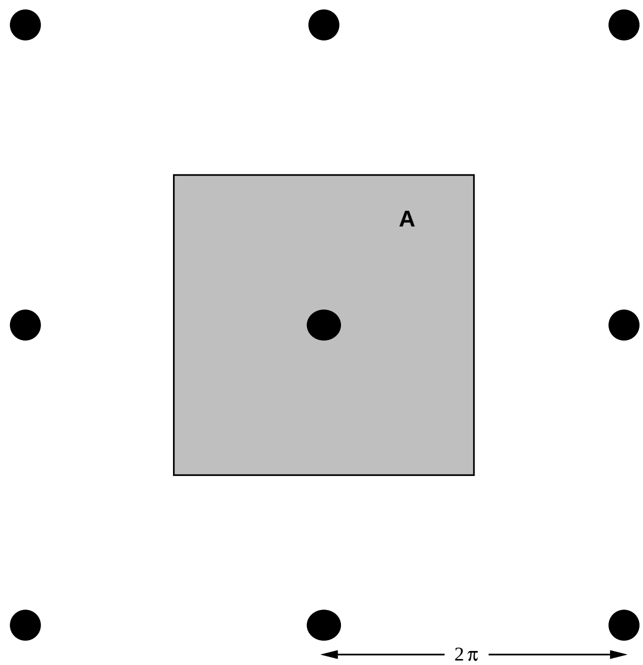
Mathematics 4: Square Density of State

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

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

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, $c_1 = \cos k_1$ and $c_2 = \cos k_2$:

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

where it proves useful in this type of calculation to use $\theta[x]$ functions to define the integration limits. Note that there are four values of $\mathbf{k}$, viz (k_1, k_2), $(k_1, -k_2)$, $(-k_1, k_2)$, $(-k_1, -k_2)$, for each value of (c_1, c_2). Performing the integration over c_2 yields:

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

Employing $c_1 \mapsto -c_1$, we can see that $\rho(-f) = \rho(f)$, and so we may assume that $f > 0$. For this case the limits yield:

$$\rho(f) = \frac{2}{\pi^2} \int_{2f-1}^{1} \frac{dc_1}{\sqrt{[1-c_1^2]}\sqrt{[1-(2f-c_1)^2]}}$$

and we can see that the integral vanishes when $f > 1$. This is a simple example of an *elliptic integral*. The best way to represent this type of integral is to rescale, so that the integration variable ranges over $x \in (-1, 1)$. This is chosen using:

$$c_1 = \alpha + \beta x$$

and $2f - 1 = \alpha - \beta$ together with $1 = \alpha + \beta$. This yields, $\alpha = f$ and $\beta = 1 - f$, and hence:

$$\begin{aligned} c_1 &= f + (1-f)x \\ 1 - c_1 &= (1-f)(1-x) \\ 1 - 2f + c_1 &= (1-f)(1+x) \\ 1 + c_1 &= (1+f) + (1-f)x \\ 1 + 2f - c_1 &= (1+f) - (1-f)x \end{aligned}$$

from which:

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

At this point one might think that the best representation has been achieved, but *numerically* this is not the case. The integrand has *singularities*, in this case square root divergences. These ought to be eradicated before attempting a numerical integration. For the present case this is straightforward. We use $x = \cos \pi y$ from which:

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

where we have used the obvious reflection symmetry to provide the final representation. This is now in a numerically amenable form. Remember that this result is for $f > 0$, that $\rho(-f) = \rho(f)$ and that $\rho(f) = 0$ for $f > 1$.