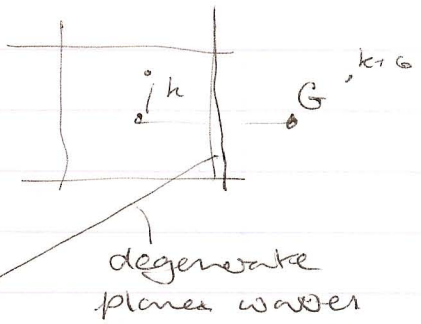
Bands in 3D

k-space partitioned into B.Z.

Zone plane

$\underline{k} \cdot \frac{1}{2}\underline{G} = \left|\frac{1}{2}\underline{G}\right|^2$



degenerate planes waves — Bragg refl^{n}

Energy bands periodic

$E_{nk} = E_{nk+G} \quad \forall \underline{G}$

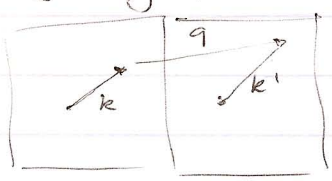
Eigenstates - Bloch

$\psi_{nk} = e^{i\underline{k}\cdot\underline{r}} u_{nk}(r)$ — periodic f^{n}

NB $|\psi_{nk}|^2 = |u_{nk}|^2$

Crystal momⁿ: Only $\hbar k$ conserved (modulo G)

e.g. scattering by phonons.



$k' \Rightarrow k+q$

Counting states : Vol per k state $(2\pi)^3/V$

Vol per BZ $= (2\pi)^3/\Omega_{cell}$

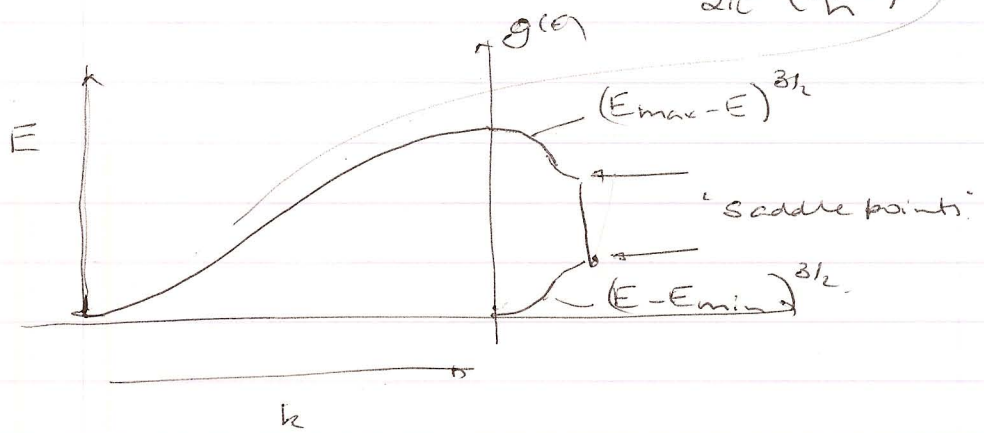
k states / BZ $= \frac{\Omega_{cell}}{V} = N$

× 2 for spin.

— even # rule

Density of states

Parabolic band edge $g(E) \sim \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(E-E_{min})^{1/2}$



— generic singularities in DOS.

Real Bands

S-p Metals

Li Ca
Na, Mg
K.

Al.

I II III
1e 2e 3e.

Transition metals eg.
+ Cu

Overlapping d-bands — narrow
S-bands — wide.

— complicated F.S.

Semiconductors / Insulators.

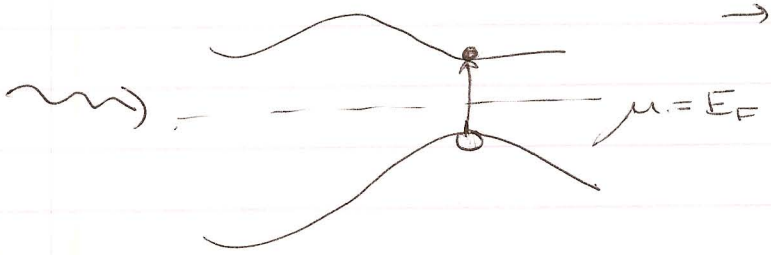
eg C, Si Ge — 2 atoms/cell.
GaAs — 4 e/atom
ZnSe. — 8 electrons/cell → 4 bands.

Si Ge → Indirect gap
Valenceband max at Γ (000)
Cond band min near Z.B. (L in Ge)
(~X in Si).

Complicated though it looks, the gap on B.Z. boundary just like the diatomic chain (in fact a diatomic molecule)

Optical transitions

photon absorbed → electron-hole pair.



