Density of States:

The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy.
\[ \psi_2 = \beta \phi_1 - \alpha \phi_2 \]
\[ \psi_1 = \alpha \phi_1 + \beta \phi_2 \]
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Energy levels:
- \( E = 0 \)
- \( E = -0.618 \)
- \( E = 1.618 \)
Density of States:

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Projected/Partial Density of States:

The projected/partial density of states (PDOS) is the relative contribution of a particular atom/orbital to the total DOS.
\[ \psi_2 = \beta \phi_1 - \alpha \phi_2 \]

\[ \psi_1 = \alpha \phi_1 + \beta \phi_2 \]

Contribution of \( \phi_1 \) in \( \psi_1 = \alpha^2 \)
Contribution of \( \phi_2 \) in \( \psi_2 = \beta^2 \)

Projected density of states

\[ \psi_1 = \left\{ \begin{array}{l}
\frac{-\Delta - \sqrt{4 t^2 + \Delta^2}}{t \sqrt{8 + \frac{2 \Delta (\Delta + \sqrt{4 t^2 + \Delta^2})}{t^2}}} \\
\frac{2}{8 + \frac{2 \Delta (\Delta + \sqrt{4 t^2 + \Delta^2})}{t^2}}
\end{array} \right. \]
\( \beta^2(E=0) = 0.5 \quad \alpha^2(E=1) = 0.5 \)

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First moment:

The first moment is the center of gravity of PDOS. In other words, first moment is exactly the on-site energy.
\[ (-1 \times 0.5) + (1 \times 0.5) = 0 \]

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\[ (-0.618 \times 0.723) + (1.618 \times 0.276) = 0 \]

\[ (-0.618 \times 0.276) + (1.618 \times 0.723) = 1 \]
DOS = \frac{1}{N} e^{-\left(\frac{E-\epsilon_i}{\Gamma}\right)^2}