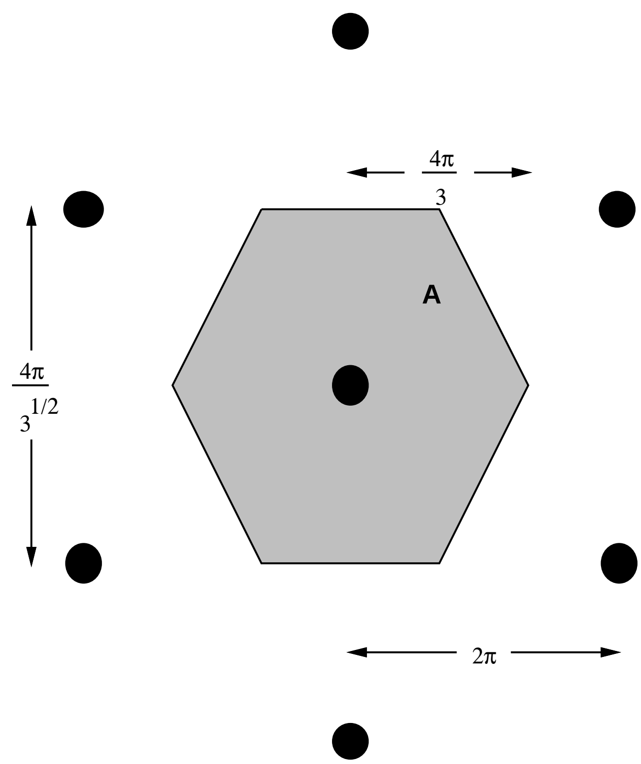
Mathematics 5: Triangular Density of State

In this section we will transform the nearest-neighbour hopping *triangular lattice density of states* into a form whereby it can be found as a one-dimensional integral. This density of states is defined as:

$$\rho(f) = \int_A \frac{d^2\mathbf{k}}{A} \delta\left[f - \frac{1}{3}\left(\cos k_1 + \cos\frac{k_1 + \sqrt{3}k_2}{2} + \cos\frac{k_1 - \sqrt{3}k_2}{2} \right)\right]$$

where the area of integration A is as depicted in the figure:



The dirac delta-function may be integrated out if we employ the variables, $c_1 = \cos k_1/2$ and $c_2 = \cos\sqrt{3}k_2/2$:

$$\rho(f) = \frac{1}{\pi^2} \int \frac{dc_1}{\sqrt{[1-c_1^2]}} \int \frac{dc_2}{\sqrt{[1-c_2^2]}} \theta[1-c_1^2]\theta[1-c_2^2]\delta\left[f + \frac{1}{3} - \frac{2c_1(c_1+c_2)}{3}\right]$$

where again we use $\theta[x]$ functions to define the integration limits. Once again, there are several values of $\mathbf{k}$ corresponding to each (c_1, c_2), this time two, due to various subtleties to do with the sign of c_1c_2. Performing the integration over c_2 yields:

$$\rho(f) = \frac{3}{2\pi^2} \int \frac{dc_1}{\sqrt{[1-c_1^2]}} \frac{\theta[1-c_1^2]\theta\left[c_1^2 - \left(\frac{3f+1}{2} - c_1^2\right)^2\right]}{\sqrt{\left[c_1^2 - \left(\frac{3f+1}{2} - c_1^2\right)^2\right]}}$$

The 'edges' or boundaries to the integration region occur when, $c_1 = \pm 1$, $c_1 = \pm\frac{1}{2} \pm \frac{\sqrt{[3+6f]}}{2} \equiv \frac{\pm 1 \pm g}{2}$, in terms of the natural variable $g = \sqrt{[3+6f]}$. *Careful* study of these

points leads to *two* types of behaviour:
(1) $f \in \left(-\frac{1}{2}, -\frac{1}{3}\right)$ for which $c_1 \in \left(\frac{1-g}{2}, \frac{1+g}{2}\right)$ and $c_1 \mapsto -c_1$.
(2) $f \in \left(-\frac{1}{3}, 1\right)$ for which $c_1 \in \left(\frac{g-1}{2}, 1\right)$ and $c_1 \mapsto -c_1$.

For each case we need to rescale the integration variable:
(1) $c_1 = \alpha + \beta x$, and since $\alpha - \beta = \frac{1-g}{2}$ and $\alpha + \beta = \frac{1+g}{2}$, we find:

$$\begin{aligned}
c_1 &= \frac{1+gx}{2} \\
\frac{1+g}{2} - c_1 &= \frac{g}{2}(1-x) \\
c_1 - \frac{1-g}{2} &= \frac{g}{2}(1+x) \\
1 - c_1 &= \frac{1}{2}(1-gx) \\
1 + c_1 &= \frac{1}{2}(3+gx) \\
c_1 + \frac{1}{2}(1+g) &= \frac{1}{2}(2+g+gx) \\
c_1 + \frac{1}{2}(1-g) &= \frac{1}{2}(2-g+gx)
\end{aligned}$$

from which we obtain:

$$\rho(f) = \frac{2\sqrt{3}}{\pi^2}\int_{-1}^{1}\frac{dx}{\sqrt{[1-x^2]}}\frac{1}{\sqrt{\left[(1-gx)\left(1+g\frac{x}{3}\right)\left(1+g\frac{1+x}{2}\right)\left(1-g\frac{1-x}{2}\right)\right]}}$$

which, with the singularities removed reduces to:

$$\rho(f) = \frac{2\sqrt{3}}{\pi}\int_{0}^{1}\frac{dz}{\sqrt{\left[(1-g\cos\pi z)\left(1+g\frac{\cos\pi z}{3}\right)\left(1+g\frac{1+\cos\pi z}{2}\right)\left(1-g\frac{1-\cos\pi z}{2}\right)\right]}}$$

(2) $c_1 = \alpha + \beta x$, and since $\alpha - \beta = \frac{g-1}{2}$ and $\alpha + \beta = 1$, we find, $\alpha = \frac{1}{4}[1+g]$ and $\beta = \frac{1}{4}[3-g]$:

$$\begin{aligned}
c_1 &= \frac{1}{4}[1+3x+g(1-x)] \\
1 - c_1 &= \frac{1}{4}[3-g](1-x) \\
c_1 + \frac{1-g}{2} &= \frac{1}{4}[3-g](1+x) \\
1 + c_1 &= \frac{1}{4}[5+3x+g(1-x)] \\
c_1 + \frac{1+g}{2} &= \frac{1}{4}[3+3x+g(3-x)] \\
c_1 + \frac{g-1}{2} &= \frac{1}{4}[3x-1+g(3-x)] \\
\frac{1+g}{2} - c_1 &= \frac{1}{4}[1-3x+g(1+x)]
\end{aligned}$$

from which we obtain:

$$\rho(f) = \frac{48}{\pi^2}\int_{-1}^{1}\frac{dx}{\sqrt{[1-x^2]}}\frac{1}{\sqrt{[(5+3x+g(1-x))\,(3+3x+g(3-x))]}}$$

$$\times\frac{1}{\sqrt{[(1-3x+g(1+x))\,(3x-1+g(3-x))]}}$$

which, with the singularities removed reduces to:

$$\rho(f) = \frac{48}{\pi}\int_{0}^{1}\frac{dz}{\sqrt{[(5+g+(3-g)\cos\pi z)\,(3+3g+(3-g)\cos\pi z)]}}$$

$$\times\frac{1}{\sqrt{[(1+g+(g-3)\cos\pi z)\,(3g-1+(3-g)\cos\pi z)]}}$$