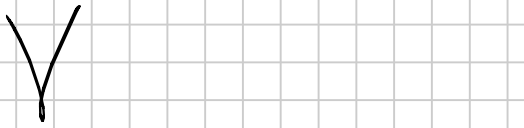
LECTURE # 16

Note Title 2/17/2010

TIGHT - BINDING



$$V(\vec{r}) = \sum_{R} V_{AT}(\vec{r} - \vec{R})$$

BASIS OF LOCALIZED ORBITALS $\varphi_m(\vec{r})$ ε_m

BLOCH FUNCTIONS

$$\psi_{km}(\vec{r}) = \sum_{R} e^{i\vec{k}\cdot\vec{R}} \varphi_m(\vec{r} - \vec{R})$$

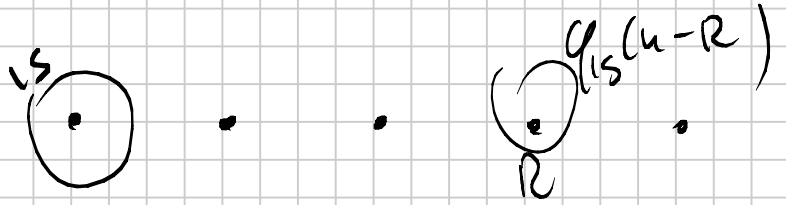
$$H\psi_k = E(k)\psi_k$$

$$\psi_k = \sum_{m \to \text{ORBITALS}} b_m(k)\, \psi_{km}(\vec{r})$$

$$\left\| \langle \psi_{mk} | H | \psi_{m'k} \rangle - E(k) \langle \psi_{mk} | \psi_{m'k} \rangle \right\| = 0$$

$$= 0$$

EXAMPLE 1 ORBITAL



$\varphi_{1s}(u)$

$$\psi_{1s,k}(\vec{u}) = \sum_R e^{ik\cdot R} \varphi_s(\vec{u} - \vec{R})$$

$R \quad R'' \quad R'$

$$\langle \psi_{1sk} | H | \psi_{1sk} \rangle = E(k) \langle \psi_{1sk} | \psi_{1sk} \rangle \sim 1 \qquad (1)$$

$$H = T + \sum_R V_{AT}(\vec{u} - \vec{R})$$

$$(1) = N \int d^3r \sum_{R R'} \varphi_{1s}(r-R) \left[T + \sum_{R''} V_{AT}(\vec{r}-\vec{R}'') \right] \varphi_{1s}(r-R') \, e^{iK(R-R')}$$

FIX $R' = 0$ AND MULTIPLY BY TOTAL # OF SITES

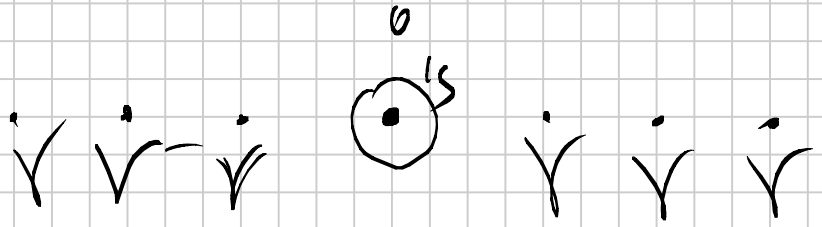
DIFFERENT TERMS

$R' = 0$

① $R = 0$, $R'' = 0$ $\rightarrow N \int d^3\vec{r} \; \varphi_{1s}(r) \left[T + V_{AT}(r) \right] \varphi_{1s}(r) =$

$\varepsilon_{1s} \rightarrow$ "ON SITE" TERM

② $R' = 0$, $R = 0$, $R'' \neq 0$ $\rightarrow N \int d^3r \; \varphi_{1s}(r) \left[\sum_{R'' \neq 0} V_{AT}(r-R'') \right] \varphi_{1s}(r)$



