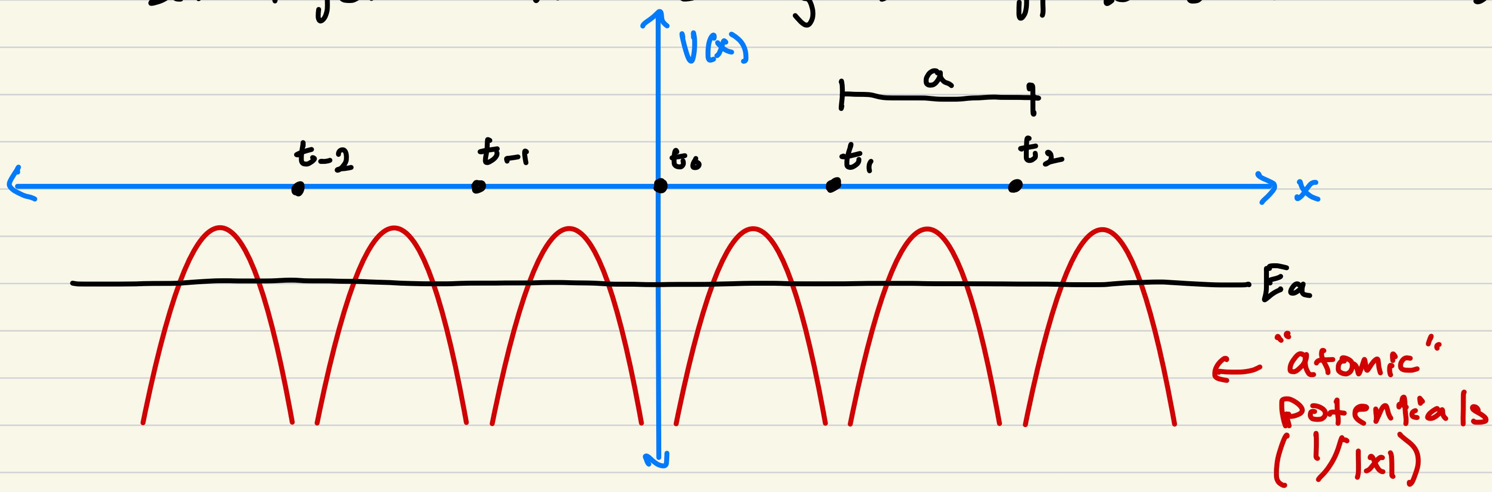
Yet another picture of 1D solids: Tight-Binding Approximation

- Before, we described solids as electrons and barriers
- In real life we have electrons and nuclei
  * electrons and nuclei attract each other!
  * Sometimes group nuclei with core electrons to form "ions"
  * Other electrons that participate in bonding are called "valence"

- Consider a set of identical atoms
  * Far apart → no interaction → same energy levels
  * Closer together → interacting → energy levels form bands



* N atomic-like potentials at lattice positions $t_n = na$
* ϕ_a is orbital of single atom, energy E_a
  • Assume nondegenerate and real
* crystal wave function using basis: $\phi_a(x - t_n)$

* Assume ϕ_a's are orthonormal

$\langle \phi_a^{t_n} | \phi_a^{t_m} \rangle = \delta_{mn}$ [notation: $\langle x | \phi_a^{t_n} \rangle = \phi(x - t_n)$]

* Represent crystal Hamiltonian in basis of atomic orbitals:

$\langle \phi_a^{t_n} | H | \phi_a^{t_n} \rangle = E_0$ ← onsite energy

$\langle \phi_a^{t_n} | H | \phi_a^{t_{n\pm 1}} \rangle = \gamma$ ← nearest neighbor hopping (<0)

* Let's make a linear combination of ϕ that satisfies Bloch's theorem:

$$\Phi(k,x) = \frac{1}{\sqrt{N}} \sum_n e^{ikt_n} \phi_a(x - t_n)$$ ← Bloch sum (k's cannot mix!)

• check Bloch's theorem:

$$\Phi(k, x+t_m) = \frac{1}{\sqrt{N}} \sum_n e^{ikt_n} \phi_a(x + t_m - t_n)$$

$\tilde{t}_n = t_n - t_m$

$= x - \tilde{t}_n$

$$= \frac{1}{\sqrt{N}} e^{ikt_m} \sum_n e^{ik(t_n - t_m)} \phi_a(x + t_m - t_n)$$

$$= e^{ikt_m} \Phi(k,x)$$

just shifted by t_m!

