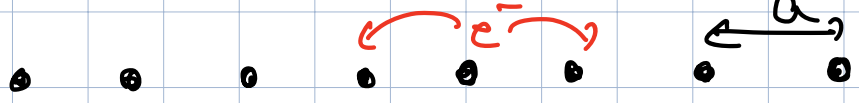
Chapter 3 : electrons in crystals

Additional references: Kittel : 7, 8, 9
A & M : 8-15

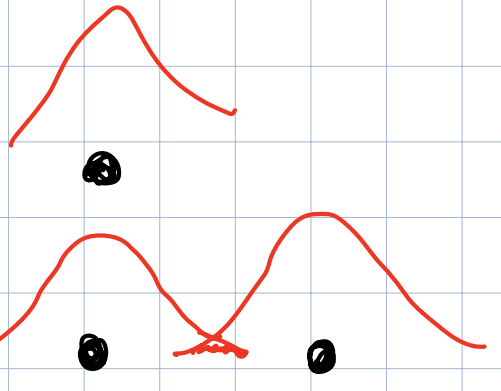


For a single nucleus, e^- is bound to it
For multiple nuclei, e^- hops around

How can we model this?

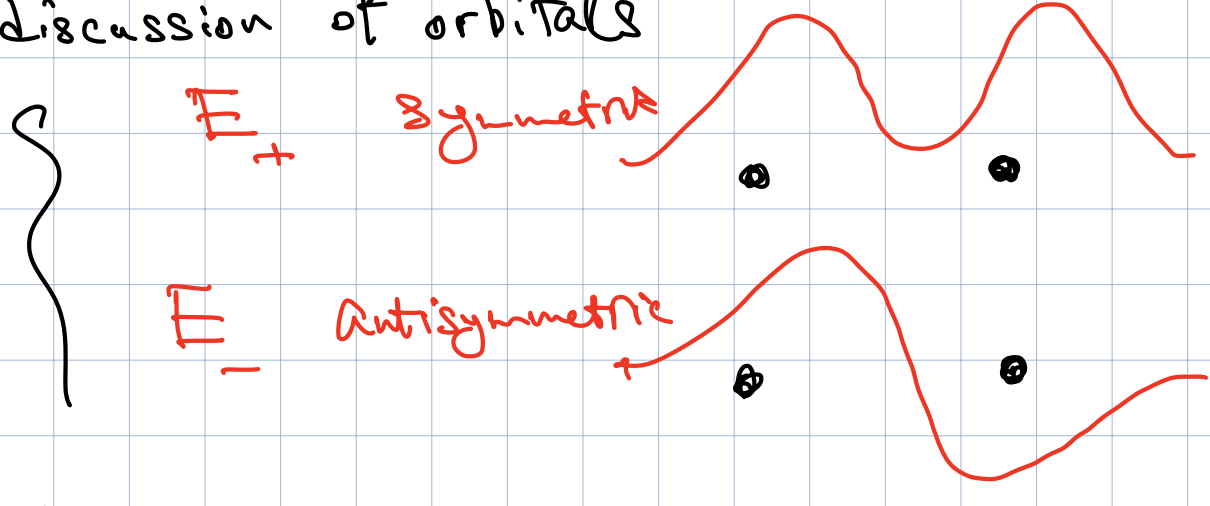
Tight-binding model

Single nucleus ⟶



Two nuclei

Reminder, discussion of orbitals



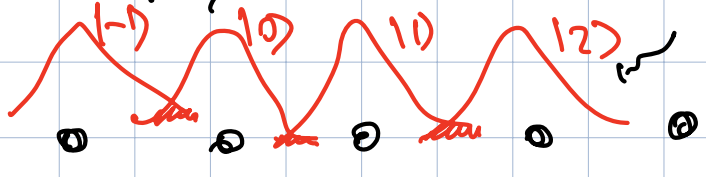
Extend this to a crystal

$$H = \frac{\vec{p}^2}{2m} + \sum_n V(\vec{r} - \vec{R}_n)$$

$\vec{R}_n$: position of nucleus n

$\vec{r}$ & $\vec{p}$: position & momentum of e^-

We take $|n\rangle$ as the orbital around nucleus n



$|n\rangle$ is an eigenstate of $\frac{\vec{p}^2}{2m} + V(\vec{r} - \vec{R}_n)$

We represent the Hamiltonian in the basis $|n\rangle$

$$\begin{cases} \langle n|H|n\rangle = E_0 \\ \& \quad \langle n|H|n\pm1\rangle = -t \\ \& \quad \langle n|H|m\rangle = 0 \qquad |n-m|>1 \end{cases}$$

We also assumed translation invariance

no dependence of E_0 & t on n

Also for simplicity, we assume orthogonality

$$\langle n|m\rangle = \delta_{nm}$$

$$H_{nm} \equiv \langle n|H|m\rangle$$

$$= E_0 \delta_{nm} - t(\delta_{n,m+1} + \delta_{n,m-1})$$

To diagonalize the Hamiltonian

$$H|\psi\rangle = E|\psi\rangle$$

$$|\psi\rangle = \sum_n \psi_n |n\rangle$$

$$H = \begin{pmatrix} \ddots & & & \\ & H_{00} & H_{01} & \cdots \\ & H_{10} & H_{11} & \\ & \vdots & & \ddots \end{pmatrix}_{nm} \qquad \begin{pmatrix} \vdots \\ \psi_0 \\ \psi_1 \\ \vdots \end{pmatrix}$$

matrix

$$\rightarrow \sum_m H_{nm} \psi_m = E \psi_n \leftarrow$$

$$\sum_m E_0 \delta_{nm} \psi_m + \cdots$$

$$\rightarrow \boxed{E_0 \psi_n - t\left(\psi_{n+1} + \psi_{n-1}\right) = E\psi_n}$$

To solve this equation, assume $\psi_n \sim e^{-ikna}$

$$E_0 e^{-ikna} - t\left(e^{-ik(n+1)a} + e^{-ik(n-1)a}\right) = E e^{-ikna}$$

$$\rightarrow \quad E = E_0 - 2t\cos(ka)$$

$k \rightarrow$ wavevector

$E = E(k)$ dispersion relation