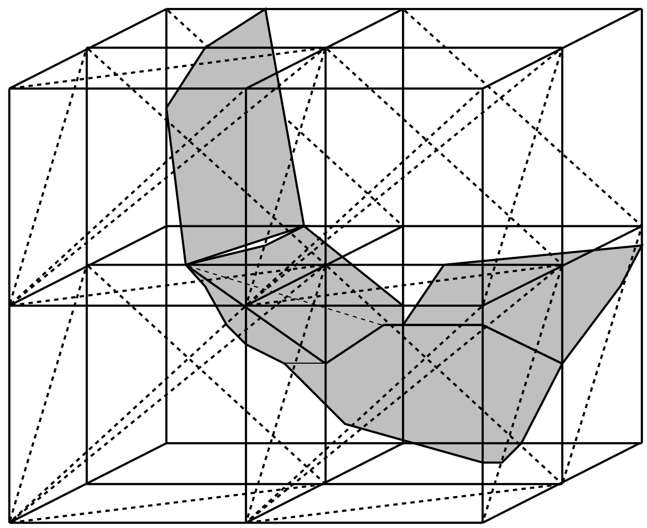
Mathematics 9: Linearised 3-d Density of States

A simple numerical technique for evaluating a three-dimensional density of states is to break up the area of integration into tetrahedra, using the calculational discretisation, and then to linearise the function inside each tetrahedron and evaluate the *exact* density of states for the linearisation. For each density required, the method amounts to finding the triangles of intersection of a polygonal surface across the integration region, as depicted in the figure:



where a cubic grid and 'odd'-shaped tetrahedra have been chosen.

The density of states:

$$\rho(f) = \int_V \frac{dV}{V} \delta\left[f - f(\mathbf{r})\right]$$

may then be rewritten:

$$\rho(f) = \frac{1}{V} \sum_t \int_{V_t} dV \, \delta\left[f - f(\mathbf{r})\right]$$

where the summation is over all the tetrahedra, t with volume V_t, which make up the integration volume, V. The function $f(\mathbf{r})$ must then be linearised in the unique way which yields the correct values at the four vertices. This is best done using quadruples of numbers, $\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$, to represent a vector, where each spatial vector is represented as:

$$\mathbf{r} = \lambda_1 \mathbf{r_1} + \lambda_2 \mathbf{r_2} + \lambda_3 \mathbf{r_3} + \lambda_4 \mathbf{r_4}$$

in terms of the position vectors of the vertices, $\mathbf{r}_i$ for the i'th vertex and the λ's are constrained to satisfy:

$$\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 1$$

This choice ensures that $\lambda_i = 1$ corresponds to the point $\mathbf{r}_i$ and $\lambda_i = 0$ corresponds to the triangle connecting the other three points. The *inside* of the tetrahedron corresponds to $\lambda_i \in (0, 1)$. Any function is then linearised by:

$$f(\mathbf{r}) \mapsto \lambda_1 f_1 + \lambda_2 f_2 + \lambda_3 f_3 + \lambda_4 f_4$$

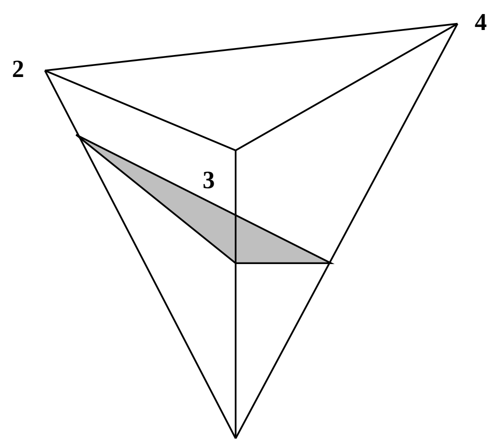
where f_i is it's value at the i'th vertex.

