

BARE BONE TIGHT BINDING

Hydrogen 1s in 1D

$$H = T + V \quad V: \text{periodic pot.}$$

$$|\psi\rangle = \sum_n e^{ikna} |n\rangle$$

$$\langle n|H|n\rangle \equiv \epsilon \quad \left(\begin{array}{l} \text{throw in atomic energy} \\ -2\beta \text{ and so on} \end{array} \right)$$

$$\langle m|H|n\rangle = -t \quad \text{if } m-n = \pm 1$$

(keep nearest neighbor only)

t is called a "hopping" matrix element

$$\langle m|n\rangle = \delta_{mn} \quad \left(\begin{array}{l} \text{somewhat of a over-simplification} \\ \text{but an often-used approx} \end{array} \right)$$

$$H|\psi\rangle = \epsilon_k |\psi\rangle$$

$$\langle m|H|\psi\rangle \stackrel{\Downarrow}{=} e^{ikna} \epsilon_k$$

$$\boxed{\epsilon_k = \epsilon - 2t \cos ka}$$

If $t \rightarrow 0$, ϵ_k becomes flat

$$m^* \rightarrow \infty$$

$t \rightarrow \infty$, ϵ_k becomes very wide

$$m^* \rightarrow 0$$

↑
ease of hopping or hopping probability
or tunneling probability