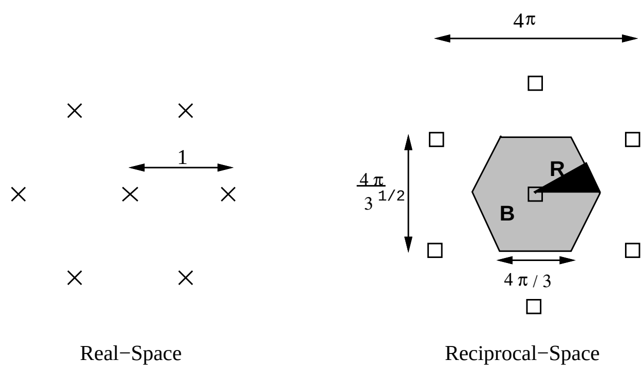
Mathematics 10: The Brillouin Zone

Any Bravais lattice has a so-called *reciprocal lattice*, defined by the requirement that for all $\mathbf{R}$ in the Bravais lattice then $\mathbf{G}$ is in the reciprocal lattice provided that:

$$e^{i\mathbf{G}.\mathbf{R}} = 1$$

The *Brillouin zone* is then the region in reciprocal space closer to the origin than any other reciprocal lattice vector.

Example: The triangular lattice in two-dimensions.
Real-Space: $\mathbf{R} = n_1\hat{\mathbf{x}}_1 + n_2\left[\frac{1}{2}\hat{\mathbf{x}}_1 + \frac{\sqrt{3}}{2}\hat{\mathbf{x}}_2\right]$
Reciprocal-Space: $\mathbf{G} = m_1\frac{4\pi}{3}\left[\frac{1}{2}\hat{\mathbf{x}}_2 + \frac{\sqrt{3}}{2}\hat{\mathbf{x}}_1\right] + m_2\frac{4\pi}{3}\hat{\mathbf{x}}_2$



The Brillouin zone is marked, $\mathbf{B}$. When a system has *point-group symmetry*, one only need calculate in the irreducible zone, which is marked $\mathbf{R}$ and constitutes a twelth of the full zone.

Any three-dimensional band-structure calculation involves finding the 'electron-bands' in an irreducible Brillouin zone.

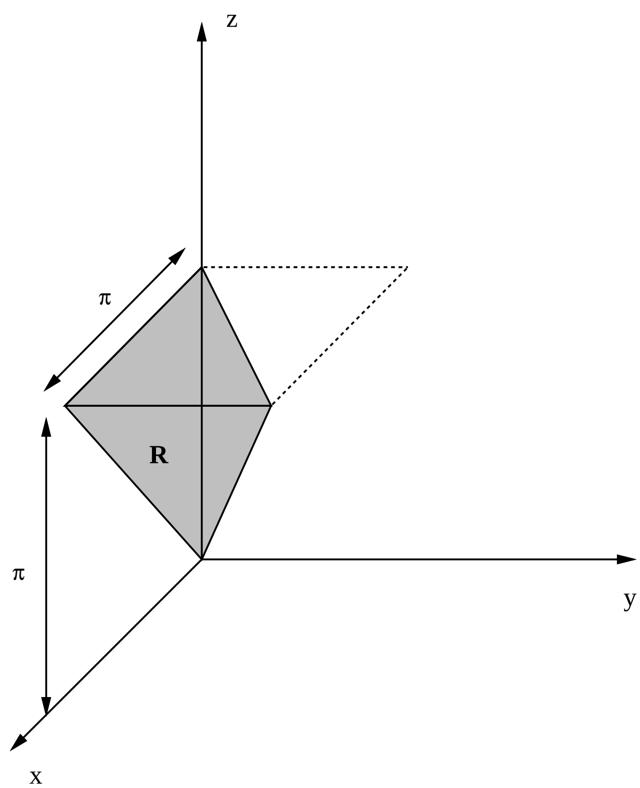
The simplest is:

$$\gamma_{\mathbf{k}} = \frac{1}{Z}\sum_{n.n.} e^{i\mathbf{k}.\mathbf{R}_{n.n.}}$$

where $\mathbf{R}_{n.n.}$ are the nearest-neighbours to the origin, and Z is the number of such neighbours.