Using this choice, the density of states becomes:

$$\int_{V_t} dV \delta\left[f - f(\mathbf{r})\right] \mapsto 6V_t \int_0^1 d\lambda_1 \int_0^1 d\lambda_2 \int_0^1 d\lambda_3 \int_0^1 d\lambda_4 \delta[1 - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4]$$

$$\times \delta[f - \lambda_1 f_1 - \lambda_2 f_2 - \lambda_3 f_3 - \lambda_4 f_4]$$

which is quite simple to evaluate. If the surface $f(\mathbf{r}) = f$ cuts the tetrahedron across the first vertex, as depicted:



then with the choice that $f_1 \le f_2 \le f_3 \le f_4$, the 'best' method to proceed is to find the points on the lines where the interpolated surface strikes, and then to employ new variables which linearly interpolate the function across this associated triangle.

It is easy to see that the interpolated function f cuts the line $1 \mapsto 2$ at the point:

$$\boldsymbol{\lambda}_{12} = \left[\frac{f_2 - f}{f_2 - f_1}, \frac{f - f_1}{f_2 - f_1}, 0, 0\right]$$

and there are analogous results for the other five lines: $x \mapsto y$.

For the current case of $f \in (f_1, f_2)$ we can then use:

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}_{12}\mu_{12} + \boldsymbol{\lambda}_{13}\mu_{13} + \boldsymbol{\lambda}_{14}\mu_{14}$$

We integrate out λ_1 and then use the μ_{1x} as our integration variables:

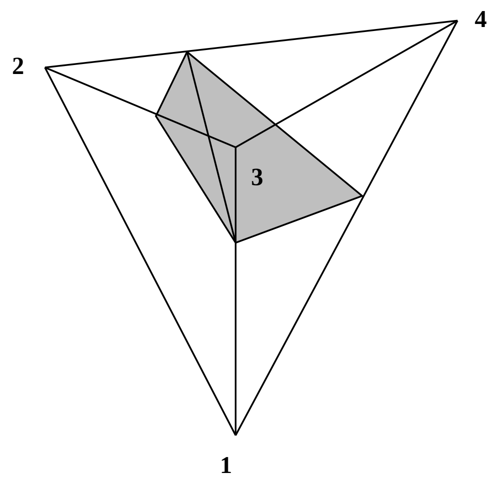
$$6\int_0^1 d\lambda_2 \int_0^1 d\lambda_3 \int_0^1 d\lambda_4 \delta[f - f_1 - \lambda_2(f_2 - f_1) - \lambda_3(f_3 - f_1) - \lambda_4(f_4 - f_1)]$$

combined with:

$$\lambda_2 = \frac{f - f_1}{f_2 - f_1}\mu_{12} \qquad \lambda_3 = \frac{f - f_1}{f_3 - f_1}\mu_{13} \qquad \lambda_4 = \frac{f - f_1}{f_4 - f_1}\mu_{14}$$

$$\mapsto 6\int_0^1 d\mu_{12}\int_0^1 d\mu_{13}\int_0^1 d\mu_{14}\frac{(f-f_1)^3}{(f_2-f_1)(f_3-f_1)(f_4-f_1)}\delta[(f-f_1)(1-\mu_{12}-\mu_{13}-\mu_{14})]$$
$$=\frac{3(f-f_1)^2}{(f_2-f_1)(f_3-f_1)(f_4-f_1)} \qquad (**)$$

For the case of $f\in(f_2,f_3)$ we have a pair of triangles as depicted in the figure:



and we therefore need $\boldsymbol{\lambda}_{13},\boldsymbol{\lambda}_{14},\boldsymbol{\lambda}_{23},\boldsymbol{\lambda}_{24}$. For the first triangle we use:

$$\boldsymbol{\lambda}=\boldsymbol{\lambda}_{24}\mu_{24}+\boldsymbol{\lambda}_{13}\mu_{13}+\boldsymbol{\lambda}_{23}\mu_{23}$$

and integrate out λ_3, whereas for the second triangle we use:

$$\boldsymbol{\lambda}=\boldsymbol{\lambda}_{24}\mu_{24}+\boldsymbol{\lambda}_{13}\mu_{13}+\boldsymbol{\lambda}_{14}\mu_{14}$$

and integrate out λ_4.

