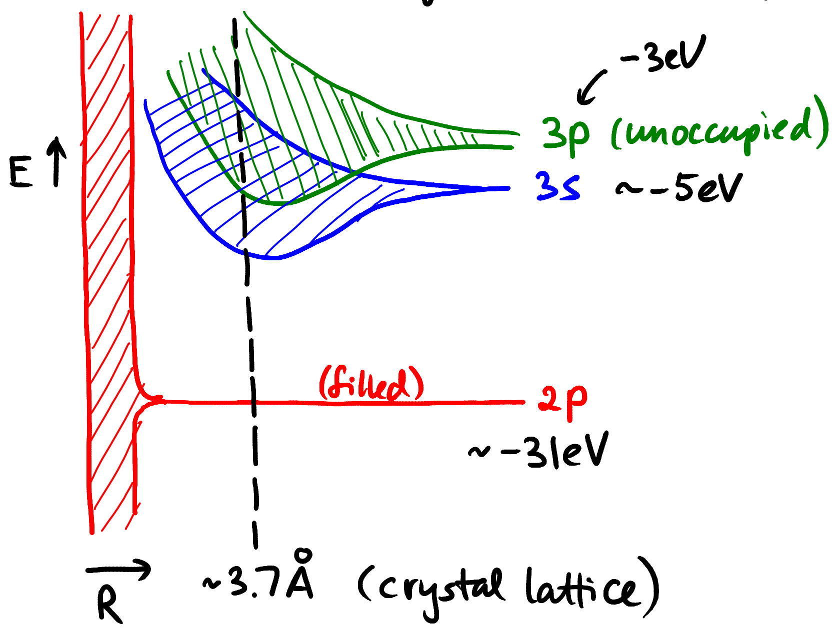
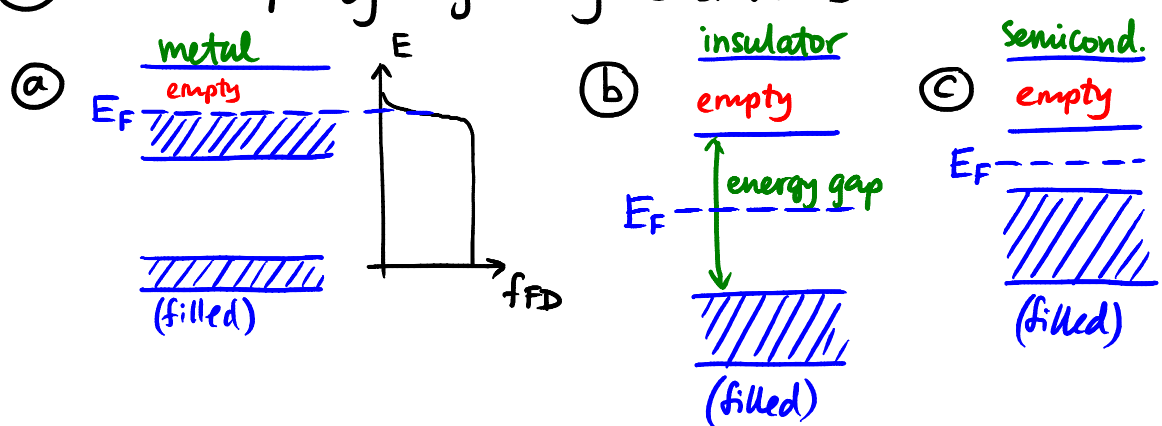
Energy band structure

① Sodium Na ($Z=11$)

Ground state configuration $1s^2 2s^2 2p^6 3s^1$



② level occupancy is given by FD statistics



some terminology

"valence band" (VB) : highest filled band

"Conduction band" (CB) : lowest empty band

"energy gap" = CB minimum − VB maximum

ⓐ E_F level inside valence band (= conduction band)

$\Rightarrow$ energy gap $= 0$ (or $\sim$ eV/10^{23})

small energy needed to move e^- into unoccupied level

<u>metals</u> resistivity $\rho = \frac{1}{\sigma} \sim 10^{-8}\,\Omega\text{m}$

ⓑ E_F inside energy gap.

