For a given $\mathcal{H}$, $\sum_{\mu} \frac{1}{E-\mu}$

Resolvent of the Hamiltonian

$$\rightarrow G(z) = (zI - \mathcal{H})^{-1} \rightarrow \text{Green operator}$$

$z \rightarrow$ Complex numbe

$G_{ss}(z) \rightarrow |s\rangle$ (Complete Basis set)

$$G_{ss}(z) = \langle s | G(z) | s \rangle$$

$\downarrow$

"Green's Function"

$|\mu\rangle \rightarrow$ Complet eigen ket of $\mathcal{H}$

$$\mathrm{Tr}\, G(z) = \sum_{s} \langle s | G(z) | s \rangle$$

$$= \sum_{s} \sum_{\mu\mu'} \langle s | \mu \rangle \underbrace{\langle \mu | G(z) | \mu' \rangle}_{} \langle \mu' | s \rangle$$

$$= \sum_{s} \sum_{\mu\mu'} \langle s|\mu\rangle \frac{\delta_{\mu\mu'}}{(z-\mu)} \langle \mu'|s\rangle$$

$$= \sum_{s} \sum_{\mu} \langle s|\mu\rangle \frac{1}{(z-\mu)} \langle \mu|s\rangle$$

$$\mathrm{Tr}\left[G(z)\right] = \sum_{s}\sum_{\mu} \frac{\overbrace{\langle \mu | s\rangle\langle s|\mu\rangle}}{(z-\mu)}$$

$$= \sum_{\mu} \frac{\langle \mu|\mu\rangle}{(z-\mu)}$$

$$\mathrm{Tr}\left[G(z)\right] = \sum_{\mu} \frac{1}{(z-\mu)}$$

$$-\frac{1}{\pi}\frac{1}{N}\underset{z\to E+i\delta^+}{\mathrm{Im}}\left\{\mathrm{Tr}\left[G(z)\right]\right\} = -\frac{1}{\pi}\frac{1}{N}\sum_{\mu} \underbrace{\underset{z\to E+i\delta^+}{\mathrm{Im}}\left[\frac{1}{(z-\mu)}\right]}$$

$$= \frac{1}{N}\sum_{\mu}\delta(E-\mu) = n(E)$$

Basis Density of States

$$n(E) = \frac{1}{N}\sum_{\mu}\delta(E-\mu)$$

$$\underbrace{\int_{E}^{E+\Delta E} dE'\, n(E')} = \frac{1}{N}\sum_{\mu}\underbrace{\int_{E}^{E+\Delta E}\delta(E'-\mu)\,dE'}$$

$$= \frac{1}{N}\left[\#\text{ of states with energy between } E \text{ and } E+\Delta E\right]$$

In the thermodynamic limit

$N \to \infty$, $\mu \to$ dense and compact

$$n(E)\,\Delta E = \frac{1}{N}\left[\begin{array}{l}\#\text{ of states lying} \\ \text{with } E \ \& \ E+\Delta E\end{array}\right]$$

$\downarrow$

Basis density of states.

$s \to$ indicates the labelling for atomic sites in a tight binding system

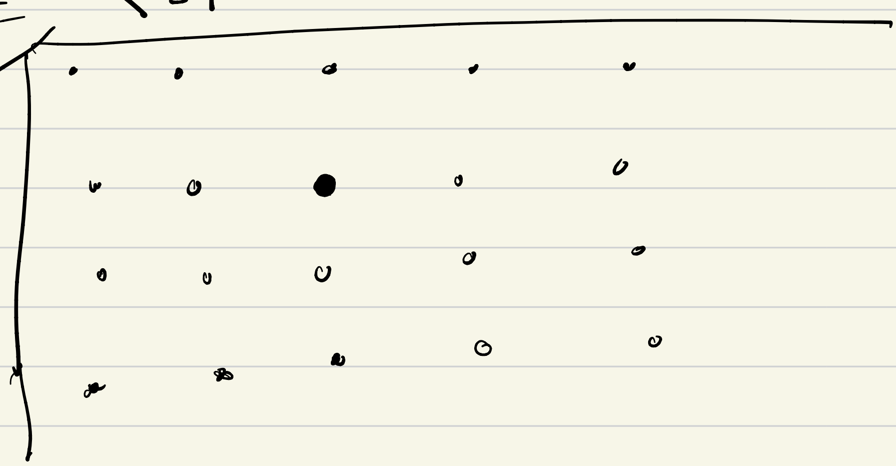
$n(E) \to$ Local density of states

$$n(E) = \sum_s \langle s | G(z) | s \rangle \to \text{Total DOS}$$

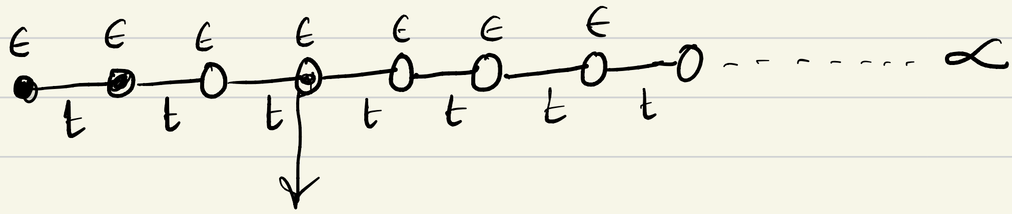
"Crystals"