The first contribution is:

$$6\int_0^1 d\lambda_1\int_0^1 d\lambda_2\int_0^1 d\lambda_4\delta[f-f_3-\lambda_1(f_1-f_3)-\lambda_2(f_2-f_3)-\lambda_4(f_4-f_3)]$$

combined with:

$$\lambda_1=\frac{f_3-f}{f_3-f_1}\mu_{13} \qquad \lambda_4=\frac{f-f_2}{f_4-f_2}\mu_{24} \qquad \lambda_2=\frac{f_4-f}{f_4-f_2}\mu_{24}+\frac{f_3-f}{f_3-f_2}\mu_{23}$$

$$\mapsto 6\int_0^1 d\mu_{13}\int_0^1 d\mu_{24}\int_0^1 d\mu_{23}\frac{(f_3-f)^2(f-f_2)}{(f_3-f_1)(f_4-f_2)(f_3-f_2)}\delta[(f-f_3)(1-\mu_{13}-\mu_{24}-\mu_{23})]$$
$$=\frac{3(f_3-f)(f-f_2)}{(f_3-f_1)(f_4-f_2)(f_3-f_2)} \qquad (**)$$

The second contribution is:

$$6\int_0^1 d\lambda_1\int_0^1 d\lambda_2\int_0^1 d\lambda_3\delta[f-f_4-\lambda_1(f_1-f_4)-\lambda_2(f_2-f_4)-\lambda_3(f_3-f_4)]$$

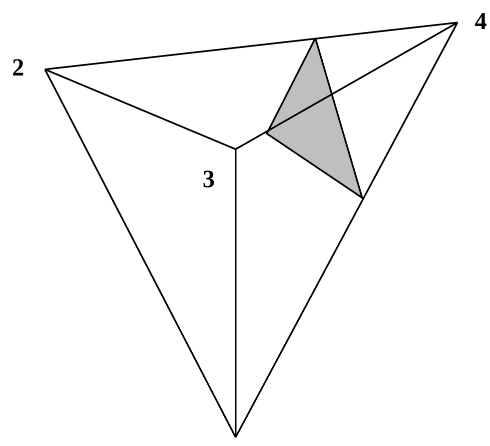
combined with:

$$\lambda_2 = \frac{f_4 - f}{f_4 - f_2}\mu_{24} \qquad \lambda_3 = \frac{f - f_1}{f_3 - f_1}\mu_{13} \qquad \lambda_1 = \frac{f_4 - f}{f_4 - f_1}\mu_{14} + \frac{f_3 - f}{f_3 - f_1}\mu_{13}$$

$$\mapsto 6\int_0^1 d\mu_{13}\int_0^1 d\mu_{24}\int_0^1 d\mu_{14}\frac{(f_4 - f)^2(f - f_1)}{(f_3 - f_1)(f_4 - f_2)(f_4 - f_1)}\delta[(f - f_4)(1 - \mu_{13} - \mu_{24} - \mu_{14})]$$

$$= \frac{3(f_4 - f)(f - f_1)}{(f_3 - f_1)(f_4 - f_2)(f_4 - f_1)} \qquad (**)$$

For the case of $f \in (f_3, f_4)$ we have a single triangle close to the top vertex as depicted in the figure:



and we therefore need $\boldsymbol{\lambda}_{14}, \boldsymbol{\lambda}_{24}, \boldsymbol{\lambda}_{34}$ and choose to integrate out λ_4

$$6\int_0^1 d\lambda_1\int_0^1 d\lambda_2\int_0^1 d\lambda_3\delta[f - f_4 - \lambda_1(f_1 - f_4) - \lambda_2(f_1 - f_3) - \lambda_3(f_1 - f_4)]$$

combined with:

$$\lambda_1 = \frac{f_4 - f}{f_4 - f_1}\mu_{14} \qquad \lambda_2 = \frac{f_4 - f}{f_4 - f_2}\mu_{24} \qquad \lambda_3 = \frac{f_4 - f}{f_4 - f_3}\mu_{34}$$

$$\mapsto 6\int_0^1 d\mu_{14}\int_0^1 d\mu_{24}\int_0^1 d\mu_{34}\frac{(f_4 - f)^3}{(f_4 - f_1)(f_4 - f_2)(f_4 - f_3)}\delta[(f - f_4)(1 - \mu_{14} - \mu_{24} - \mu_{34})]$$

$$= \frac{3(f_4 - f)^2}{(f_4 - f_1)(f_4 - f_2)(f_4 - f_3)} \qquad (**)$$

In each of the three regions, all we need do is calculate using the formulae marked (**).