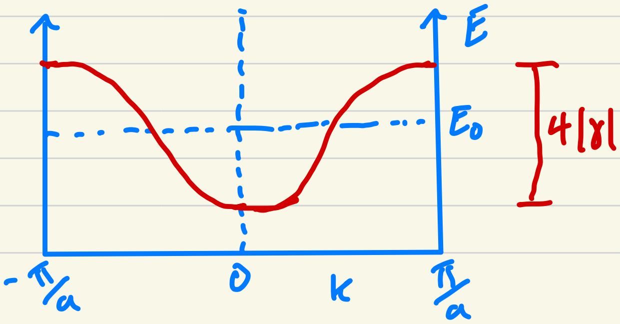
* Note: Bloch sums w/ different k are orthonormal

* Energy dispersion of band: (e.g., see next page)

$E(k) = \langle \Phi^k | H | \Phi^k \rangle$ [notation: $\langle x | \Phi^k \rangle = \Phi(k,x)$]

* For nearest neighbor hopping:

$$E(k) = E_0 + 2\gamma \cos(ka)$$



- Dispersion: $E(k) = E_0 + 2\gamma\cos(ka)$

  * Expand to second order around $k=0$

    $$E(x) \approx E_0 + 2\gamma - \gamma a^2 k^2 \cong E_0 + 2\gamma - \frac{\hbar^2 k^2}{2m^*}$$

    where "effective mass" $m^* = \dfrac{\hbar^2}{2|\gamma| a^2}$ ← larger hopping, smaller m^*

- Tight-binding Hamiltonian as an operator:

$$\boxed{\hat{H} = E_0 \sum_n |\phi^n\rangle\langle\phi^n| + \gamma \sum_n \left[|\phi^n\rangle\langle\phi^{n+1}| + |\phi^{n+1}\rangle\langle\phi^n|\right]}$$

* Bloch sum is:

$$|\Phi^k\rangle = \frac{1}{\sqrt{N}} \sum_m e^{ikt_m} |\phi_m\rangle$$

* Can calculate the dispersion:

$$\hat{H}|\Phi^k\rangle = \frac{1}{\sqrt{N}} \sum_m e^{ikt_m}\Big[E_0 \sum_n |\phi^n\rangle\langle\phi^n|\phi^m\rangle$$

$$+ \gamma \sum_n \left(|\phi^n\rangle\langle\phi^{n+1}|\phi^m\rangle + |\phi^{n+1}\rangle\langle\phi^n|\phi^m\rangle\right)\Big]$$

$$= \frac{1}{\sqrt{N}} \sum_m e^{ikt_m}\left[E_0|\phi^m\rangle + \gamma\left(|\phi^{m-1}\rangle + |\phi^{m+1}\rangle\right)\right]$$

$$= E_0|\Phi^k\rangle + \gamma\left(e^{-ika} + e^{ika}\right)|\Phi^k\rangle$$

$$= \left[E_0 + 2\gamma\cos(ka)\right]|\Phi^k\rangle$$

* We can write H as a N×N matrix (assume γ is real)

$$4\times4: \begin{bmatrix} E_0 & \gamma & 0 & 0 \\ \gamma & E_0 & \gamma & 0 \\ 0 & \gamma & E_0 & \gamma \\ 0 & 0 & \gamma & E_0 \end{bmatrix} \leftarrow \text{"tridiagonal" matrix}$$

- Many physics problems expressed as a tridiagonal matrix
- Most general form:

$$M = \begin{bmatrix} \alpha_0 & \beta_1 & 0 & 0 & \cdots \\ \beta_1 & \alpha_1 & \beta_2 & 0 & \cdots \\ 0 & \beta_2 & \alpha_2 & \beta_3 & \cdots \\ 0 & 0 & \beta_3 & \alpha_3 & \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

← Assume M is large but finite

* Suppose we would like to determine

$$\left(\frac{1}{M}\right)_{00}$$

← Top left element of inverse of M

(we see why below)

- Can show that (see G and P sec. I.4.2):

$$\left(\frac{1}{M}\right)_{00} = \cfrac{1}{\alpha_0 - \underbrace{\cfrac{\beta_1^2}{\alpha_1 - \cfrac{\beta_2^2}{\cdots}}} - \underbrace{\cfrac{\beta_0^2}{\alpha_{-1} - \cfrac{\beta_{-1}^2}{\cdots}}}}$$

(for n in positive or negative directions)

"continued fractions"