

## Density of States and Green's functions

- Consider system described by  $H|\psi_m\rangle = E_m|\psi_m\rangle$
- Density of states (DOS) is important attribute!

$$D(E) = \sum_m \delta(E - E_m)$$

↑ eigenvalues of  $H$

\* "Projected DOS" for orbital  $f_0$  is:

$$n_0(E) = \sum_m |\langle f_0 | \psi_m \rangle|^2 \delta(E - E_m)$$

some basis function ↑ eigenfunctions of  $H$

- Define the (retarded) Green's function:

$$G(E + i\varepsilon) \equiv \frac{1}{(E + i\varepsilon)\mathbb{I} - H}$$

infinitesimal  
 $\varepsilon > 0$

↑  
 $N \times N$  identity  
matrix

↑  
 $N \times N$  matrix

\* Since  $H$  is a matrix, so is  $G$

\* Consider upper left element:

$$G_{00}(E + i\varepsilon) \equiv \langle f_0 | \frac{1}{(E + i\varepsilon)\mathbb{I} - H} | f_0 \rangle$$

$$= \langle f_0 | \sum_m |\psi_m\rangle \langle \psi_m| \frac{1}{E + i\varepsilon - H} | f_0 \rangle$$

$$= \sum_m |\langle f_0 | \psi_m \rangle|^2 \frac{1}{E + i\varepsilon - E_m} \left( \frac{E - E_m - i\varepsilon}{E - E_m - i\varepsilon} \right)$$

$$= \sum_m |\langle f_0 | \psi_m \rangle|^2 \frac{E - E_m - i\varepsilon}{(E - E_m)^2 + \varepsilon^2}$$

$$G_{00}(E+i\epsilon) = \sum_n |\langle f_0 | \psi_n \rangle|^2 \frac{E - E_n - i\epsilon}{(E - E_n)^2 + \epsilon^2}$$

• Using:  $\lim_{\epsilon \rightarrow 0^+} \frac{1}{\pi} \frac{\epsilon}{(E - E_n)^2 + \epsilon^2} = \delta(E - E_n)$

projected DOS:  $n_0(E) = -\frac{1}{\pi} \lim_{\epsilon \rightarrow 0^+} \text{Im } G_{00}(E+i\epsilon)$

• Summing diagonal elements gives total DOS:

$$D(E) = -\frac{1}{\pi} \lim_{\epsilon \rightarrow 0^+} \text{Im Tr } G(E+i\epsilon)$$

- Let's do the calculation for the tight-binding Hamiltonian:

\* Take  $E_0 = 0$

$$G_{00}(\tilde{E}) = \langle f_0 | \frac{1}{\tilde{E} - H} | f_0 \rangle = \frac{1}{\tilde{E} - \frac{2\gamma^2}{\tilde{E} - \frac{\gamma^2}{\tilde{E} - \frac{\gamma^2}{\tilde{E} - \dots}}}}$$

define:  $t(E) = \frac{\gamma^2}{\tilde{E} - \frac{\gamma^2}{\tilde{E} - \frac{\gamma^2}{\tilde{E} - \dots}}} = \frac{\gamma^2}{\tilde{E} - t(\tilde{E})} \Rightarrow t(\tilde{E}) = \frac{1}{2} (\tilde{E} \pm \sqrt{\tilde{E}^2 - 4\gamma^2})$

$$\text{so } G_{00}(\tilde{E}) = \frac{1}{\tilde{E} - 2t(\tilde{E})} = \frac{1}{\pm \sqrt{\tilde{E}^2 - 4\gamma^2}}$$

• Choose sign so that proj. DOS is positive

$$n^{\text{TB}}(E) = \frac{1}{\pi} \frac{1}{\sqrt{4\gamma^2 - E^2}}, |E| < 2|\gamma|$$

↑ Band width!

- Can also get DOS from summing dispersion over  $k$ :

$$D(E) = \sum_k \delta[E - 2\gamma \cos(ka)] \quad (E_0 = 0)$$

\* Convert to continuous  $k$  version:

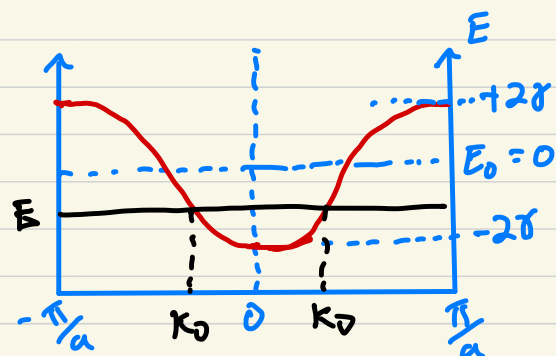
$$\sum_k \rightarrow \frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk \quad (\text{recall, } k = \frac{2\pi}{Na} n)$$

$$\text{So: } D(E) = \frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} \delta[E - 2\gamma \cos(ka)] dk$$

$$\text{Using: } \delta[f(x)] = \sum_{x_0 \text{ zeros of } f(x)} \frac{\delta(x - x_0)}{|f'(x_0)|}$$

$$D(E) = \frac{Na}{2\pi} 2 \frac{1}{|2\gamma a \sin(ka)|}$$

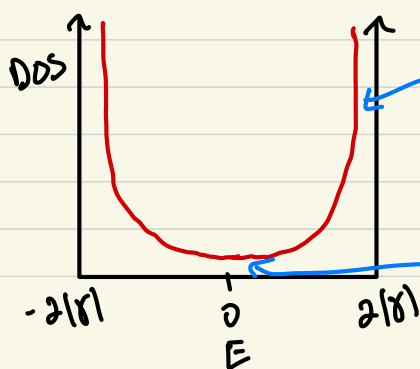
$$k_0 = \frac{1}{a} \arccos\left(\frac{E}{2\gamma}\right) \quad \text{so:}$$



$$D(E) = \frac{Na}{\pi} \left| 2\gamma a \sin\left[\arccos\left(\frac{E}{2\gamma}\right)\right] \right|^{-1}$$

$$= \frac{N}{\pi} \frac{1}{\sqrt{4\gamma^2 - E^2}} = N * n(E) \quad (\text{for } |E| < 2|\gamma|)$$

\* Plotting the DOS: ( $E_0 = 0$ )



large near areas of flat dispersion (top and bottom of bands)

smallest when slope of bands is maximum