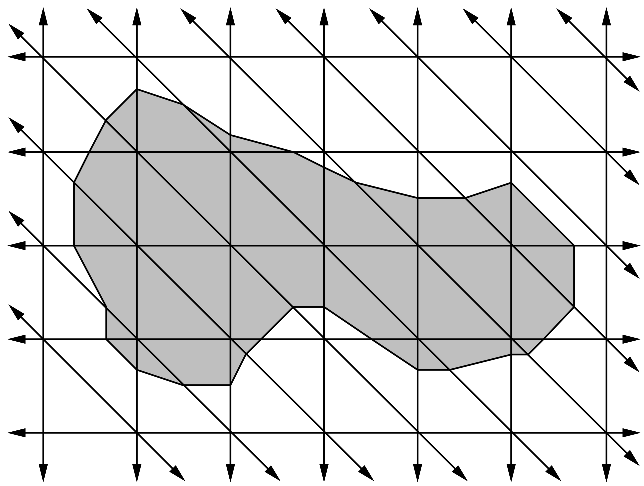
Mathematics 6: Linearised Density of States

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



where a square grid and 'odd'-shaped triangles have been chosen.

The density of states:

$$\rho(f) = \int_A \frac{dA}{A} \delta\left[f - f(\mathbf{r})\right]$$

may then be rewritten:

$$\rho(f) = \frac{1}{A} \sum_t \int_{A_t} dA \delta\left[f - f(\mathbf{r})\right]$$

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

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

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:

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

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

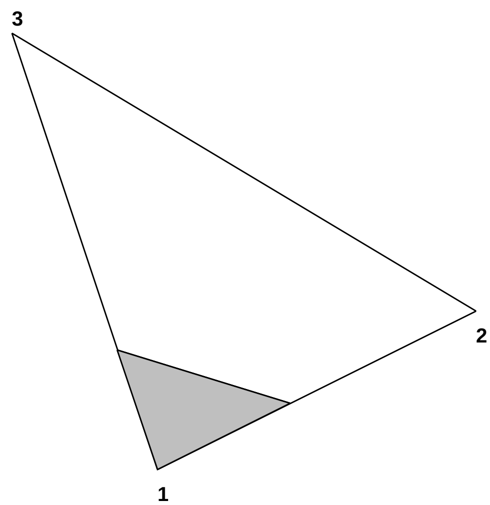
$$f(\mathbf{r}) \mapsto \lambda_1 f_1 + \lambda_2 f_2 + \lambda_3 f_3$$

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

Using this choice, the density of states becomes:

$$\int_{A_t} dA\delta\left[f - f(\mathbf{r})\right] \mapsto 2A_t \int_0^1 d\lambda_1 \int_0^1 d\lambda_2 \int_0^1 d\lambda_3 \delta[1-\lambda_1-\lambda_2-\lambda_3]\delta[f-\lambda_1 f_1-\lambda_2 f_2-\lambda_3 f_3]$$

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



then it is natural to use $s = \lambda_1 + \lambda_2 + \lambda_3$, $f = \lambda_1 f_1 + \lambda_2 f_2 + \lambda_3 f_3$ and λ_1 as the basis. The 'Jacobian' is:

$$J = \frac{\partial[s, f]}{\partial[\lambda_2, \lambda_3]} = det \begin{bmatrix} 1 & 1 \\ f_2 & f_3 \end{bmatrix} = \mid f_3 - f_2 \mid$$

from which we find:

$$\int_{A_t} dA\delta\left[f - f(\mathbf{r})\right] \mapsto 2A_t \int \frac{d\lambda_1}{\mid f_3 - f_2 \mid} = 2A_t abs\left[\frac{\lambda_1^+ - \lambda_1^-}{f_3 - f_2}\right]$$

and we need to find the value of λ_1 at the 'edges' of the triangle, $\lambda_1^\pm$. This occurs when either $\lambda_2 = 0$ or $\lambda_3 = 0$.