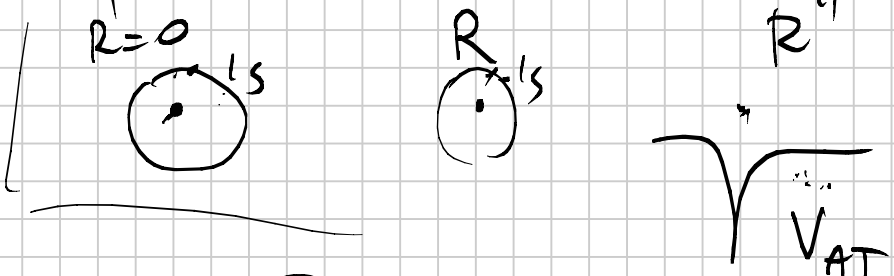
CRYSTAL FIELD TERM → K INDEPENDENT

ONLY GIVES ENERGY SHIFTS _

(3) $R' = 0$, $R \neq 0$; $R'' \neq 0$

$$\int d^3r \, \varphi_{1s}(\vec{r} - \vec{R}) \sum_{R''} V_{AT}(\vec{r} - \vec{R}'') \, \varphi_{1s}(\vec{r}) \, e^{i k \cdot R}$$

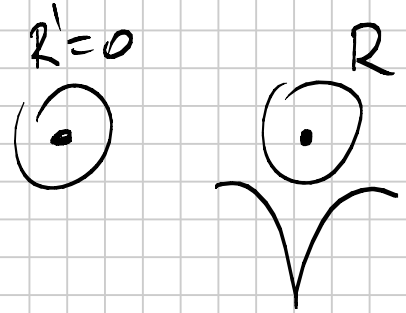
HOPPING INTEGRALS



FURTHER APPROXIMATIONS FOR (3)

(A) 2 CENTERS :

R'' ONLY AT R OR AT 0 .

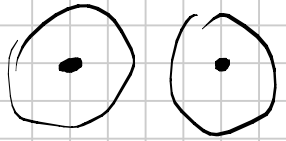


(B)

$\sum_{R''}$ → 0 R AND R'' ARE FIRST NEIGHBORS

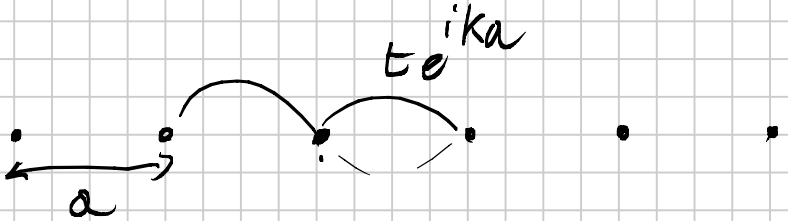
(C)

