5.7: A Model Graphene Diffraction Pattern

The purpose of this tutorial is to model graphene as seven fused benzene rings (see below) and use a Fourier transform of the atomic positions to calculate its diffraction pattern.

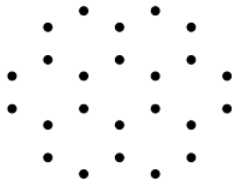
Number of atoms:	$A = 24$	Atomic dimension:	$d = .25$	Atomic positions:	
$x_1 = 0$	$y_1 = 1.386$	$x_2 = 0$	$y_2 = -1.386$	$x_{15} = 0$	$y_{15} = 2.772$
$x_3 = -1.2$	$y_3 = 0.693$	$x_4 = 1.2$	$y_4 = 0.693$	$x_{16} = 1.2$	$y_{16} = 3.465$
$x_5 = 1.2$	$y_5 = -0.693$	$x_6 = -1.2$	$y_6 = -0.693$	$x_{17} = 2.4$	$y_{17} 2.772$
$x_7 = 2.4$	$y_7 = 1.386$	$x_8 = 3.6$	$y_8 = 0.693$	$x_{18} = 0$	$y_{18} = -2.772$
$x_9 = 3.6$	$y_9 = -0.693$	$x_{10} = 2.4$	$y_{10} = -1.386$	$x_{19} = 1.2$	$y_{19} = -3.465$
$x_{11} = -2.4$	$y_{11} = 1.368$	$x_{12} = -3.6$	$y_{12} = 0.693$	$x_{20} = 2.4$	$y_{20} = -2.772$
$x_{13} = -3.6$	$y_{13} = -0.693$	$x_{14} = -2.4$	$y_{14} = -1.386$	$x_{21} = -2.4$	$y_{21} = 2.772$
$x_{22} = -1.2$	$y_{22} = 3.465$	$x_{23} = -2.4$	$y_{23} = -2.772$	$x_{24} = -1.2$	$y_{24} = -3.465$

The diffraction pattern is the Fourier transform of the atomic positions into momentum space.

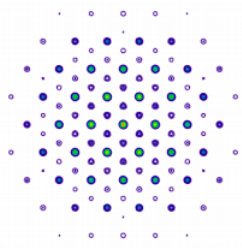
$$\Delta = 20 \quad N = 200 \quad j = 0..N \quad px_j = -\Delta + \frac{2\Delta j}{N} \quad k = 0..N \quad py_k = -\Delta + \frac{2\Delta k}{N}$$

$$\Psi(p_x,\, p_y) = \sum_{m=1}^{A} \left(\int_{x_m - \frac{d}{2}}^{x_m + \frac{d}{2}} exp(-ip_x x)dx \int_{y_m - \frac{d}{2}}^{y_m + \frac{d}{2}} exp(-ip_y y)dx \right) \quad p_{j,\,k} = \left(|\Psi(px_j,\, py_j)|\right)^2$$

$i = 1..A$



Graphene Model



Diffraction Pattern

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