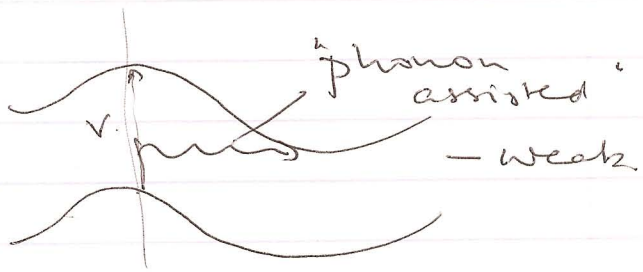
$$\hbar\omega = E_c(k+q) - E_v(k)$$

$q_{photon} = \omega/c \ll \frac{2\pi}{a}$.

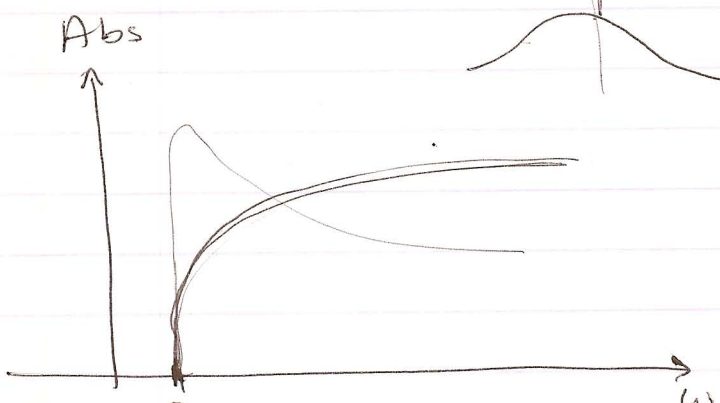
"Vertical"

Direct gap — vertical transition between lowest c & highest v states (GaAs)

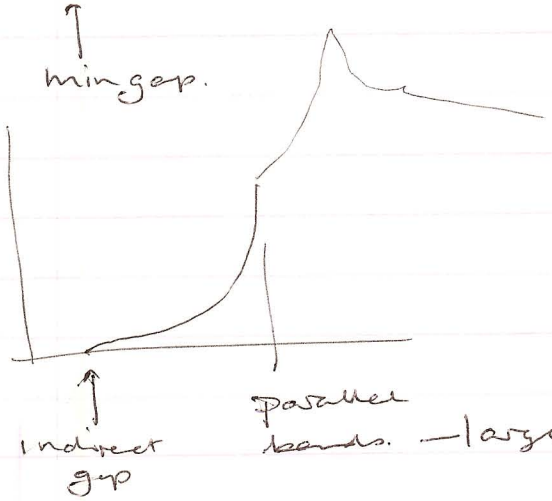
Indirect gap.
eg. Si



See Fig 7.6



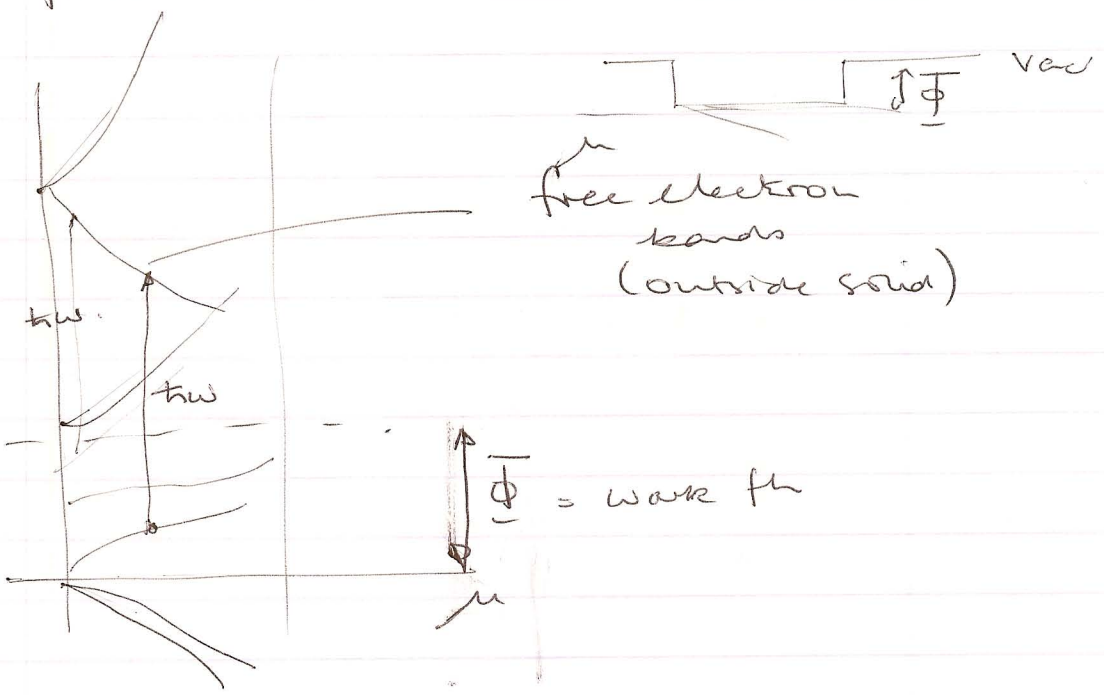
Direct gap semiconductor.



