Modeling the Diffraction Pattern of Solid C_{60}

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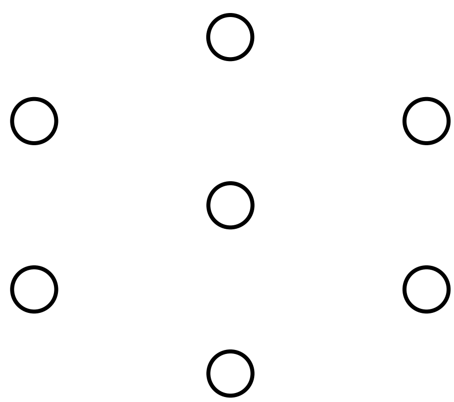
In this tutorial a model diffraction pattern for C_{60} is calculated and compared with the experimental diffraction pattern.

Solid C_{60} has the cubic close-packed crystal structure. For the sake of computational convenience this structure will be modeled as a planar close-packed array consisting of seven C_{60} molecules represented by squares (see the mask geometry shown below). According to quantum mechanical principles, radiat illuminating this geometrical arrangement interacts with all its members simultaneously thus being cas the spatial superposition, Ψ, given below. This spatial wave function is then projected into momentum space by a Fourier transform. Therefore what is measured at the detector can be interpreted as the two-dimensional momentum distribution created by the spatial localization that occurrs at the mask up illumination.

Create mask geometry: $A := 6$ $R := 1.4$ $m := 1..A$ $\Theta_m := \frac{2\cdot\pi\cdot m}{A}$

$x_m := R\cdot\sin(\Theta_m)$ $y_m := R\cdot\cos(\Theta_m)$ $x_7 := 0$ $y_7 := 0$ Molecule size: $d := .3$

Display coordinate wave function (mask geometry): $m := 1..7$



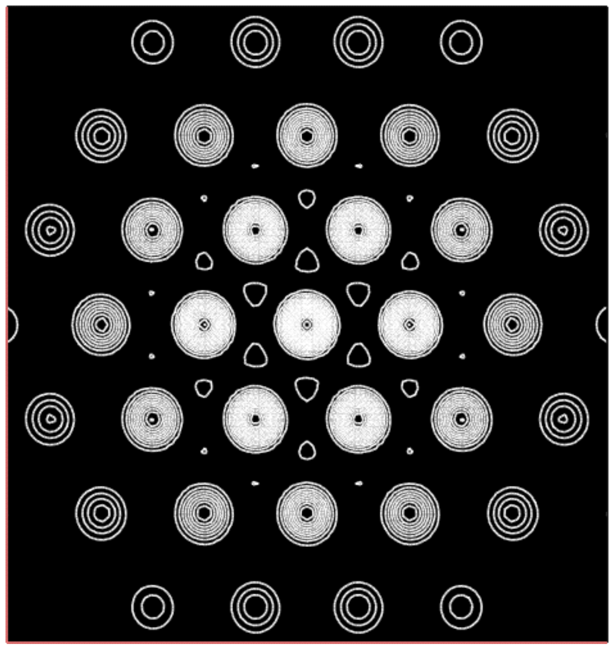
Fourier transform the coordinate wave function into the momentum representation:

$$\Phi(p_x, p_y) := \sum_{m=1}^{A+1} \int_{x_m-\frac{d}{2}}^{x_m+\frac{d}{2}} \exp(-i\cdot p_x\cdot x)\,dx\cdot \int_{y_m-\frac{d}{2}}^{y_m+\frac{d}{2}} \exp(-i\cdot p_y\cdot y)\,dy$$

Display diffraction pattern:

$\Delta := 15 \qquad N := 100 \qquad j := 0..N \qquad px_j := -\Delta + \frac{2 \cdot \Delta \cdot j}{N} \qquad k := 0..N \qquad py_k := -\Delta + \frac{2 \cdot \Delta \cdot k}{N}$

$$\mathrm{DiffractionPattern}_{j,k} := \left(\left|\Phi\left(px_j, py_k\right)\right|\right)^2$$



DiffractionPattern

The calculated diffraction pattern above compares favorably with the experimental diffraction pattern shown below, indicating that the simple planar model proposed for C_{60} captures the essential element the actual solid structure. See page 154 of *Perfect Symmetry* by Jim Baggot for further information.