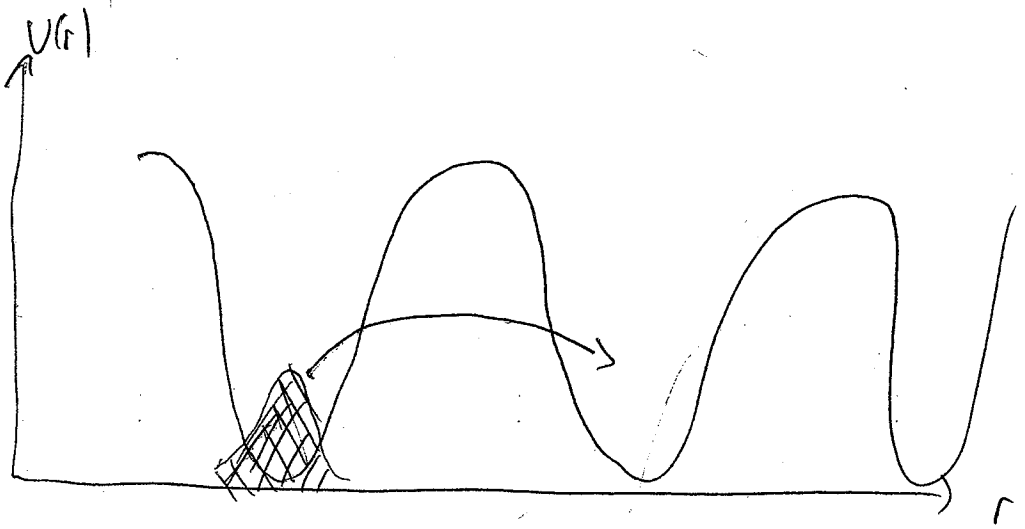
Tight-Binding Band Structure

- Consider opposite limit from nearly free electrons
  → very strong potential $U(r)$
- We will give a very heuristic treatment, a more systematic discussion is given in A&M Ch. 10.



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 $\vec{R}$, $|\vec{R}\rangle$.

- Crucial assumption: $\langle \vec{R}|\vec{R}'\rangle = 0$ if $\vec{R} \neq \vec{R}'$
- 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~~ Anyway, if wells are deep / far apart, the overlap is exponentially small. See A&M Ch. 10 for more careful discussion.

- However, the Hamiltonian induces transitions between these states, $\langle \vec{R}|H|\vec{R}'\rangle = -t$, if $\vec{R}$ and $\vec{R}'$ are nearest neighbors.

- $$H_{eff} = -t \sum_{\langle \vec{R}\vec{R}' \rangle} \left[|\vec{R}\rangle\langle\vec{R}'| + H.c. \right]$$

↑ sum over nearest-neighbor pairs

• We usually write such Hamiltonians using 2nd quantization.

- Let $C^{\dagger}_{\vec{R}\sigma}$ create electron at $\vec{R}$ with spin σ, then...

$$H_{eff} = -t \sum_{\langle \vec{R}\vec{R}' \rangle} \left[C^{\dagger}_{\vec{R}\sigma} C_{\vec{R}'\sigma} + C^{\dagger}_{\vec{R}'\sigma} C_{\vec{R}\sigma} \right]$$

Q: Where do these localized states come from more physically?

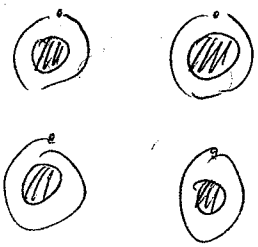
A: They're atomic orbitals.

Example: Na atoms form BCC lattice.

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

$$-t \sum_{\langle RR' \rangle} \left[|\vec{R}\rangle\langle\vec{R}'| + H.c. \right]$$

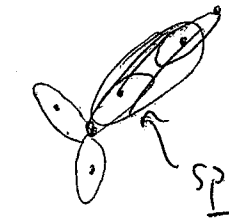
• $H_{eff} = -t \sum_{\langle \vec{R}\vec{R}' \rangle} (C^{\dagger}_{\vec{R}\sigma} C_{\vec{R}'\sigma} + H.c.)$



• $C^{\dagger}_{\vec{R}\sigma}$ creates s-state orbital at site $\vec{R}$.

More
One ~~first~~ example: graphene

- Carbon atoms, which are $2s^2 2p^2$, form honeycomb lattice.



sp^2 orbitals. "σ-bonding"

Also "π" orbital, $\perp$ to plane

- σ-bonding orbitals are like core levels, filled with pairs of electrons, one from each C-atom. → inert

- But the π-orbital has only single electron per atom.
- Call honeycomb sites $\vec{r}$, let $c^\dagger_{\vec{r}\sigma}$ create electron in $\vec{r}$ orbital. Then:

$$H_{TB} = -t \sum_{\langle \vec{r}\vec{r}' \rangle} \left[c^\dagger_{\vec{r}\sigma} c_{\vec{r}'\sigma} + c^\dagger_{\vec{r}'\sigma} c_{\vec{r}\sigma} \right]$$

$|\vec{r}\rangle\langle\vec{r}'|$ + H.c.

Solving for tight-binding band structure:

Square lattice:

$$H = -t \sum_{\langle \vec{R}\vec{R}' \rangle} \left[|\vec{R}\rangle\langle\vec{R}'| + H.c. \right]$$

$$= -t \sum_{\vec{R}} \left[\left(|\vec{R}\rangle\langle \vec{R} + a\hat{x}| + H.c. \right) + \left(|\vec{R}\rangle\langle \vec{R} + a\hat{y}| + H.c. \right) \right]$$

This is tight-binding Bloch state!

$$|\vec{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} |\vec{k}\rangle \quad ; \quad |\vec{k}\rangle = \frac{1}{\sqrt{N_c}} \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} |\vec{R}\rangle$$

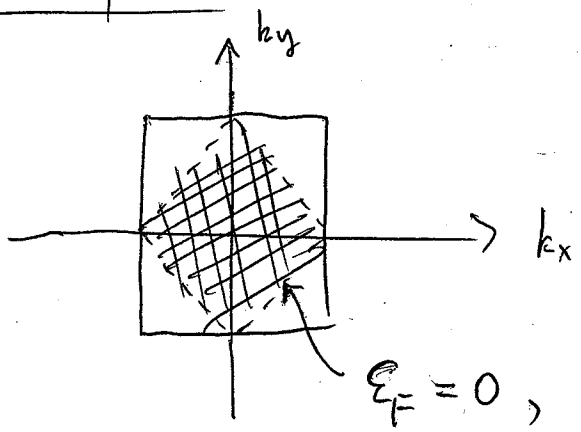
Plug in:

$$H = \sum_{\vec{k}} \left[-2t \left(\cos(ak_x) + \cos(ak_y) \right) \right] |\vec{k}\rangle\langle\vec{k}|$$

$$\varepsilon(\vec{k}) = -2t \left[\cos(ak_x) + \cos(ak_y) \right]$$

- Only one band $\longrightarrow$ # bands = # orbitals / unit cell.

One electron per site:



$\varepsilon_F = 0$, "diamond shaped" Fermi surface

- This diamond shape is pathological, it goes away if we add diagonal hopping.