1 Linear Tetrahedron

We compute the DOS for all three dimensions using the Linear Tetrahedron method. Considering a reciprocal space Hamiltonian $H_{\mathbf{k}}$ with M degrees of freedom, we denote $\varepsilon_{m\mathbf{k}}$ its m-th eigenvalue for $m \in [\![1, M]\!]$.

1.1 1D Linear Tetrahedron

In 1D the Brillouin zone is split into subintervals of equal length where eigenvalues are interpolated as

$$\varepsilon_{mk} = a + bk, \ \forall m \in [\![1, M]\!], k \in \mathcal{B} \tag{1}$$

Therefore the expression of the DOS is

$$D(E) = \frac{1}{|\mathcal{B}|} \int_{S(E)} \frac{1}{|\nabla \varepsilon_k|} \mathrm{d}\sigma(k) = \frac{1}{|\mathcal{B}|} \int_{S(E)} \frac{1}{|b|} \mathrm{d}\sigma(k) \tag{2}$$

Which leads to the following contribution at each interval T_i for the m-th eigenvalue between the points k_i and $k_{i+1} \in [0, 1]$

$$D_{T_i}(E) = \begin{cases} \frac{|T_i|}{|b|} & \text{if } \varepsilon_{mk_i} < E < \varepsilon_{mk_{i+1}} \\ 0 & \text{else} \end{cases} \tag{3}$$

1.2 2D Linear Tetrahedron

In 2D, the reduced Brillouin zone is a square. We can subdivide this square into multiple squares that can all be subdivided into two triangles. Let's place ourselves in a triangle where we want to interpolate the eigenvalues on it. Let ε be an eigenvalue on T our triangle. We have in cartesian coordinates

$$\varepsilon(k_x, k_y) = ak_x + bk_y + c \tag{4}$$

Now using the interpolated values of ε on each vertex that we will call ε_i and such that $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_3$ (for convenience).

We have in barycentric coordinates that

$$\varepsilon(e, u) = \varepsilon_1(1 - e - u) + \varepsilon_2 e + \varepsilon_3 u \tag{5}$$

Now we want to interpolate the DOS

$$D(E) = \frac{1}{|\mathcal{B}|} \int_{S(E)} \frac{1}{|\nabla \varepsilon(e, u)|} \frac{\partial(k_x, k_y)}{\partial(e, u)} \mathrm{d}\sigma(e, u) \tag{6}$$

Now splitting the Brillouin zone into triangles, we can exhibit the contribution of each triangle T_i to the DOS and using that $|\nabla \varepsilon(e, u)| = \sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2}$

$$D_{T_i}(E) = \frac{2|T_i|}{|\mathcal{B}|} \frac{1}{\sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2}} \int_{S(E) \cap T_i} \mathrm{d}\sigma(e, u) \tag{7}$$

Herethe intersection of the Fermi surface and the triangles are (depending on E) either empty, straight lines or points.

- $E < \varepsilon_1$ or $E > \varepsilon_3$, in this case $S(E) \cap T_i = \emptyset$ thus the contribution to the DOS is 0.

- $\varepsilon_1 < E < \varepsilon_2$, here we have $S(E) \cap T_i$ which is a line between two points as shown in (rajouter figure).
  We have for c_1 that $u = 0$ and for c_2 we have $e = 0$, thus giving us both equations

$$c_1 : E = \varepsilon_1(1-e) + \varepsilon_2 e,\ \ u = 0 \tag{8}$$
$$c_2 : E = \varepsilon_1(1-u) + \varepsilon_3 u,\ \ e = 0 \tag{9}$$

  So $c_1 = \left(\frac{E-\varepsilon_1}{\varepsilon_2-\varepsilon_1}, 0\right)$ and $c_2 = \left(0, \frac{E-\varepsilon_1}{\varepsilon_3-\varepsilon_1}\right)$.
  Therefore the length A of the segment $[c_1, c_2]$ is

$$A = \sqrt{\left(\frac{E-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right)^2 + \left(\frac{E-\varepsilon_1}{\varepsilon_3-\varepsilon_1}\right)^2} \tag{10}$$
$$A = (E-\varepsilon_1)\sqrt{\frac{(\varepsilon_2-\varepsilon_1)^2 + (\varepsilon_3-\varepsilon_1)^2}{(\varepsilon_2-\varepsilon_1)^2(\varepsilon_3-\varepsilon_1)^2}} \tag{11}$$
$$A = \frac{(E-\varepsilon_1)}{(\varepsilon_2-\varepsilon_1)(\varepsilon_3-\varepsilon_1)}\left|\nabla\varepsilon(e,u)\right| \tag{12}$$