$$n_s(E) = \langle s | G(z) | s \rangle$$

Local DOS.



Tight Binding Model



$\langle i|j\rangle = \delta_{ij}$

$$H = \sum_i \epsilon P_i + \sum_i \sum_{j \in nn} t \, T_{ij}$$

$P_i \to$ Projection operator $\to |i\rangle\langle i|$

$T_{ij} \to$ Transfer operator $\to |i\rangle\langle j|$

$|j\rangle\langle i|$

$$H = \sum_i \epsilon \, |i\rangle\langle i| + \sum_i \sum_{j \in nn} t \, |i\rangle\langle j|$$

$\langle i|H|i\rangle = \epsilon$; $\langle i|H|j\rangle = t$ if j belongs to the nn of i

$= 0$ otherwise

$$
H = \begin{pmatrix}
\epsilon & t & & & & & \\
t & \epsilon & t & & & 0 & \\
 & t & \epsilon & t & & & \\
 & & t & \epsilon & t & & \\
 & & & t & \epsilon & t & \\
 & 0 & & & t & \epsilon & \\
 & & & & & & \ddots
\end{pmatrix}
$$

$$
G(z) = (zI - H)^{-1}
$$

$$
G_{11}(z) = \underbrace{\langle 1 | (zI - H)^{-1} | 1 \rangle}
$$

$$
(zI - H)^{-1} = \begin{pmatrix}
(z-\epsilon) & -t & 0 & 0 & 0 & 0 & 0 \\
-t & (z-\epsilon) & -t & 0 & 0 & 0 & 0 \\
0 & -t & (z-\epsilon) & -t & 0 & 0 & 0 \\
0 & 0 & -t & (z-\epsilon) & -t & 0 & 0 \\
 & & \ddots & & \ddots & &
\end{pmatrix}^{-1}
$$

$$G_{11}(z) = (zI - H)^{-1}_{11} = \frac{1}{D}\left[\text{Matrix of Co-factor of } (Z-\epsilon)\right]$$

$$(zI - H) = \begin{pmatrix} z-\epsilon & -t & 0 & 0 & 0 & 0 & 0 \\ -t & z-\epsilon & -t & 0 & 0 & 0 & 0 \\ 0 & -t & z-\epsilon & -t & 0 & 0 & 0 \\ 0 & 0 & -t & z-\epsilon & -t & 0 & 0 \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

$$D = (Z-\epsilon)\, D^{(1)} - (-t)\, \det \begin{vmatrix} -t & -t & 0 & 0 & 0 & \cdots \\ 0 & (Z-\epsilon) & -t & 0 & 0 & \\ 0 & -t & z-\epsilon & -t & 0 & \cdots \end{vmatrix}$$

$$D = D^{(0)} = (Z-\epsilon)\, D^{(1)} - (-t)(-t)\, D^{(2)}$$

$$\boxed{D^{(n)} = (Z-\epsilon)\, D^{(n+1)} - t^2 D^{(n+2)}}$$

$$G_{11}(z) = \frac{\text{Cofactors of } (Z-\epsilon)}{D^{(0)}}$$

$$= \frac{D^{(1)}}{(Z-\epsilon)\, D^{(1)} - t^2 D^{(2)}}$$

$$D^{(n)} = (z-\epsilon) D^{(n+1)} - t^2 D^{(n+2)}$$

$$G_{11}(z) = \frac{D^{(1)}}{(z-\epsilon) D^{(1)} - t^2 D^{(2)}}$$

$$= \frac{1}{(z-\epsilon) - t^2 \dfrac{D^{(2)}}{D^{(1)}}}$$

$$= \frac{1}{(z-\epsilon) - \dfrac{t^2 D^{(2)}}{(z-\epsilon) D^{(2)} - t^2 D^{(3)}}}$$

$$= \frac{1}{(z-\epsilon) - \dfrac{t^2}{(z-\epsilon) - \dfrac{t^2}{(z-\epsilon) - \dfrac{t^2}{(z-\epsilon)}}}}$$