(1) Simple Cubic:

Real-Space: $\mathbf{R} = n_1\hat{\mathbf{x}}_1 + n_2\hat{\mathbf{x}}_2 + n_3\hat{\mathbf{x}}_3$
Reciprocal-Space: $\mathbf{G} = 2\pi[m_1\hat{\mathbf{x}}_1 + m_2\hat{\mathbf{x}}_2 + m_3\hat{\mathbf{x}}_3]$

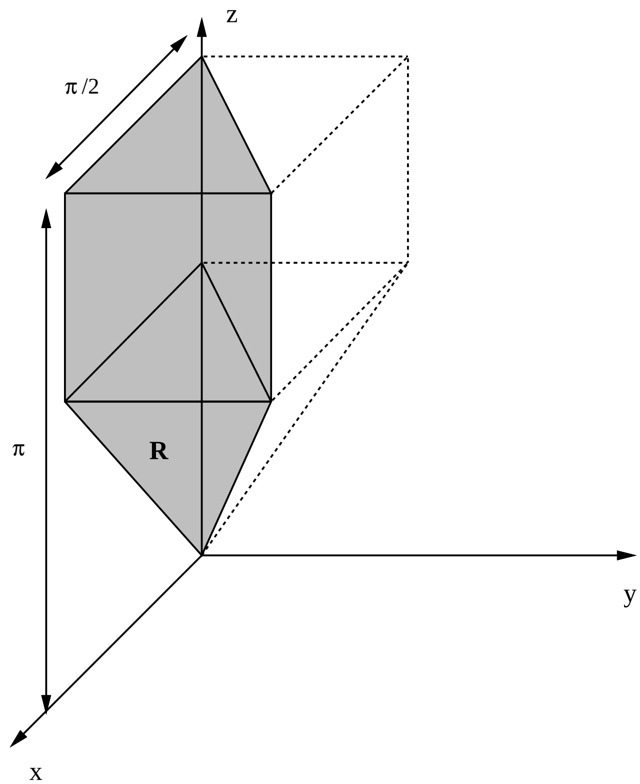


$k_2 < k_1$, $k_3 > k_1$, $k_3 > k_2$, $k_3 \in (0, \pi)$ and the simplest dispersion from one degree of freedom per atom and nearest-neighbour hopping yields:

$$\gamma_{\mathbf{k}} = \frac{1}{3}\left[\cos k_1 + \cos k_2 + \cos k_3\right]$$

(2) Face-centre cubic:

Real-Space: $\mathbf{R} = n_1\hat{\mathbf{x}}_1 + n_2\hat{\mathbf{x}}_2 + n_3\hat{\mathbf{x}}_3$
with $n_1 + n_2 + n_3 = 2i$ is even
Reciprocal-Space: $\mathbf{G} = \pi[m_1\hat{\mathbf{x}}_1 + m_2\hat{\mathbf{x}}_2 + m_3\hat{\mathbf{x}}_3]$
with $m_2 + m_3 = 2i_1$, $m_3 + m_1 = 2i_2$, $m_1 + m_2 = 2i_3$, are all even

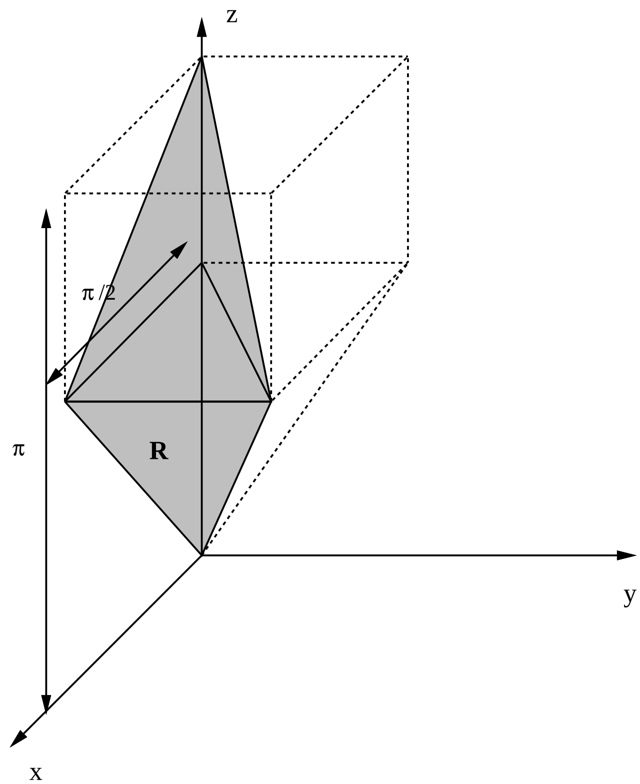


$k_2 < k_1$, $k_1 < \min(k_3, \pi/2)$, $k_2 < \min(k_3, \pi/2)$, $k_3 \in (0, \pi)$ and the simplest dispersion from one degree of freedom per atom and nearest-neighbour hopping yields:

$$\gamma_{\mathbf{k}} = \frac{1}{3}\left[\cos k_2 \cos k_3 + \cos k_3 \cos k_1 + \cos k_1 \cos k_2\right]$$

