A Model Graphene Diffraction Pattern

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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:

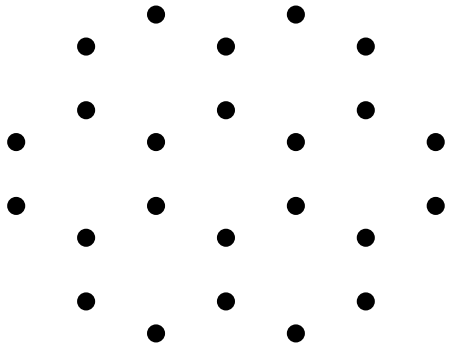
$x_1 := 0$	$y_1 := 1.386$	$x_2 := 0$	$y_2 := -1.386$	$x_{15} := 0$	$y_{15} := 2.772$
$x_3 := -1.2$	$y_3 := .693$	$x_4 := 1.2$	$y_4 := .693$	$x_{16} := 1.2$	$y_{16} := 3.465$
$x_5 := 1.2$	$y_5 := -.693$	$x_6 := -1.2$	$y_6 := -.693$	$x_{17} := 2.4$	$y_{17} := 2.772$
$x_7 := 2.4$	$y_7 := 1.386$	$x_8 := 3.6$	$y_8 := .693$	$x_{18} := 0$	$y_{18} := -2.772$
$x_9 := 3.6$	$y_9 := -.693$	$x_{10} := 2.4$	$y_{10} := -1.386$	$x_{19} := 1.2$	$y_{19} := -3.465$
$x_{11} := -2.4$	$y_{11} := 1.386$	$x_{12} := -3.6$	$y_{12} := .693$	$x_{20} := 2.4$	$y_{20} := -2.772$
$x_{13} := -3.6$	$y_{13} := -.693$	$x_{14} := -2.4$	$y_{14} := -1.386$	$x_{21} := -2.4$	$y_{21} := 2.772$
$x_{22} := -1.2$	$y_{22} := 3.465$	$x_{23} := -2.4$	$y_{23} := -2.772$	$x_{24} := -1.2$	$y_{24} := -3.465$

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

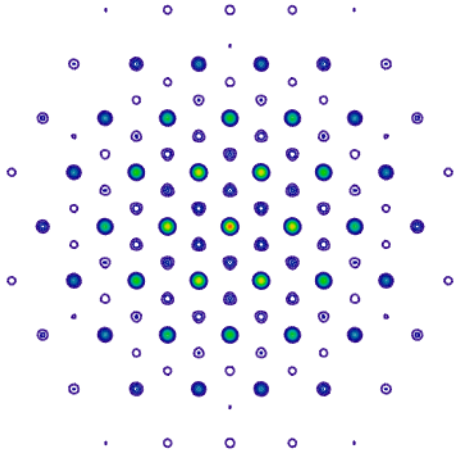
$\Delta := 20$ $N := 200$ $j := 0 .. N$ $p_{x_j} := -\Delta + \frac{2 \cdot \Delta \cdot j}{N}$ $k := 0 .. N$ $p_{y_k} := -\Delta + \frac{2 \cdot \Delta \cdot k}{N}$

$$\Psi(p_x, p_y) := \sum_{m=1}^{A} \left(\int_{x_m - \frac{d}{2}}^{x_m + \frac{d}{2}} \exp(-i \cdot p_x \cdot x)\, dx \cdot \int_{y_m - \frac{d}{2}}^{y_m + \frac{d}{2}} \exp(-i \cdot p_y \cdot y)\, dy \right) \qquad P_{j,k} := \left(\left| \Psi(p_{x_j}, p_{y_k}) \right| \right)^2$$

$i := 1 .. A$



Graphene Model



Diffraction Pattern