— large DOS.

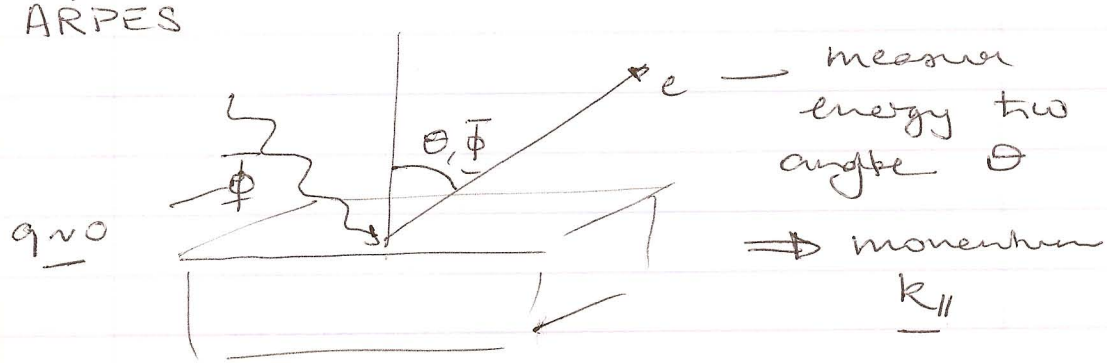
Photoemission

Incident photon energy high — electron ejected from solid



→ Approximately measures the total density of states

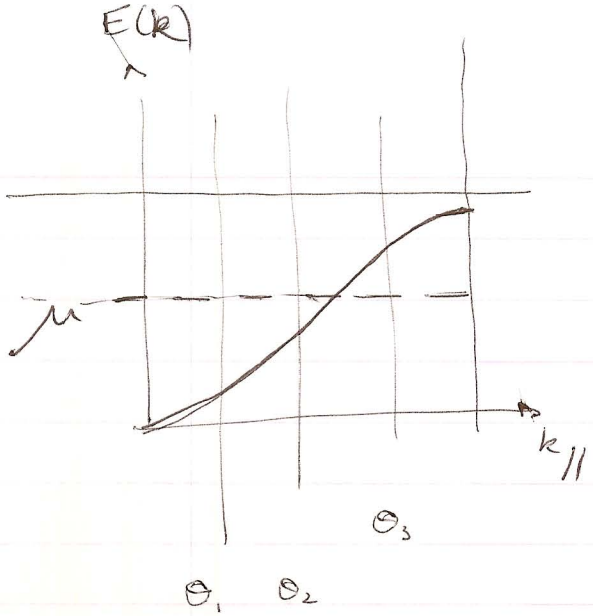
→ Angle Resolved Photo Emission Spectroscopy ARPES