(i) $\lambda_2 = 0$

$$\begin{bmatrix} 1 & 1 \\ f_1 & f_3 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} 1 \\ f \end{bmatrix}$$

from which:

$$\lambda_1 = \frac{f_3 - f}{f_3 - f_1}$$

(ii) $\lambda_3 = 0$

$$\begin{bmatrix} 1 & 1 \\ f_1 & f_2 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 1 \\ f \end{bmatrix}$$

from which:

$$\lambda_1 = \frac{f_2 - f}{f_2 - f_1}$$

Since:

$$\frac{f_2 - f}{f_2 - f_1} - \frac{f_3 - f}{f_3 - f_1} = \frac{(f_1 - f)(f_3 - f_2)}{(f_3 - f_1)(f_2 - f_1)}$$

we eventually deduce that:

$$\rho(f) \mapsto \frac{1}{A} \sum_t 2A_t abs \left[\frac{(f - f_1)}{(f_2 - f_1)(f_3 - f_1)} \right]$$

when $f \in (f_1, min(f_2, f_3))$ or when $f \in (max(f_2, f_3), f_1)$.

There is only one 'pathology', when $f_1 = f_2 = f_3$ and the δ-function remains. This situation leads to a very 'spiky' density of states and must be avoided.

We also require to evaluate a 'partial' density of states:

$$\rho(f) = \int_A \frac{dA}{A} \delta \left[f - f(\mathbf{r}) \right] w(\mathbf{r})$$

where $w(\mathbf{r})$ is a 'weight' function. The triangularisation is equivalent to before, but the linearisation of the density of states becomes:

$$\int_{A_t} dA \delta \left[f - f(\mathbf{r}) \right] w(\mathbf{r}) \mapsto$$

$$2A_t \int_0^1 d\lambda_1 \int_0^1 d\lambda_2 \int_0^1 d\lambda_3 \delta[1 - \lambda_1 - \lambda_2 - \lambda_3] \delta[f - \lambda_1 f_1 - \lambda_2 f_2 - \lambda_3 f_3](\lambda_1 w_1 + \lambda_2 w_2 + \lambda_3 w_3)$$

and the natural basis is $s = \lambda_1 + \lambda_2 + \lambda_3$, $f = \lambda_1 f_1 + \lambda_2 f_2 + \lambda_3 f_3$ and $w = \lambda_1 w_1 + \lambda_2 w_2 + \lambda_3 w_3$, for which:

$$J = \frac{\partial[f, s, w]}{\partial[\lambda_1, \lambda_2, \lambda_3]} = det \begin{bmatrix} 1 & 1 & 1 \\ f_1 & f_2 & f_3 \\ w_1 & w_2 & w_3 \end{bmatrix} = \mid w_1(f_3 - f_2) + w_2(f_1 - f_3) + w_3(f_2 - f_1) \mid$$

and then:

$$\int_{A_t} dA \delta \left[f - f(\mathbf{r}) \right] w(\mathbf{r}) \mapsto$$

$$\int_{A_t} \frac{2w dw}{J} = A_t(w^+ + w^-) abs \left[\frac{w^+ - w^-}{w_1(f_3 - f_2) + w_2(f_1 - f_3) + w_3(f_2 - f_1)} \right]$$

and we need the values of $w(\mathbf{r})$ at the 'edges', $w^{\pm}$.

(i) $\lambda_2 = 0$

$$w = \frac{f_3 - f}{f_3 - f_1} w_1 + \frac{f - f_1}{f_3 - f_1} w_3 = w_1 + (f - f_1) \frac{w_3 - w_1}{f_3 - f_1}$$

(ii) $\lambda_3 = 0$

$$w = \frac{f_2 - f}{f_2 - f_1} w_1 + \frac{f - f_1}{f_2 - f_1} w_2 = w_1 + (f - f_1) \frac{w_2 - w_1}{f_2 - f_1}$$

These values may be used directly in the evaluation of the partial density of states.

There is one new 'pathology' in this problem, when $J = 0$. The vanishing of J means a linear dependence:

$$w_i = \alpha + \beta f_i$$

and then $w(\mathbf{r})$ is **constant** along the line $f(\mathbf{r}) = f$ and so:

$$\int_{A_t} dA\delta\left[f - f(\mathbf{r})\right] w(\mathbf{r}) \mapsto 2A_t abs\left[\frac{(f - f_1)}{(f_2 - f_1)(f_3 - f_1)}\right] w^\sigma$$

for this case, with either value of $w^\pm$, since $w^+ = w^-$.