no available levels except with large excitation energy

gap ~ 10eV

<u>insulators</u> $\rho \sim 10^{14}\,\Omega\text{m}$

ⓒ same as ⓑ but energy gap ~1eV

e^-'s can be thermally excited into CB,

there they become n (–) carriers

(empty vacancies in VB act as p (+) carriers = "holes")

<u>semiconductors</u> $\rho \sim 10^{-2}$ to $10^{9}\,\Omega\text{m}$

<u>Resistivity temperature dependence</u>

metals: ρ increases with T

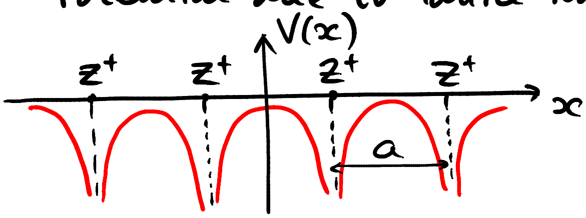
semiconductors: ρ decreases with T

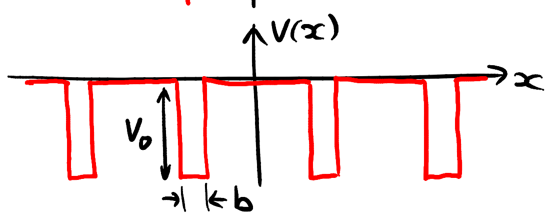
③ QM model (1D)

Potential due to lattice ions: $V(x+a) = V(x)$

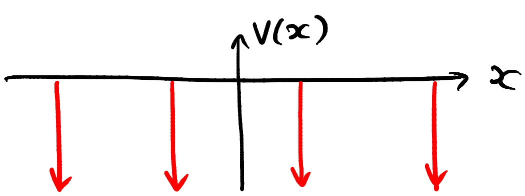
periodic with a

a = lattice const.





"Kronig-Penney"

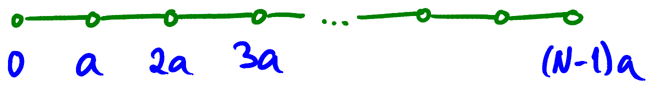


Dirac comb

Solve $\hat{\mathcal{H}}\Psi = E\Psi$ with $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(x)$

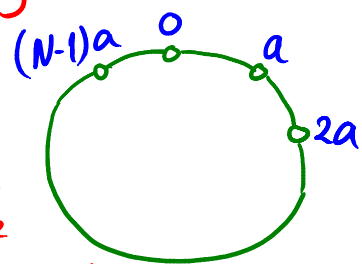
Q: what to do with boundaries on either end ?

1D lattice
N atoms



A: mathematically convinient

N>>1 approaches
1D linear lattice



truly periodic

<u>Bloch theorem</u> : soln. is of the form $\psi(x) = e^{ikx}u(x)$

k is a real quantity

$u(x+a) = u(x)$ periodic with a

use Bloch theorem to "extend" results for $0<x<a$ to the entire lattice

$\psi(x+a) = e^{ik(x+a)}u(x+a) = e^{ika}\psi(x)$

$|\psi(x+a)|^2 = |\psi(x)|^2 \leftarrow$ as anticipated for meas quant.

k - quantized , not continuous

$\psi(x+Na) = e^{ikNa}\psi(x) = \psi(x)$ (same pt)

$e^{ikNa} = 1$, $\Rightarrow$ $kNa = 2\pi n$, n any integer

$k_n = \frac{2\pi}{Na} n$ discrete

a) $-\frac{N}{2} \leq n < \frac{N}{2}$, N possible states

$-\frac{\pi}{a} < k_n < \frac{\pi}{a}$ 1^{st} Brillouin zone

$\rightarrow E(k_n)$ = first energy band

b) $-N \leq n < -\frac{N}{2}$ or $\frac{N}{2} \leq n < N$

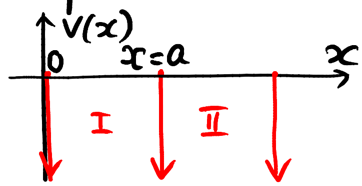
$\frac{\pi}{a} < |k_n| < 2\frac{\pi}{a}$ 2nd Brillouin zone

$\rightarrow E(k_n)$ = second energy band

c) etc.