$$\alpha$$

$$G_{11}(z) = \frac{1}{(z-\epsilon) - t^2 G_{11}(z)}$$

$$\boxed{G_{11}(z) = \frac{(z-\epsilon) \pm \sqrt{(z-\epsilon)^2 - 4t^2}}{2t^2}}$$

$$G_{11}(z) = \frac{(z-\epsilon) \pm \sqrt{(z-\epsilon)^2 - 4t^2}}{2t^2}$$

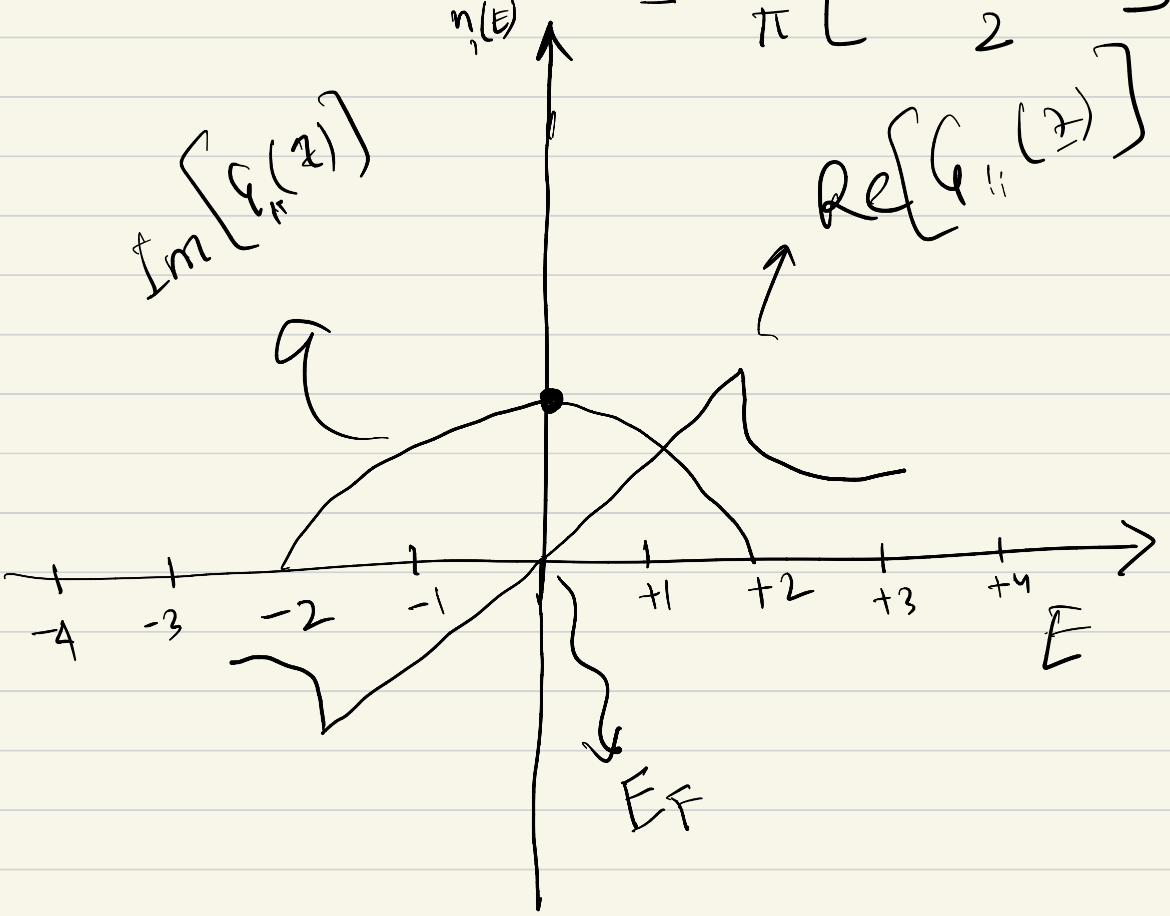
$\epsilon = 0, \quad t = 1$ ✓

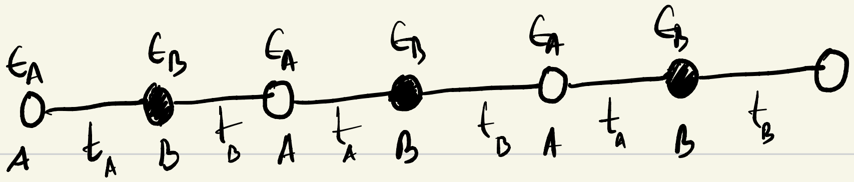
$$G_{11}(z) = \frac{z \pm \sqrt{z^2 - 4}}{2}$$ ✓