With the addition of a weight function, the calculation proceeds along a similar line, but with an addition of a 'weight' in the integration:

$$w \mapsto w_1 + (f - f_1)\left[\frac{w_2 - w_1}{f_2 - f_1}\mu_{12} + \frac{w_3 - w_1}{f_3 - f_1}\mu_{13} + \frac{w_4 - w_1}{f_4 - f_1}\mu_{14}\right]$$

for $f \in (f_1, f_2)$, which integrates to:

$$3w_1 + (f - f_1)\left[\frac{w_2 - w_1}{f_2 - f_1} + \frac{w_3 - w_1}{f_3 - f_1} + \frac{w_4 - w_1}{f_4 - f_1}\right] \qquad (**)$$

a mutiplicative factor to augment the previous result (replacing the factor 3).

For the case of $f \in (f_2, f_3)$, we need two such weights, one for each triangle. The first triangle yields:

$$w \mapsto w_3 - (f_3 - f)\left[\frac{w_3 - w_1}{f_3 - f_1}\mu_{13} + \frac{w_3 - w_2}{f_3 - f_2}\mu_{23}\right] + \mu_{24}\left[\frac{w_4 - w_3}{f_4 - f_2}(f - f_2) + \frac{w_2 - w_3}{f_4 - f_2}(f_4 - f)\right]$$

$$= w_3 + (w_2 - w_3)\mu_{24} - (f_3 - f)\left[\frac{w_3 - w_1}{f_3 - f_1}\mu_{13} + \frac{w_3 - w_2}{f_3 - f_2}\mu_{23}\right] + (f - f_2)\left[\frac{w_4 - w_2}{f_4 - f_2}\right]\mu_{24}$$

which integrates to:

$$2w_3 + w_2 + (f - f_2)\left[\frac{w_4 - w_2}{f_4 - f_2}\right] - (f_3 - f)\left[\frac{w_3 - w_1}{f_3 - f_1} + \frac{w_3 - w_2}{f_3 - f_2}\right] \qquad (**)$$

a mutiplicative factor to augment the previous result (replacing the factor 3). The second triangle yields:

$$w \mapsto w_4 - (f_4 - f)\left[\frac{w_4 - w_1}{f_4 - f_1}\mu_{14} + \frac{w_4 - w_2}{f_4 - f_2}\mu_{24}\right] + \mu_{13}\left[\frac{w_1 - w_4}{f_3 - f_1}(f_3 - f) + \frac{w_3 - w_4}{f_3 - f_1}(f - f_1)\right]$$

$$= w_4 + (w_1 - w_4)\mu_{13} - (f_4 - f)\left[\frac{w_4 - w_1}{f_4 - f_1}\mu_{14} + \frac{w_4 - w_2}{f_4 - f_2}\mu_{24}\right] + (f - f_1)\left[\frac{w_3 - w_1}{f_3 - f_1}\right]\mu_{13}$$

which integrates to:

$$2w_4 + w_1 + (f - f_1)\left[\frac{w_3 - w_1}{f_3 - f_1}\right] - (f_4 - f)\left[\frac{w_4 - w_1}{f_4 - f_1} + \frac{w_4 - w_2}{f_4 - f_2}\right] \qquad (**)$$

a mutiplicative factor to augment the previous result (replacing the factor 3).

For the case $f \in (f_3, f_4)$

$$w \mapsto w_4 - (f_4 - f)\left[\frac{w_4 - w_1}{f_4 - f_1}\mu_{14} + \frac{w_4 - w_2}{f_4 - f_2}\mu_{24} + \frac{w_4 - w_3}{f_4 - f_3}\mu_{34}\right]$$

which integrates to:

$$3w_4 - (f_4 - f)\left[\frac{w_4 - w_1}{f_4 - f_1} + \frac{w_4 - w_2}{f_4 - f_2} + \frac{w_4 - w_3}{f_4 - f_3}\right] \qquad (**)$$

a mutiplicative factor to augment the previous result (replacing the factor 3).

There are no pathologies in this calculation, other than the special case of $f_1 = f_2 = f_3 = f_4 = f$, for which the density remains a δ-function.