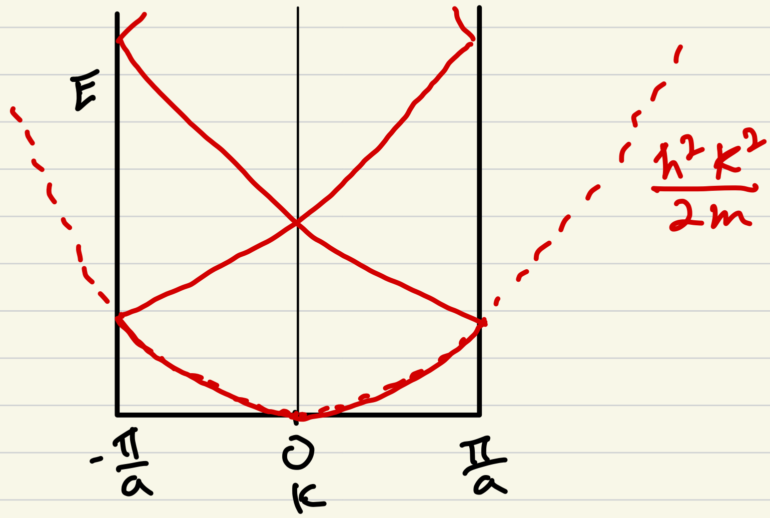
Expanding in a plane wave basis for periodic potentials:

- Recall the "empty lattice" dispersion
- We know that a periodic potential can only couple states at same k
- Use empty lattice eigenfunctions (plane waves) as the basis to expand



- Consider 1D Hamiltonian w/ generic periodic potential

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \leftarrow V(x) = V(x+ma) \quad m \in \mathbb{Z}$$

* Plane waves as a basis:

$$W_k^n(x) = \frac{1}{\sqrt{L}} e^{i(k+h_n)x} \qquad h_n = \frac{2\pi n}{a} \qquad L = Na$$

* Matrix elements:

$$\langle W_k^m | H | W_k^n \rangle = \frac{\hbar^2 (k+h_n)^2}{2m}\delta_{mn} + \frac{1}{L}\int_0^L e^{-i(h_m - h_n)x} V(x)\,dx$$

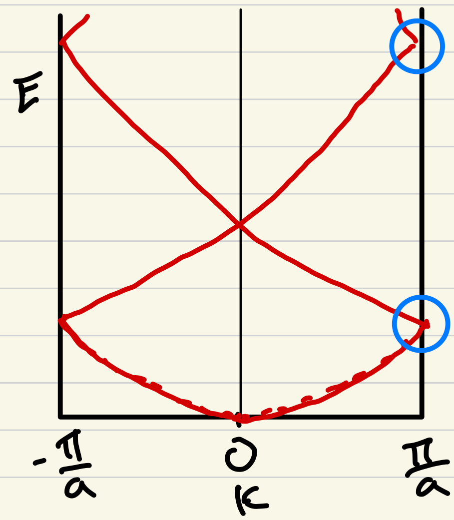
$$= \frac{\hbar^2 (k+h_n)^2}{2m}\delta_{mn} + V(h_m - h_n)$$

Fourier transform of V

So to get eigenvalues E, need to solve:

$$\det\left[\left(\frac{\hbar^2 (k+h_n)^2}{2m} - E\right)\delta_{mn} + V[h_m - h_n]\right] = 0$$

Nearly free electron approximation:



- Lets focus on $k = \pi/a$:

  * Plane waves: $\pm \frac{\pi}{a}$, $E_0 = \frac{\hbar^2}{2m}\left(\frac{\pi^2}{a^2}\right)$

    $\pm \frac{3\pi}{a}$, $E = 9E_0$

    ...

  * Consider just two basis functions:

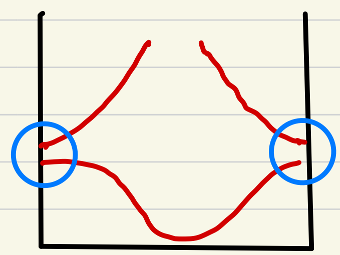
$$\psi_1 = \frac{1}{\sqrt{L}} \exp\left(i \frac{\pi}{a} x\right), \quad \psi_2 = \frac{1}{\sqrt{L}} \exp\left(-i \frac{\pi}{a} x\right)$$

  • secular equation becomes:

Fourier transform of V at $2\pi/a$

$$\det \begin{bmatrix} E_0 - E & V_1 \\ V_1^* & E_0 - E \end{bmatrix} = 0$$

note $V(-2\pi/a) = V^*(2\pi/a)$ (for $V(x)$ real)



$$\Rightarrow E = E_0 \pm |V_1|$$

Periodic potential splits degeneracy and opens a gap!

* What is behavior near (but not at) $\pm \pi/a$?
  Choose basis functions:

$$\psi_1 = \frac{1}{\sqrt{L}} \exp\left[i(\pi/a - \Delta k)x\right] \qquad \left[E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a} - \Delta k\right)^2\right]$$

$$\psi_2 = \frac{1}{\sqrt{L}} \exp\left[i(-\pi/a - \Delta k)x\right] \qquad \left[E_2 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a} + \Delta k\right)^2\right]$$

- Secular equation:

$$\det\begin{bmatrix} E_1 - E & V_1 \\ V_1^* & E_2 - E \end{bmatrix} = 0$$

$$\frac{1}{2}(E_1+E_2) = \frac{\hbar^2}{4m}\left[2\left(\frac{\pi}{a}\right)^2 + 2\Delta k^2\right] = E_0 + \frac{\hbar^2 \Delta k^2}{2m}$$

$$(E_1-E_2)^2 = \left[\frac{\hbar^2}{2m}\left(4\frac{\pi}{a}\Delta k\right)\right]^2 = 16\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\frac{\hbar^2}{2m}\Delta k^2 = 16E_0\frac{\hbar^2\Delta k^2}{2m}$$

$$\Rightarrow E = \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1-E_2)^2 + 4|V_1|^2}\right]$$

dispersion near zone boundary

$$E(\Delta k) = E_0 + \frac{\hbar^2\Delta k^2}{2m} \pm \frac{1}{2}\sqrt{16E_0\frac{\hbar^2\Delta k^2}{2m} + 4|V_1|^2}$$

- Expand for small Δk:

$$E(\Delta k) = E_0 + \frac{\hbar^2\Delta k^2}{2m} \pm |V_1|\sqrt{\frac{4E_0}{|V_1|^2}\frac{\hbar^2\Delta k^2}{2m} + 1}$$

$\sqrt{x+1} \approx 1 + \frac{x}{2} + \cdots$ for small x

$$\approx E_0 + \frac{\hbar^2\Delta k^2}{2m} \pm |V_1|\left[1 + \frac{2E_0}{|V_1|^2}\frac{\hbar^2\Delta k^2}{2m}\right] + \cdots$$

$$= E_0 \pm |V_1| + \frac{\hbar^2\Delta k^2}{2m}\left(1 \pm \frac{2E_0}{|V_1|}\right)$$

- Can define "effective masses" of two bands:

$$\frac{1}{m^*} = \frac{1}{m}\left(1 \pm \frac{2E_0}{|V_1|}\right)$$ - Small nonzero $V_1 \rightarrow$ small m^*