$z \to E + \delta$

$$n_1(E) = -\frac{1}{\pi} \operatorname{Im} G_{11}(z)$$

$$= \frac{1}{\pi}\left[\frac{\sqrt{4 - z^2}}{2}\right]$$



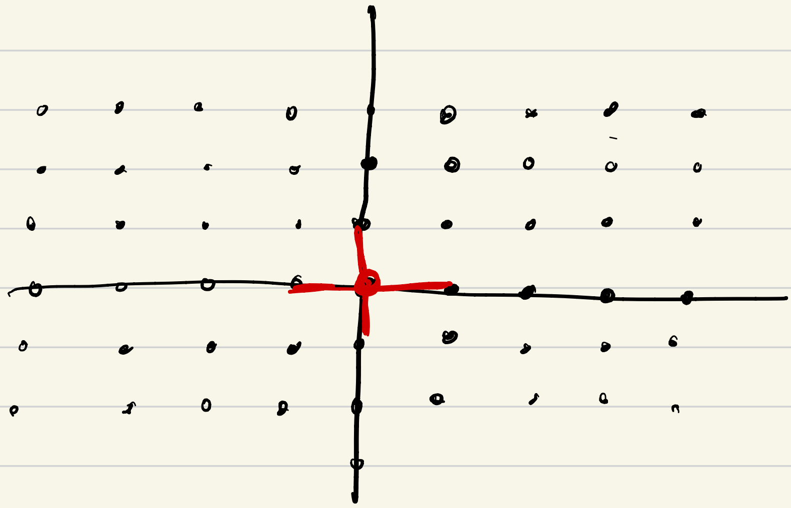


Alternating Tight binding Semiinfinite Linear chain

$$G_{11}(z) = \frac{(z-\epsilon_A)^2 - t_A^2 + t_B^2 \pm \sqrt{(z-z_1)(z-z_2)(z-z_3)(z-z_4)}}{2(z-\epsilon)\, t_B^2}$$

where, $z_1 = (\epsilon - t_B + t_A)$; $z_2 = \epsilon - t_B - t_A$

$z_3 = \epsilon - t_A + t_B$; $z_4 = \epsilon + t_B + t_A$



$$\mathcal{H} = \sum_i \epsilon P_i + \sum_i \sum_{j \in nn} t\, T_{ij}$$

$$|i\rangle$$

$$\begin{array}{cc} & \begin{array}{ccccccc} 1 & & & & & & \end{array} \\ H = & \begin{pmatrix} \epsilon & t & t & t & t & 0 & 0 \\ t & & & & & & \vdots \\ t & & & & & & \\ t & & & & & & \\ t & & & & & & \\ 0 & & & & & & \\ \vdots & & & & & & \end{pmatrix} \end{array}$$

$|i\rangle$

Lanczos Algorithm

$$H = \begin{pmatrix} \text{Sparse} & \\ & \text{Matrix.} \end{pmatrix}$$

$$|n\rangle$$

New basis; $|n\rangle\rangle$ $\langle\langle m|n\rangle\rangle = \delta_{mn}$

$$\boxed{|n+1\rangle\rangle = H|n\rangle\rangle - \alpha_n |n\rangle\rangle - \beta_n^2 |n-1\rangle\rangle}$$

$$\begin{cases} |0\rangle\rangle = 0, \quad \beta_1^2 = 1 \\ |n\rangle\rangle = |1\rangle \end{cases}$$

$$\cancel{\langle\langle n|n+1\rangle\rangle}^{\,0} = \langle\langle n|H|n\rangle\rangle - \alpha_n \langle\langle n|n\rangle\rangle$$

$$\alpha_n = \frac{\langle\langle n|H|n\rangle\rangle}{\langle\langle n|n\rangle\rangle}$$

$$\langle\langle n-1 | \cancel{n+1} \rangle\rangle^{0} = \langle\langle n-1 | H | n \rangle\rangle - \beta_n^2 \langle\langle n-1 | n-1 \rangle\rangle$$

$$\beta_n^2 = \frac{\langle\langle n-1 | H | n \rangle\rangle}{\langle\langle n-1 | n-1 \rangle\rangle} = \frac{\langle\langle n | n \rangle\rangle}{\langle\langle n-1 | n-1 \rangle\rangle}$$

$$\alpha_n = \frac{\langle\langle n | H | n \rangle\rangle}{\langle\langle n | n \rangle\rangle}$$

$$|n\rangle\rangle : H = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & 0 & 0 & 0 & 0 \\ \beta_1 & \alpha_2 & \beta_2 & & 0 & 0 & 0 \\ 0 & \beta_2 & \alpha_3 & \beta_3 & & 0 & 0 \\ 0 & 0 & \beta_3 & \alpha_4 & \beta_4 & 0 & 0 \\ 0 & 0 & 0 & \beta_4 & & 0 & 0 \\ & & & & \ddots & & \end{pmatrix}$$