5.14: Model Diffraction Pattern for Napthalene

Ten holes in a two-dimensional mask are used to model the diffraction pattern for napthalene. It is assumed that only the carbon atoms scatter radiation.

Establish mask geometry:

$$R = 2 \quad m = 1..6 \quad \Theta_m = \frac{2\pi m}{6} \quad x_m = R\sin(\Theta_m) - \sqrt{3} \quad y_m = R\cos(\Theta_m)$$

$$m = 7..10 \quad \Theta_m = \frac{2\pi(m-0.5)}{6} \quad x_m = R\sin(\Theta_m) + \sqrt{3} \quad y_m = R\cos(\Theta_m - \frac{\pi}{\sqrt{3}})$$
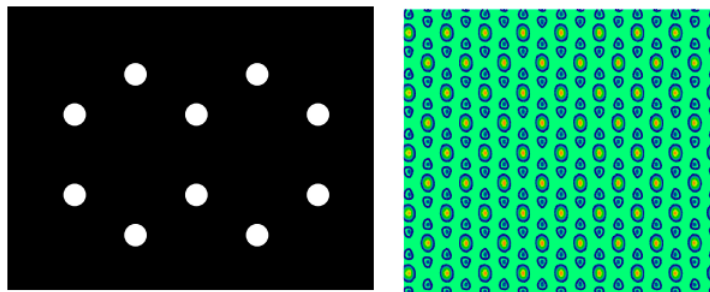
Fourier transform of position wave function (mask geometry) into the momentum representation. Initially the carbon atoms are considered to be point scatterers.

$$m = 1..10 \quad \Phi(p_x,\ p_y) = \frac{1}{2\pi d\sqrt{10}} \left[\sum_{m=1} \left(\int_{x_m-\frac{d}{2}}^{x_m+\frac{d}{2}} exp(-ip_x x)dx \int_{y_m-\frac{d}{2}}^{y_m+\frac{d}{2}} exp(-ip_y y)dy \right) \right]$$

Display mask geometry and diffraction pattern:

$$N = 100 \quad \Delta p = 15 \quad j = 0..N \quad k = 0..N \quad px_j = -\Delta + \frac{2\Delta pj}{N} \quad py_k = -\Delta p + \frac{2\Delta pk}{N}$$

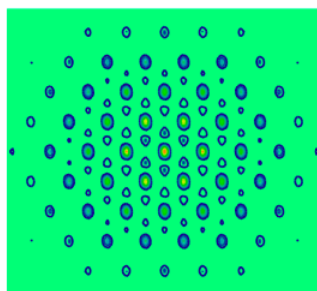$$\text{Diffraction pattern}_{j,\ k} = (|\Phi(px_j,\ py_k)|)^2$$

This calculation illustrates the uncertainty principle. There is no attenuation in the diffraction pattern (momentum distribution) because there is no uncertainty in the carbon atom positions.

Now the diffraction pattern is recalculated assuming an arbitrary finite dimension for the carbon atoms.

$$r = .15 \quad \Phi(p_x,\ p_y) = \frac{1}{2\pi d\sqrt{10}} \left[\sum_{m=1} \left(\int_{x_m-r}^{x_m+r} exp(-ip_x x)dx \int_{y_m-r}^{y_m+r} exp(-ip_y y)dy \right) \right]$$

$$\text{Diffraction pattern}_{j,\ k} = (|\Phi(px_j,\ py_k)|)^2$$

There is attenuation in the momentum distribution (less uncertainty) because there is more uncertainty in the carbon atom positions.