$$\int d^3r\ \varphi_{1s}(r)\ \varphi_{1s}(r-R) \sim \delta_{R,0}$$



→

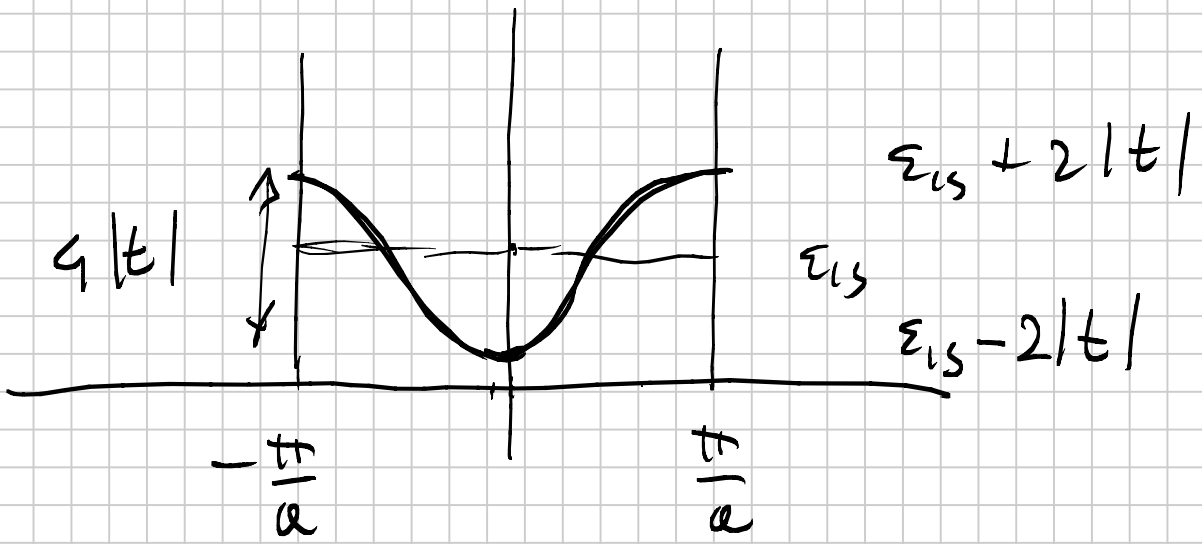
φ_{1s} ε_{1s}



$$E(k) = \langle \psi_{1s,k} | H | \psi_{1s,k} \rangle = \overset{\text{ON SITE}}{\varepsilon_{1s}} + \underline{t}\, e^{ik\cdot a} + t\, e^{-ika}$$

$$t = \int d^3r\ \varphi_{1s}(r)\, V_{AT}(r)\, \varphi_{1s}(r-a) \qquad < 0$$

$$E(k) = \varepsilon_{1s} + 2t\cos ka$$



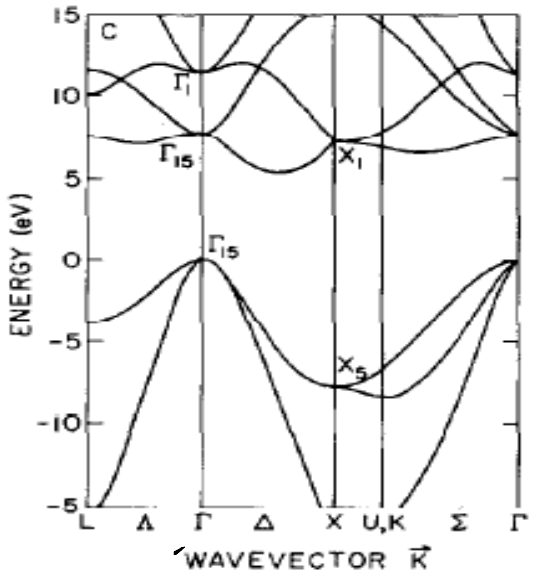


Fig. 11(k).

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TIGHT BINDING BANDS FOR DIAMOND (C)

5 ORBITALS / ATOM

1S P_x P_y P_z S^*

TOTAL 10 ORBITALS

SEMICLASSICAL MODEL FOR ELECTRON DYNAMICS

DRUDE / SOMMERFELD

$\vec{p} = \hbar\vec{k}$

$\Delta k = \frac{(2\pi)^3}{V} \quad \vec{k} \in \mathbb{R}^3$

$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$

$\psi_{\vec{k}} = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

BLOCH ELECTRONS

$\hbar\vec{k}$ → CRYSTAL MOMENTUM

$\neq \vec{p}$ LINEAR MOMENTUM

$\Delta k = \frac{(2\pi)^3}{V} \quad \vec{k} \in 1^{ST}$ BRILLOUIN ZONE

$\varepsilon_m(\vec{k}) = \varepsilon_m(\vec{k} + \vec{G})$

$\forall\, \vec{G} \in$ RECIPROCAL LATTICE VECTOR

$\psi_{mk}(\vec{r})$

$\psi_{mk}(\vec{r} + \vec{R}) = e^{i\vec{k}\vec{R}} \psi_m(\vec{k})$

COLLISIONS WITH IONS

RESET VELOCITY AFTER EACH COLLISION

NO "COLLISIONS" WITH IONS

$\Rightarrow$ IONS DO NOT AFFECT DYNAMICS

$$\dot{\vec{p}} = -e\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{H}\right)$$

BETWEEN COLLISION

ψ_{mk} STEADY STATES

$\tau = \infty \qquad \sigma = \infty$

BLOCH ELECTRONS STILL HAVE τ FINITE BECAUSE OF

① IMPURITIES AND DEFECT

② LATTICE VIBRATIONS

$\Big\} \rightarrow \tau < \infty$