1 Tetrahedra

Let us assume that we want to calculate a quantity (e.g. the partial DOS):

$$I(\epsilon) = \sum_n \int F(\mathbf{k})\delta(\epsilon - \epsilon_n(\mathbf{k}))d\mathbf{k}$$

where n is the sum over Kohn-Sham states with eigenvalues $\epsilon_n(\mathbf{k})$, calculated for a discrete set of k-points. Within the tetrahedron method, the k-point grid forms N tetrahedra, whose vertices are $\mathbf{k}_k^{(i)}, k = 1,4$ (i is the tetrahedron index). The integral is calculated by summing over all tetrahedra:

$$I(\epsilon) = \sum_{i=1}^{N} V_T^{(i)} g^{(i)} \sum_{k=1}^{4} I_k^{(i)} F_k^{(i)}$$

where $F_k^{(i)} = F(\mathbf{k}_k^{(i)})$, $V_T^{(i)}$ is the volume of the $i-$th tetrahedron, $g^{(i)}$ and $I_k^{(i)}$ are weights (note that $\sum_{k=1}^4 I_k^{(i)} = 1$) that depend on the energy ϵ as follows. Let us consider a specific tetrahedron and drop the tetrahedron index i. Let us call $\epsilon_k, k = 1,4$ the values of the Kohn-Sham states eigenvalues corresponding to the four tetrahedra corners, in order of increasing energy, and let us introduce the notations $f_{ij} = (\epsilon - \epsilon_j)/(\epsilon_i - \epsilon_j)$ (note that$f_{ij} + f_{ji} = 1$).

- if $\epsilon < \epsilon_1$ or $\epsilon > \epsilon_4$, the contribution of this tetrahedron is zero.

- if $\epsilon_1 < \epsilon < \epsilon_2$:

$$g = 3\frac{f_{21}f_{31}f_{41}}{\epsilon - \epsilon_1} = 3\frac{(\epsilon - \epsilon_1)^2}{(\epsilon_2 - \epsilon_1)(\epsilon_3 - \epsilon_1)(\epsilon_4 - \epsilon_1)}$$

$$I_1 = \frac{1}{3}(f_{12} + f_{13} + f_{14}) = \frac{1}{3}\left(\frac{\epsilon - \epsilon_2}{\epsilon_1 - \epsilon_2} + \frac{\epsilon - \epsilon_3}{\epsilon_1 - \epsilon_3} + \frac{\epsilon - \epsilon_4}{\epsilon_1 - \epsilon_4}\right)$$

$$I_2 = \frac{1}{3}f_{21} = \frac{1}{3}\frac{\epsilon - \epsilon_1}{\epsilon_2 - \epsilon_1}, \qquad I_3 = \frac{1}{3}f_{31} = \frac{1}{3}\frac{\epsilon - \epsilon_1}{\epsilon_3 - \epsilon_1}, \qquad I_4 = \frac{1}{3}f_{41} = \frac{1}{3}\frac{\epsilon - \epsilon_1}{\epsilon_4 - \epsilon_1}$$

- if $\epsilon_2 < \epsilon < \epsilon_3$:

$$g = 3\frac{f_{23}f_{31} + f_{32}f_{24}}{\epsilon_4 - \epsilon_1} = \frac{3}{\epsilon_4 - \epsilon_1}\left(\frac{\epsilon - \epsilon_3}{\epsilon_2 - \epsilon_3}\frac{\epsilon - \epsilon_1}{\epsilon_3 - \epsilon_1} + \frac{\epsilon - \epsilon_2}{\epsilon_3 - \epsilon_2}\frac{\epsilon - \epsilon_4}{\epsilon_2 - \epsilon_4}\right)$$

$$I_1 = \frac{f_{14}}{3} + \frac{f_{13}f_{31}f_{23}}{g(\epsilon_4 - \epsilon_1)}, \qquad I_2 = \frac{f_{23}}{3} + \frac{f_{24}^2 f_{32}}{g(\epsilon_4 - \epsilon_1)}, \qquad I_3 = \frac{f_{32}}{3} + \frac{f_{31}^2 f_{23}}{g(\epsilon_4 - \epsilon_1)}, \qquad I_4 = \frac{f_{41}}{3} + \frac{f_{42}f_{24}f_{32}}{g(\epsilon_4 - \epsilon_1)}$$

- if $\epsilon_3 < \epsilon < \epsilon_4$:

$$g = 3\frac{f_{14}f_{24}f_{34}}{\epsilon_4 - \epsilon} = 3\frac{(\epsilon - \epsilon_4)^2}{(\epsilon_4 - \epsilon_1)(\epsilon_4 - \epsilon_2)(\epsilon_4 - \epsilon_3)}$$

$$I_1 = \frac{1}{3}f_{14} = \frac{1}{3}\frac{\epsilon - \epsilon_4}{\epsilon_1 - \epsilon_4}, \qquad I_2 = \frac{1}{3}f_{24} = \frac{1}{3}\frac{\epsilon - \epsilon_4}{\epsilon_2 - \epsilon_4}, \qquad I_3 = \frac{1}{3}f_{34} = \frac{1}{3}\frac{\epsilon - \epsilon_4}{\epsilon_3 - \epsilon_4}$$

$$I_4 = \frac{1}{3}(f_{41} + f_{42} + f_{43}) = \frac{1}{3}\left(\frac{\epsilon - \epsilon_1}{\epsilon_4 - \epsilon_1} + \frac{\epsilon - \epsilon_2}{\epsilon_4 - \epsilon_2} + \frac{\epsilon - \epsilon_3}{\epsilon_4 - \epsilon_3}\right)$$

References:
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