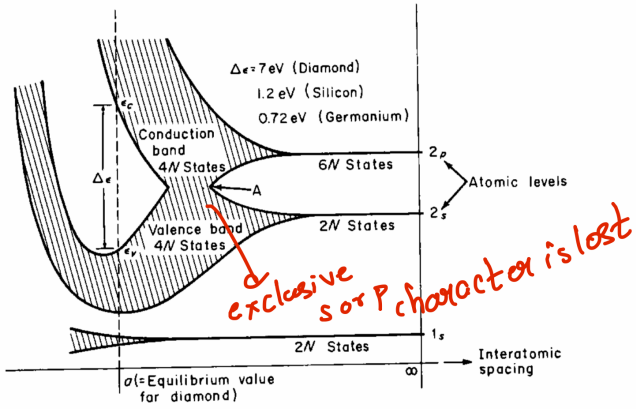
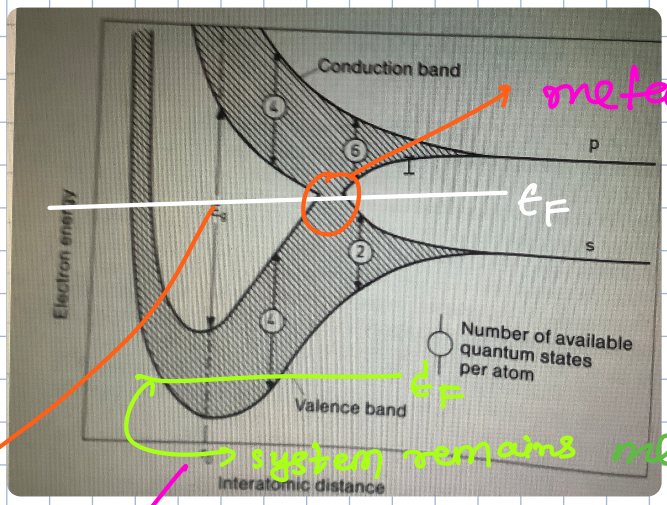


FIGURE 9.2. The bands arising from the 1*s*, 2*s*, and 2*p* atomic states of carbon (diamond) as a function of interatomic distance. [After W. Shockley, *Electrons and Holes in Semiconductors*, D. van Nostrand Co., Inc., New York (1950).]

exclusive s or P character is lost



metal

semiconducting

system remains metallic

eqm distance of solid

Goal:- we wanna understand how does one calculate these bands are?

We'll use tight binding method.

↓

not all encalculating but captures a lot of the physics of it.

Two Approaches

① Free electron

KE >>> V

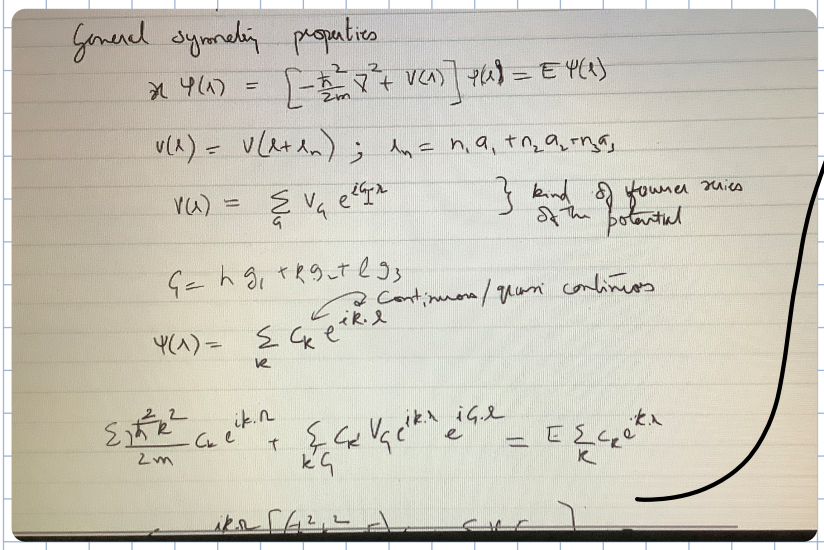
② Assume solid has AOs & electrons are allowed to hop from one to other.

V >>> KE

↓

Complementary pictures

We spend two lectures discussing this.



