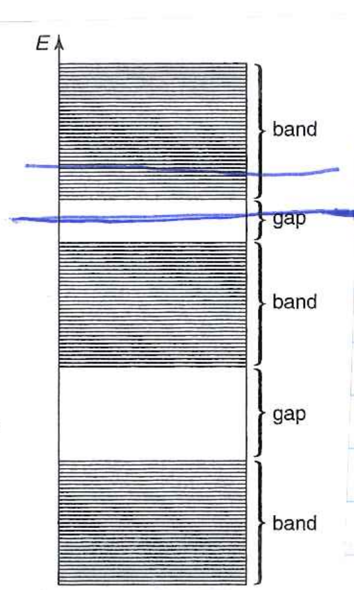
$$\cos Ka = \underbrace{\cos z + \beta\frac{\sin z}{z}}$$

must be b/w -1 and 1 to have any solutions



Shaded are → it is possible to find solutions ~~E(K)~~) (~~for~~ since $|f(z)| \le 1$) Thus, there are available states $E(K)$

lines - states with different K values, representing allowed values of electron energy $E(K)$



Fermi energy for a conductor many available states

Fermi energy for an insulator ~~conductor~~ no available states for electrons to move into