  Thus the contribution to the DOS finally becomes

$$D_{T_i}(E) = \frac{2\left|T_i\right|}{|\mathcal{B}|}\frac{(E-\varepsilon_1)}{(\varepsilon_2-\varepsilon_1)(\varepsilon_3-\varepsilon_1)} \tag{13}$$

- $\varepsilon_2 < E < \varepsilon_3$, we still have a line as shown in (mettre figure).
  Here for c_1 we have $e + u = 1$ and for c_2 we have $e = 0$

$$c_1 : E = \varepsilon_2 e + \varepsilon_3 u,\ \ e + u = 1 \tag{14}$$
$$c_2 : E = \varepsilon_1(1-u) + \varepsilon_3 u,\ \ e = 0 \tag{15}$$
$$\tag{16}$$

  $c_1 = \left(\frac{\varepsilon_3-E}{\varepsilon_3-\varepsilon_2}, \frac{E-\varepsilon_2}{\varepsilon_3-\varepsilon_2}\right)$, $c_2 = \left(0, \frac{E-\varepsilon_1}{\varepsilon_3-\varepsilon_1}\right)$.
  Now the length A of the segment is

$$A = \sqrt{\left(\frac{\varepsilon_3-E}{\varepsilon_3-\varepsilon_2}\right)^2 + \left(\frac{E-\varepsilon_2}{\varepsilon_3-\varepsilon_2} - \frac{E-\varepsilon_1}{\varepsilon_3-\varepsilon_1}\right)^2} \tag{17}$$
$$A = \sqrt{\left(\frac{(\varepsilon_3-\varepsilon_1)(\varepsilon_3-E)}{(\varepsilon_3-\varepsilon_2)(\varepsilon_3-\varepsilon_1)}\right)^2 + \left(\frac{(E-\varepsilon_2)(\varepsilon_3-\varepsilon_1) - (E-\varepsilon_1)(\varepsilon_3-\varepsilon_2)}{(\varepsilon_3-\varepsilon_2)(\varepsilon_3-\varepsilon_1)}\right)^2} \tag{18}$$
$$A = \frac{1}{(\varepsilon_3-\varepsilon_2)(\varepsilon_3-\varepsilon_1)}\sqrt{(\varepsilon_3-\varepsilon_1)^2(\varepsilon_3-E)^2 + (E-\varepsilon_3)^2(\varepsilon_2-\varepsilon_1)^2} \tag{19}$$
$$A = \frac{(\varepsilon_3-E)}{(\varepsilon_3-\varepsilon_2)(\varepsilon_3-\varepsilon_1)}\left|\nabla\varepsilon(e,u)\right| \tag{20}$$

  Thus the contribution to the DOS finally becomes

$$D_{T_i}(E) = \frac{2\left|T_i\right|}{|\mathcal{B}|}\frac{(\varepsilon_3-E)}{(\varepsilon_3-\varepsilon_2)(\varepsilon_3-\varepsilon_1)} \tag{21}$$

1.3 3D Linear Tetrahedron

In 3D, the reduced Brillouin zone is a cube. We can subdivide this cube into multiple cube that can all be subdivided into six regular tetrahedra. Let's place ourselves in a tetrahedron where we want to interpolate the eigenvalues on it. Let ε be an eigenvalue on T our tetrahedron. We have in cartesian coordinates

$$\varepsilon(k_x, k_y, k_z) = ak_x + bk_y + ck_z + d \tag{22}$$

Now using the interpolated values of ε on each vertex that we will call ε_i and such that $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_3 \leq \varepsilon_4$ (for convenience).