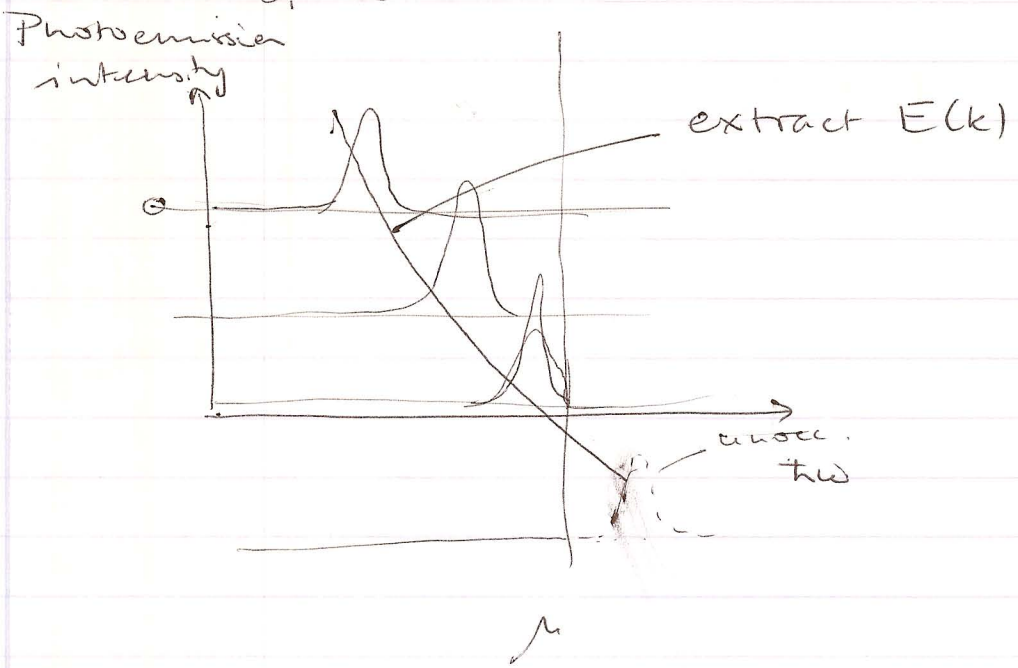


∴ Excitation remaining in solid has momentum $-k_{\parallel}$, charge $+e$, — hole in band.

→ Scan θ, ω ⇒ $E_{hole}(k_{\parallel}, \omega)$

[$k_{\perp}$ difficult to extract] — use 2D system.

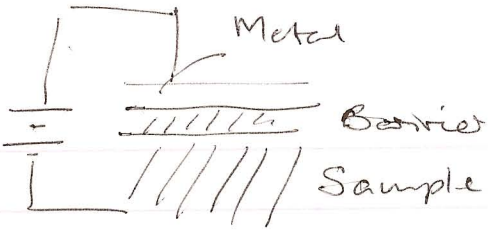


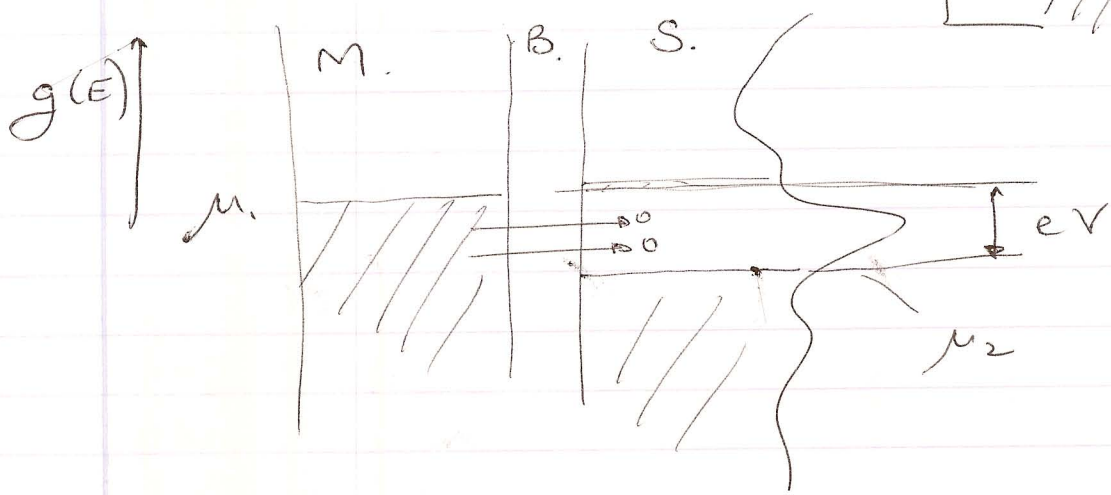


Sr_2RuO_4 — layered 2D metal
— many d-bands.

— mapping F.S.

Tunneling





If momentum conservation not important
— only conserve energy.

$$I \propto \int_{\mu_1}^{\mu_2} d\mathcal{E}\; g_{metal}(\mathcal{E})\, g_{sample}(\mathcal{E}, V)\, T(\mathcal{E})$$

(metal ele.)

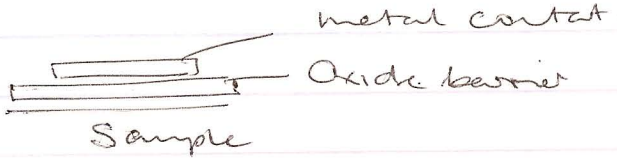
$$g_{sample}(\mathcal{E}, V) = g_{sample}(\mathcal{E} + eV)$$

(rounded by kT)

$$\therefore \frac{dI}{dV} \propto g_s(\mu + eV)$$

— easiest at low $V < \mathcal{E} \sim$ | vout or so.

— Tunnel Junctions



— STM

— imaging as fn of space.

— AFM.