(4) specific example of Dirac comb potential

$$V(x) = -V_0 a \sum_{j=0}^{N-1} \delta(x - ja)$$



* solve Sch. eq. for $0 \le x < a$ (region I), then use Bloch theorem to extend to region II, etc.

$$\psi_I(x) = A \sin k_0 x + B \cos k_0 x \quad , \text{ with } \hbar k_0 = \sqrt{2mE}$$

($k_0 \neq$ Bloch's k !!)

To find unknowns:

1. $\psi_I(a) = \psi_{II}(a) = e^{ika}\psi_I(0) = \psi_I(x=a)$

$$\Rightarrow A = B\,\frac{e^{ika} - \cos k_0 a}{\sin k_0 a}$$

2. $\frac{d\psi}{dx}$ cont. @ $x = a$, or finite jump for δ-fcn

$$\Delta\left(\frac{d\psi(a)}{dx}\right) = \frac{d\psi_{II}(a)}{dx} - \frac{d\psi_I(a)}{dx} = -\frac{2maV_0\psi(a)}{\hbar^2}$$

integrate Schr. eq. across δ-fcn

$$\frac{d\psi_I(a)}{dx} = k_0 A \cos k_0 a - k_0 B \sin k_0 a$$

$$\frac{d\psi_{II}(a)}{dx} = e^{ika}\frac{d\psi_I(0)}{dx} = k_0 A e^{ika}$$

$\Rightarrow$ two unknowns, two eqns. Eliminate A and B:

$$\cos ka = \cos k_0 a - \beta\,\frac{\sin k_0 a}{k_0 a} \quad , \text{ with } \beta = \frac{mV_0 a^2}{\hbar^2}$$

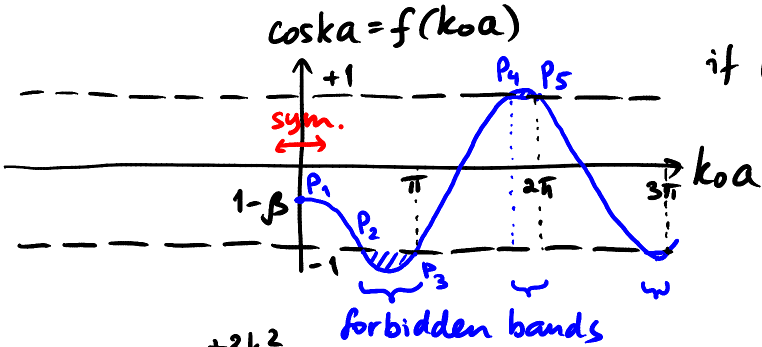
relates k and energy (thru k_0) = "dispersion relation"

β - dimensionless, measure of e^--ion interaction

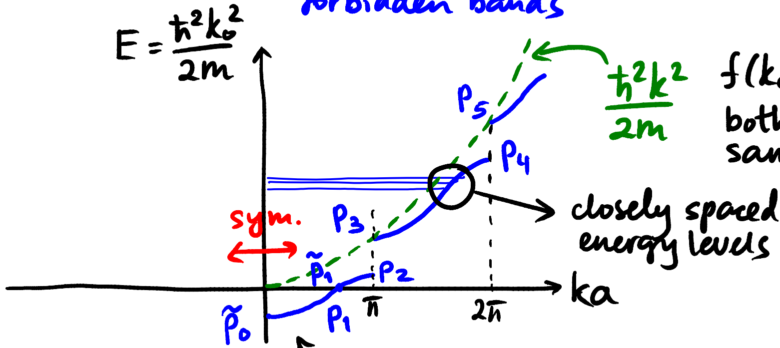
check $\beta = 0$, $\Rightarrow$ $k = k_0$ (free particle motion)