We have in barycentric coordinates that

$$\varepsilon(e, u, v) = \varepsilon_1(1 - e - u - v) + \varepsilon_2 e + \varepsilon_3 u + \varepsilon_4 v \tag{23}$$

Now we want to interpolate the DOS

$$D(E) = \frac{1}{|\mathcal{B}|} \int_{S(E)} \frac{1}{|\nabla\varepsilon(e, u, v)|} \frac{\partial(k_x, k_y, k_z)}{\partial(e, u, v)} \mathrm{d}\sigma(e, u, v) \tag{24}$$

Now splitting the Brillouin zone into triangles, we can exhibit the contribution of each triangle T_i to the DOS and using that $|\nabla\varepsilon(e, u, v)| = \sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_4 - \varepsilon_1)^2}$

$$D_{T_i}(E) = \frac{6|T_i|}{|\mathcal{B}|} \frac{1}{\sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_4 - \varepsilon_1)^2}} \int_{S(E)\cap T_i} \mathrm{d}\sigma(e, u) \tag{25}$$

- $E < \varepsilon_1$ or $E > \varepsilon_4$, in this case $S(E) \cap T_i = \emptyset$ thus the contribution to the DOS is 0.
- $\varepsilon_1 < E < \varepsilon_2$, here we have $S(E) \cap T_i$ which is a triangle whose vertex are on the ridges of the tetrahedron We have for c_1 that $u = v = 0$, for c_2 $e = v = 0$ and for c_3, $e = u = 0$, giving us the three following equations

$$c_1 : E = \varepsilon_1(1 - e) + \varepsilon_2 e,\ \ u = v = 0 \tag{26}$$

$$c_2 : E = \varepsilon_1(1 - u) + \varepsilon_3 u,\ \ e = v = 0 \tag{27}$$

$$c_3 : E = \varepsilon_1(1 - v) + \varepsilon_4 v,\ \ e = u = 0 \tag{28}$$

$c_1 = \left(\frac{E-\varepsilon_1}{\varepsilon_2-\varepsilon_1}, 0, 0\right)$, $c_2 = \left(0, \frac{E-\varepsilon_1}{\varepsilon_3-\varepsilon_1}, 0\right)$, $c_3 = \left(0, 0, \frac{E-\varepsilon_1}{\varepsilon_4-\varepsilon_1}\right)$

So the area $A = \int_{S(E)\cap T_i} \mathrm{d}\sigma(e, u)$ of the triangle spanned by our 3 points c_1, c_2 and c_3 is

$$A = \frac{|(c_2 - c_1) \times (c_3 - c_1)|}{2} \tag{29}$$

$$A = \frac{(E - \varepsilon_1)^2}{2} \frac{\sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_4 - \varepsilon_1)^2}}{(\varepsilon_2 - \varepsilon_1)(\varepsilon_3 - \varepsilon_1)(\varepsilon_4 - \varepsilon_1)} \tag{30}$$

Finally the contribution on the tetrahedron to the DOS is

$$D_{T_i}(E) = \frac{3|T_i|}{|\mathcal{B}|} \frac{(E - \varepsilon_1)^2}{(\varepsilon_2 - \varepsilon_1)(\varepsilon_3 - \varepsilon_1)(\varepsilon_4 - \varepsilon_1)} \tag{31}$$

- $\varepsilon_2 < E < \varepsilon_3$, here we have $S(E) \cap T_i$ which is a tetragon.

$$c_1 : E = \varepsilon_2 e + \varepsilon_4 v,\ \ u = 0, e + v = 1 \tag{32}$$

$$c_2 : E = \varepsilon_2 e + \varepsilon_3 u,\ \ v = 0, e + u = 1 \tag{33}$$

$$c_3 : E = \varepsilon_1(1 - u) + \varepsilon_3 u,\ \ e = v = 0 \tag{34}$$

$$c_4 : E = \varepsilon_1(1 - v) + \varepsilon_4 v,\ \ e = u = 0 \tag{35}$$

Which gives us $c_1 = \left(\frac{\varepsilon_4-E}{\varepsilon_4-\varepsilon_2}, 0, \frac{E-\varepsilon_2}{\varepsilon_4-\varepsilon_2}\right)$, $c_2 = \left(\frac{\varepsilon_3-E}{\varepsilon_3-\varepsilon_2}, \frac{E-\varepsilon_2}{\varepsilon_3-\varepsilon_2}, 0\right)$, $c_3 = \left(0, \frac{E-\varepsilon_1}{\varepsilon_3-\varepsilon_1}, 0\right)$, $c_4 = \left(0, 0, \frac{E-\varepsilon_1}{\varepsilon_4-\varepsilon_1}\right)$
Now the area A of a tetragon is as follows