(3) Body-centre cubic:

Real-Space: $\mathbf{R} = n_1\hat{\mathbf{x}}_1 + n_2\hat{\mathbf{x}}_2 + n_3\hat{\mathbf{x}}_3$
with $n_2 + n_3 = 2i_1$, $n_3 + n_1 = 2i_2$, $n_1 + n_2 = 2i_3$, are all even
Reciprocal-Space: $\mathbf{G} = \pi[m_1\hat{\mathbf{x}}_1 + m_2\hat{\mathbf{x}}_2 + m_3\hat{\mathbf{x}}_3]$
with $m_1 + m_2 + m_3 = 2i$ is even



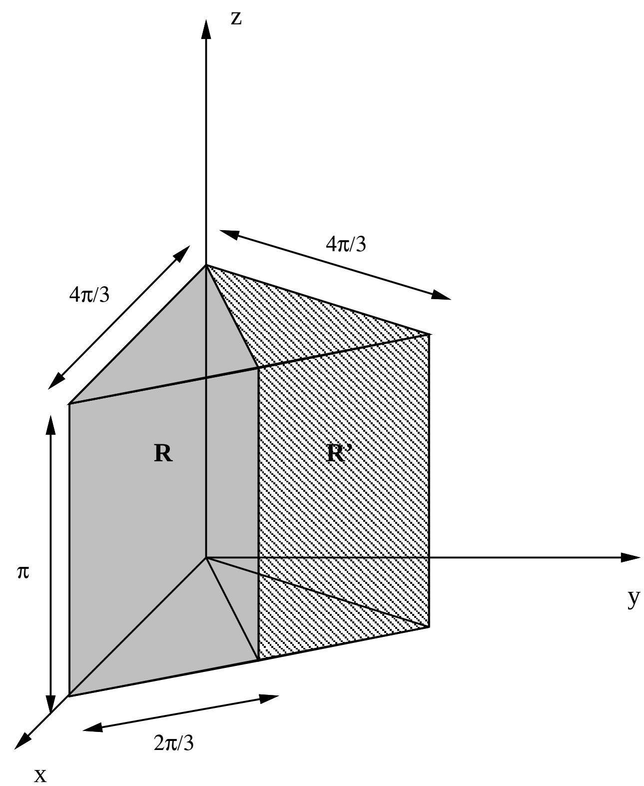
$k_2 < k_1$, $k_1 <\min(k_3, \pi - k_3)$, $k_2 <\min(k_3, \pi - k_3)$, $k_3 \in (0, \pi)$ and the simplest dispersion from one degree of freedom per atom and nearest-neighbour hopping yields:

$$\gamma_{\mathbf{k}} = \cos k_1 \cos k_2 \cos k_3$$

(4) Simple Hexagonal and Hexagonal close-pack:

Real-Space: $\mathbf{R} = n_1 \hat{\mathbf{x}}_1 + n_2 \left[\frac{1}{2}\hat{\mathbf{x}}_1 + \frac{\sqrt{3}}{2}\hat{\mathbf{x}}_2\right] + n_3 \hat{\mathbf{x}}_3$

Reciprocal-Space: $\mathbf{G} = \frac{4\pi}{\sqrt{3}} m_1 \left[\frac{\sqrt{3}}{2}\hat{\mathbf{x}}_1 + \frac{1}{2}\hat{\mathbf{x}}_2\right] + \frac{4\pi}{\sqrt{3}} m_2 \hat{\mathbf{x}}_2 + 2\pi m_3 \hat{\mathbf{x}}_3$



It may be best to use $R \cup R'$ and a triangular grid. $k_2 > 0$, $k_2 < \frac{k_1}{\sqrt{3}}$, $k_2 < \frac{4\pi}{\sqrt{3}} - \sqrt{3}k_1$, $k_1 \in (0, 4\pi/3)$ $k_3 \in (0, \pi)$ and the simplest dispersion from one degree of freedom per atom and nearest-neighbour hopping yields:

$$\gamma_{\mathbf{k}\pm} = \frac{\gamma_{\mathbf{k}}^T}{2} \pm \frac{\sqrt{[1 + 2\gamma_{\mathbf{k}}^T]}}{2\sqrt{3}} \cos\frac{k_3}{2}$$

in terms of the triangular lattice structure-factor:

$$\gamma_{\mathbf{k}}^T = \frac{1}{3}\left[2\cos\frac{k_1}{2}\left[\cos\frac{k_1}{2} + \cos\frac{\sqrt{3}k_2}{2}\right] - 1\right]$$