Let $f(k_0 a) \equiv \cos k_0 a - \beta\,\frac{\sin k_0 a}{k_0 a}$

solve graphically $\cos ka = f(k_0 a)$



if $0<\beta<2$



$f(k_0a\to\infty)\simeq\cos k_0a$

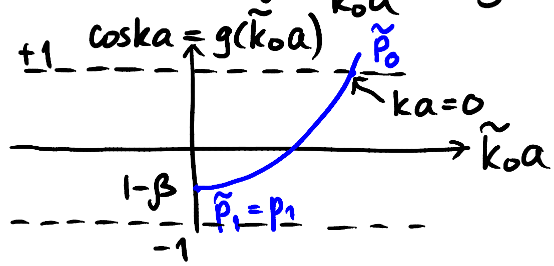
both k, k_0 are the same when $k\to\infty$

k_0 is imaginary

possible to have $k_0\to i\tilde{k}_0$ still giving real k

$$\cos ka=\cosh\tilde{k}_0a-\beta\frac{\sinh\tilde{k}_0a}{\tilde{k}_0a}\equiv g(\tilde{k}_0a)$$

negative $E=-\frac{\hbar^2\tilde{k}_0^2}{2m}$



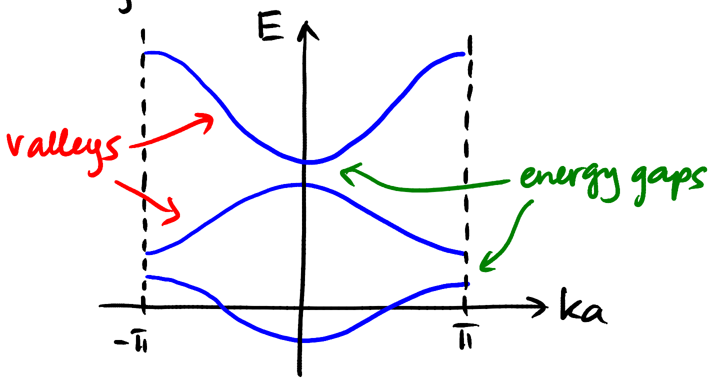
Brillouin zones: $-\pi<ka<\pi$ 1st Br. zone (or Br. zone)

$\pi<|ka|<2\pi$ 2nd Br. zone

etc.

Can express Bloch fcns within 1st Br. zone,

e.g. use $-\pi<ka<\pi$



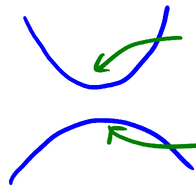
⑤ Effective mass

$\hbar k =$ crystal momentum

can represent energy in a valley

$$E = E_0 + \frac{\hbar^2 k^2}{2m^*}$$ ← now Bloch's k !

$$\frac{1}{m^*} \equiv \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$ ← related to curvature of $E(k)$



$\frac{1}{m^*} > 0$

$\frac{1}{m^*} < 0$ negative

Electron in a valley responds to ext. force $\mathcal{F}$ according to

$$\frac{dv_g}{dt} = \frac{1}{m^*}\mathcal{F}$$ ← e.g. due to electr. or magnetic field

how to measure?
measure cyclotron resonance $\omega_c = \frac{eB}{m^* c}$

⑦ Semiconductors

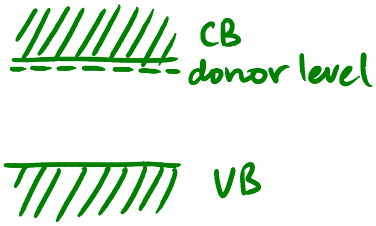
* absence of e^- in valence band = "hole" behaves as a positive charge with m^* mass

Two types : intrinsic and extrinsic (= doped)

a) intrinsic semiconductor:
thermally excited electron-hole pairs
\# electrons = # holes (e.g. pure Si)

b) extrinsic semiconductor:
mainly e^- (n) or hole (p) carriers resulting from doping

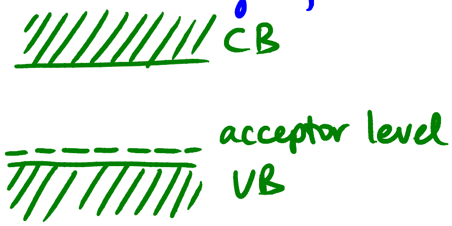
Ex1: replace one Si atom with As (group $\underline{V}$)
extra negative carrier close to CBM ($\sim 0.05\,eV$)



electron gets thermally excited to conduction band

"n-type semiconductor"

Ex2: replace one Si atom with Ga (group $\overline{\underline{III}}$)
shortage of an e^- creates acceptor level



acceptor level gets populated from VB → leaves a hole behind

"p-type semiconductor"

p-n junction = basis of most solid state electronic devices

How does a transistor work?