$$A = \frac{\Big|((c_1 - c_4) + (c_2 - c_4)) \times (c_2 - c_4)\Big|}{2} \tag{36}$$

$$\begin{aligned} A =& \frac{\sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_{41} - \varepsilon_1)^2}}{2(\varepsilon_3 - \varepsilon_1)(\varepsilon_4 - \varepsilon_1)} \times \\ & \left((\varepsilon_2 - \varepsilon_1) - 2(\varepsilon_2 - E) - \frac{(\varepsilon_2 - E)^2((\varepsilon_3 - \varepsilon_1) + (\varepsilon_4 - \varepsilon_2))}{(\varepsilon_3 - \varepsilon_2)(\varepsilon_4 - \varepsilon_2)}\right) \end{aligned} \tag{37}$$

$$\begin{aligned} D_{T_i}(E) =& \frac{3|T_i|}{|\mathcal{B}|} \frac{1}{(\varepsilon_3 - \varepsilon_1)(\varepsilon_4 - \varepsilon_1)} \times \\ & \left((\varepsilon_2 - \varepsilon_1) - 2(\varepsilon_2 - E) - \frac{(\varepsilon_2 - E)^2((\varepsilon_3 - \varepsilon_1) + (\varepsilon_4 - \varepsilon_2))}{(\varepsilon_3 - \varepsilon_2)(\varepsilon_4 - \varepsilon_2)}\right) \end{aligned} \tag{38}$$

- $\varepsilon_3 < E < \varepsilon_4$, here we have $S(E) \cap T_i$ which is a triangle whose vertex are on the ridges of the tetrahedron We have for c_1 that $u = 0$, for c_2 $e = 0$ and for c_3, $e = u = 0$, giving us the three following equations

$$c_1 : E = \varepsilon_2 e + \varepsilon_4 v, \;\; u = 0, \;\; e + v = 1 \tag{39}$$
$$c_2 : E = \varepsilon_3 u + \varepsilon_4 v, \;\; e = 0, \;\; u + v = 1 \tag{40}$$
$$c_3 : E = \varepsilon_1(1 - v) + \varepsilon_4 v, \;\; e = u = 0 \tag{41}$$

$c_1 = \left(\frac{\varepsilon_4-E}{\varepsilon_4-\varepsilon_2}, 0, \frac{\varepsilon_2-E}{\varepsilon_4-\varepsilon_2}\right)$, $c_2 = \left(0, \frac{\varepsilon_4-E}{\varepsilon_4-\varepsilon_3}, \frac{\varepsilon_3-E}{\varepsilon_4-\varepsilon_3}\right)$, $c_3 = \left(0, 0, \frac{E-\varepsilon_1}{\varepsilon_4-\varepsilon_1}\right)$

$$\int_{S(E)\cap T_i} \mathrm{d}\sigma(e, u, v) = \frac{|(c_1 - c_3) \times (c_2 - c_3)|}{2} \tag{42}$$

$$\int_{S(E)\cap T_i} \mathrm{d}\sigma(e, u, v) = \frac{(\varepsilon_4 - E)^2}{2} \frac{\sqrt{(\varepsilon_2 - \varepsilon_1)^2 + (\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_4 - \varepsilon_1)^2}}{(\varepsilon_4 - \varepsilon_1)(\varepsilon_4 - \varepsilon_2)(\varepsilon_4 - \varepsilon_3)} \tag{43}$$

$$D_{T_i}(E) = \frac{3|T_i|}{|\mathcal{B}|} \frac{(\varepsilon_4 - E)^2}{(\varepsilon_4 - \varepsilon_1)(\varepsilon_4 - \varepsilon_2)(\varepsilon_4 - \varepsilon_3)} \tag{44}$$