→ So essentially f.T. of eqn

& we get

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) C_{\vec{k}} + \sum_{\vec{G}} V_{\vec{G}}\, C_{\vec{k}-\vec{G}} = 0$$

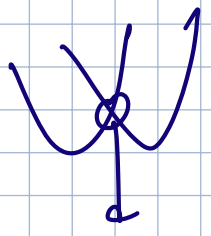
$$\psi_{\vec{k}}(\vec{r}) = \sum C_{\vec{k}-\vec{G}}\, e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$$

$$= e^{i\vec{k}\cdot\vec{r}} \left[\sum C_{\vec{k}-\vec{G}}\, e^{-i\vec{G}\cdot\vec{r}}\right]$$

Problem:- Calculating $V_{\vec{G}}$ is difficult

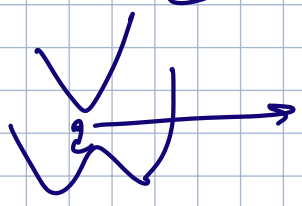
these are like the terms that couple different parabolas

$$U_{nk}(\vec{r}) = U_{nk}(\vec{r}+\vec{R})$$



← hybridises states of diff k

at crossing pnts, we'll see a level repulsion.



~ Gap $\propto V_G$

Another perspective

V_G turns on backscattering

scattering in general:

extreme example

$$|\psi_-(x)|^2 = \left|\left(\frac{e^{iGx} - e^{-iGx}}{2}\right)\right|^2$$

$$|\psi_+(x)|^2 = \left|\left(\frac{e^{iGx} + e^{-iGx}}{2}\right)\right|^2$$

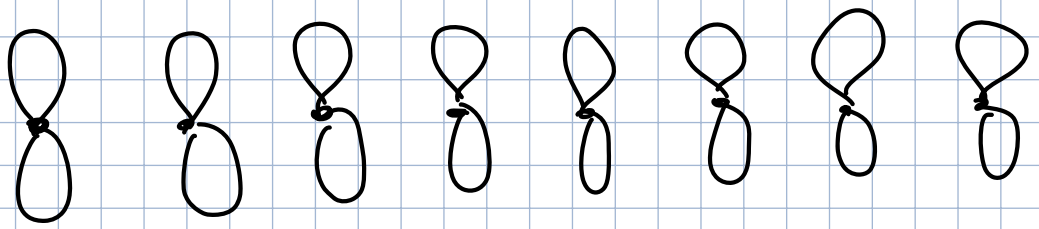
free electron → potential → bands → ⇒ eff mass

→ Gaps

f. electron misses existence of semicond-

/insulators.

Another way :- Tightbinding Approach.



AO's

So ψ_{solid} = LCAO , for eg. $\psi = \sum_i \alpha_i \phi(r-R_i)$ → AO's

$$H_A(r-r_n)\,\phi_i(r-r_m) = E_i\,\phi(r-r_m)$$

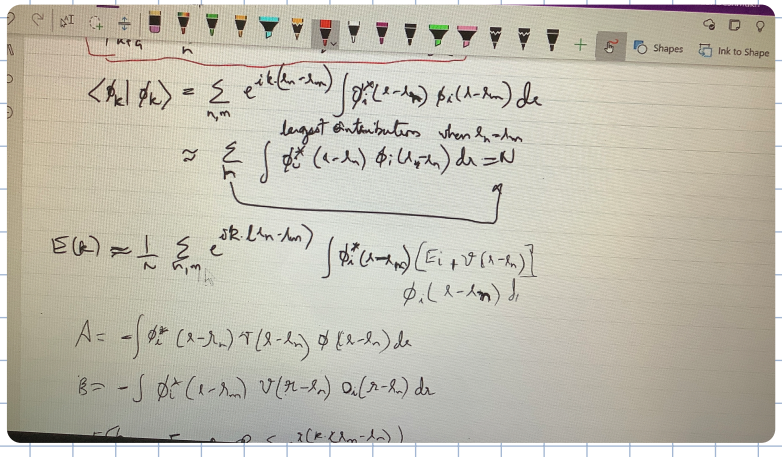
But now new H = $H_A + V$ → existence of other sides around original

