# 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:

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

infintesimal $\varepsilon > 0$

NxN identity matrix

NxN matrix

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

* Consider upper left element:

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

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

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

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

$$G_{00}(E+i\varepsilon) = \sum_m |\langle f_0|\psi_m\rangle|^2 \frac{E-E_m-i\varepsilon}{(E-E_m)^2+\varepsilon^2}$$

- Using: $\lim_{\varepsilon\to 0^+} \frac{1}{\pi}\frac{\varepsilon}{(E-E_m)^2+\varepsilon^2} = \delta(E-E_m)$

projected DOS: $\boxed{n_0(E) = -\frac{1}{\pi}\lim_{\varepsilon\to 0^+} \operatorname{Im} G_{00}(E+i\varepsilon)}$

- Summing diagonal elements gives total DOS:

$$\boxed{D(E) = -\frac{1}{\pi}\lim_{\varepsilon\to 0^+} \operatorname{Im}\operatorname{Tr} G(E+i\varepsilon)}$$

- Let's do the calculation for the tight-binding Hamiltonian (take $E_0=0$):

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

define: $t(\tilde{E}) \equiv \cfrac{\gamma^2}{\tilde{E}-\cfrac{\gamma^2}{\tilde{E}-\cfrac{\gamma^2}{\cdots}}} = \cfrac{\gamma^2}{\tilde{E}-t(\tilde{E})} \Rightarrow t(\tilde{E}) = \frac{1}{2}\left(\tilde{E} \pm \sqrt{\tilde{E}^2-4\gamma^2}\right)$

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

for $|E|<2|\gamma|$, $\operatorname{Im} G_{00} = \frac{1}{\pm\sqrt{4\gamma^2-\tilde{E}^2}}$, $\lim_{\varepsilon\to 0^+}\operatorname{Im}(G_{00}) = \frac{1}{\pm\sqrt{4\gamma^2-E^2}}$

- Choose sign so that proj. DOS is positive

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

Band width!

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

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

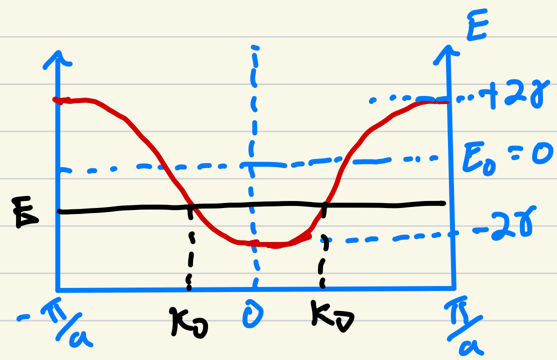
* convert to continuous $k$ version:

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

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

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

$$D(E) = \frac{Na}{2\pi}\, 2\, \frac{1}{|2\gamma a \sin(k_0 a)|}$$




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

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

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

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