Tight-Binding Band Structure

- Consider opposite limit from nearly free electrons
  \[ \rightarrow \text{very strong potential } U(r) \]
- We will give a very heuristic treatment; a more systematic discussion is given in A& M Ch. 10.

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Almost localized state tunnels from one potential well to the next, tunneling matrix element $t$. 
For simplicity, start with only a single localized state at each lattice site \[ \hat{R}, \vert \hat{R} \rangle \].

- Crucial assumption: \[ \langle \hat{R} \vert \hat{R}' \rangle = 0 \] if \( \hat{R} \neq \hat{R}' \).

- In reality, these states are non-orthogonal — we can take this into account, but it doesn’t change the structure of the resulting model significantly. Anyway, it turns out deep (for apart), the overlap is exponentially small. See A&M Ch. 10 for more careful discussion.

- However, the Hamiltonian induces transitions between these states, \( \langle \hat{R}' \vert \hat{H} \vert \hat{R} \rangle = -t \), if \( \hat{R} \) and \( \hat{R}' \) are nearest neighbors.

\[
\hat{H}_{\text{eff}} = -t \sum_{\hat{R}, \hat{R}'} \left[ \langle \hat{R} \vert \hat{R}' \rangle + \langle \hat{R}' \vert \hat{R} \rangle \right]
\]  

\[ \text{sum over nearest-neighbor pairs} \]
We usually write such Hamiltonians using 2nd quantization.

- Let $\mathbf{C}_{\mathbf{R}_0}^+$ create electron at $\mathbf{R}$ with spin $\sigma$.

Then...

$$\text{Heff} = -t \sum_{\mathbf{R}, \mathbf{R}'} \left[ \mathbf{C}_{\mathbf{R}_0}^+ \mathbf{C}_{\mathbf{R}'\sigma} + \mathbf{C}_{\mathbf{R}'\sigma}^+ \mathbf{C}_{\mathbf{R}_0} \right]$$

Q: Where do these localized states come from more physically?
A: They're atomic orbitals.

Example: Na atoms form BCC lattice.

Each Na atom has [Ne]3s$^1$ configuration.

- $\mathbf{C}_{\mathbf{R}_0}^+$ creates s-state orbital at site $\mathbf{R}$. 
Another example: Cuprates, e.g. \( \text{La}_2\text{CuO}_4 \)

- Important part is \( \text{CuO}_2 \) layers
  \[
  \begin{array}{ccc}
  \text{Cu} & \times & \text{Cu} \\
  \times & \text{O} & \times \\
  \text{Cu} & \times & \text{Cu}
  \end{array}
  \]

- \( \text{Cu} \) is \( \text{Cu}^{2+} \rightarrow 3d^9 \) configuration
- \( \text{O} \) is \( \text{O}^{2-} \rightarrow 2p^6 \)

- For each \( \text{Cu} \), important orbital is \( d_{x^2-y^2} \)

- For each \( \text{O} \), it's either \( p_x \) or \( p_y \):

- [Diagram of \( d_{x^2-y^2} \) orbital]
- [Diagram of \( p_x \) or \( p_y \) orbitals]
Let:
\[ \text{C}^+_{2s} \] create electron in Cu \( d_{x^2-y^2} \)

Let:
\[ d^+_R \] create electron in O \( p_x / p_y \)

\[ \text{Then:} \quad H_{TB} = \sum_R \left[ \varepsilon_d \text{C}^+_{2s} C_{2s} + \varepsilon_p \sum_{i=x,y} d^+_R \right] \]
\[ - t_{pd} \sum_R \left[ \left( \text{C}^+_{2s} d_R, \sigma + H.c. \right) + \ldots \right] \]

For compounds, \( \varepsilon_d - \varepsilon_p \sim 2 \text{ eV} \)
\( t_{pd} \sim 1 \text{ eV} \)
How to solve tight-binding band structures?

(i.e. what's $E_n(k)$?)

Simple example: Square lattice

$$H = -t \sum_{R} \left[ C_{R\sigma}^+ C_{R+\hat{x},\sigma} + C_{R+\hat{x},\sigma}^+ C_{R\sigma} + C_{R\sigma}^+ C_{R+\hat{y},\sigma} + C_{R+\hat{y},\sigma}^+ C_{R\sigma} \right]$$

Let's Fourier transform:

$$C_{R\sigma} = \frac{1}{\sqrt{N_c}} \sum_{k} e^{i k \cdot R} C_{k\sigma}; \quad C_{k\sigma} = \frac{1}{\sqrt{N_c}} \sum_{R} e^{-i k \cdot R} C_{R\sigma}$$

Check: $\{ C_{R\sigma}, C_{R'\sigma}^+ \} = \delta_{RR'} \delta_{\sigma\sigma'}$

Result: 

$$H = \sum_{k} \left[ -2t \left( \cos(k_x) + \cos(k_y) \right) \right] C_{k\sigma}^+ C_{k\sigma}$$
One electron per site:

\[ \epsilon_F = 0 \]  

"Diamond shaped" Fermi surface

This diamond shape is pathological, if you add diagonal hopping.

\[ t' \]
One last example: graphene.

- Carbon atoms, with an \(2s^2 2p^2\), form honeycomb lattice.

\[ \text{\(s^2\) orbitals, "\(\sigma\) bonding"} \]

\[ \text{Also "\(\pi\)" orbital, \(\perp\) to plane} \]

- \(\pi\)-bonding orbitals are like core bands, filled with pairs of electrons, one from each C-atom. \(\rightarrow\) inert

- But the \(\pi\)-orbital has only single electron per atom.

- Call honeycomb sites \(r\), let \(C^\dagger_{r\sigma}\) create electron in \(\sigma\) for orbital. Then:

\[
H_{1B} = -t \sum_{r,\sigma} \left[ C_{r\sigma}^\dagger C_{r\sigma} + C_{r\sigma}^\dagger C_{r\sigma} \right]
\]