$$= \frac{-\hbar^2}{2m}\nabla^2 + V_A(r-r_m) + \sum_{n\neq m} V_A(r-r_n)$$

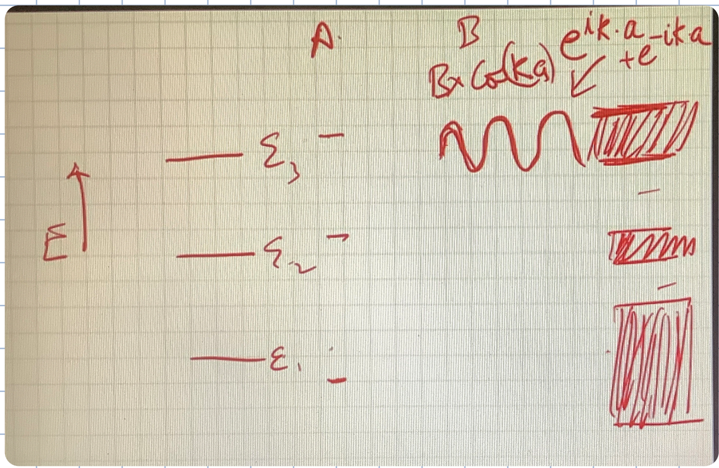
$V_A(r-r_m)$: due to site m

Variational approach

$\phi_{k+\theta}$



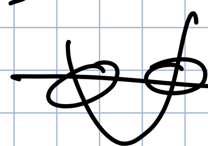
Maybe watch Siddhu's Lectures



Book :-
E back & Luth.

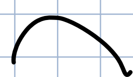
When should I apply free e^- → pedagogical
↳ not helpful for optical propr
↳ no gaps in spectrum

goes very far for **transport** →



→ transport doesn't care abt the lower band

close to band edge



But for optical propr ⇒ need TBM

free electron ⇒

Arpes
↳ shine light & look at e^-'s inside core → 10 eV below fermi energy

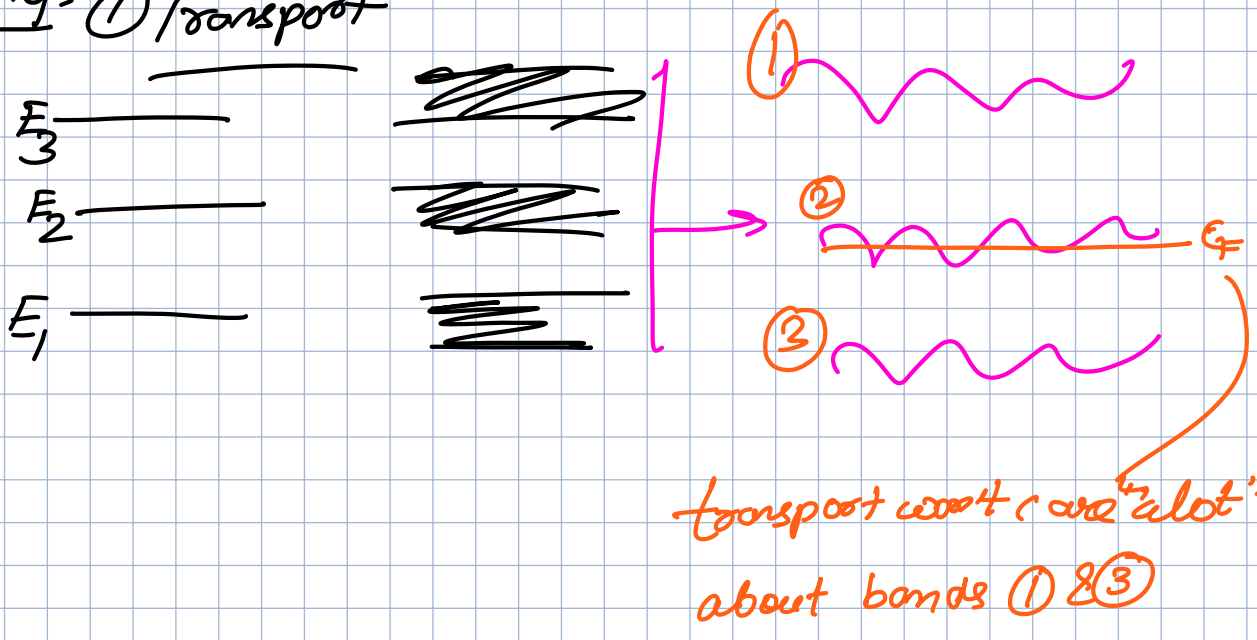
transport →

;

Q. When do we stop adding orbitals?

↳ depends on the physics of what you wanna explore.

for e.g. - ① Transport



transport won't care "a lot" about bonds ① & ③

But suppose we ARPES, which can give info on core orbitals, we have to take lower orbitals into account.