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NOTE

Calculating diffraction patterns

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Abstract

Following Marcella's approach to the double-slit experiment (Marcella T V 2002 *Eur. J. Phys.* **23** 615–21), diffraction patterns for two-dimensional masks are calculated by Fourier transform of the Mask geometry into momentum space.

I wish to describe a simple extension of Marcella's [1] recent analysis of the double-slit experiment to two dimensions.

The essential point Marcella makes in his unique treatment of this well-known experiment is that the diffraction pattern at the detection screen is actually a measurement of the momentum distribution of the diffracted particles. Therefore the calculated diffraction pattern is simply obtained from the Fourier transform of the coordinate space wavefunction (the double-slit geometry) into momentum space. Marcella considered two spatial models: (model 1) infinitesimally thin slits represented by Dirac delta functions; and (model 2) slits of finite width.

About 60 years ago Sir Lawrence Bragg [2] proposed the optical transform as an aid in the interpretation of the x-ray diffraction patterns of crystals. This required the fabrication of two-dimensional masks of various crystal or molecular geometries and the generation of the diffraction pattern using visible electromagnetic radiation. Present-day laser technology has made the generation of such diffraction patterns routine, even in the classroom.

In addition, Marcella's computational approach makes calculating the diffraction patterns conceptually and mathematically straightforward. If one considers the mask as consisting of point scatterers (model 1), the coordinate space wavefunction is a linear superposition of the scattering positions:

$$|\Psi\rangle = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}|x_i, y_i\rangle \tag{1}$$

where N is the number of point scatterers.

The Fourier transform into the momentum representation yields

$$\langle p|\Psi\rangle = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\langle p_x|x_i\rangle\langle p_y|y_i\rangle = \frac{1}{2\pi\hbar}\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\exp\left[-\frac{i}{\hbar}(p_x x_i + p_y y_i)\right]. \tag{2}$$

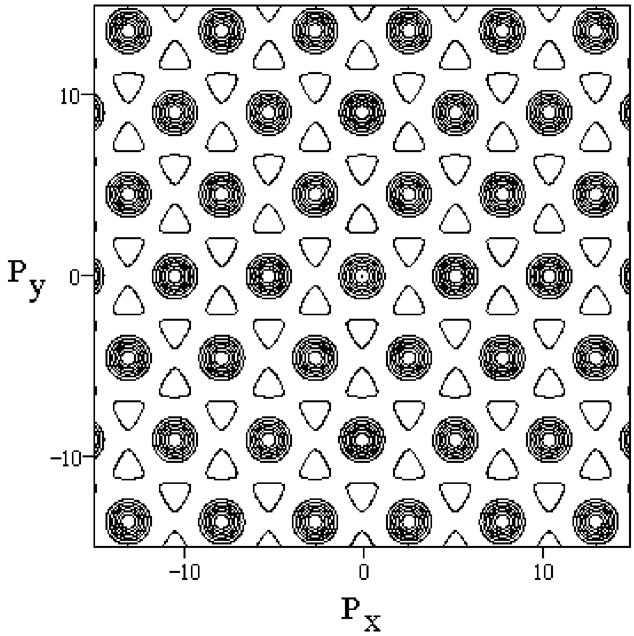

Figure 1. The diffraction pattern for a hexagonal arrangement of six point scatterers.

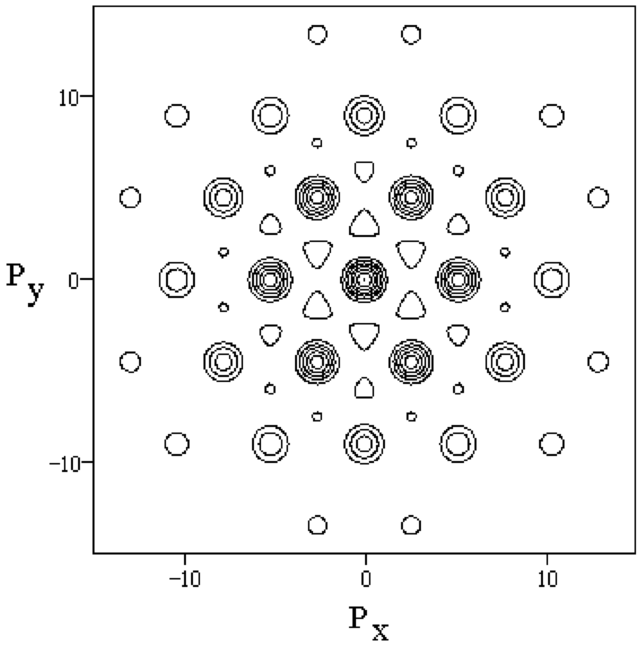

Figure 2. The diffraction pattern for a hexagonal arrangement of six finite scatterers.

For model 2, which assumes finite-sized scatterers, equation (2) becomes

$$\langle p|\Psi\rangle = \frac{1}{2\pi\hbar r\sqrt{N}} \sum_{i=1}^{N} \int_{x_i - r/2}^{x_i + r/2} \exp\left[-\frac{\mathrm{i} p_x x}{\hbar}\right] \mathrm{d}x \int_{y_i - r/2}^{y_i + r/2} \exp\left[-\frac{\mathrm{i} p_y y}{\hbar}\right] \mathrm{d}y \tag{3}$$

where r is the spatial dimension of the scatterers. In the interests of mathematical simplicity, the scatterers are assumed to be small squares rather than circles.

Figure 1 shows the diffraction pattern, $|\langle p|\Psi\rangle|^2$, for a hexagonal arrangement of six point scatterers calculated using equation (2), while figure 2 shows the pattern obtained with equation (3) for six finite hexagonal scatterers. The calculated diffraction pattern shown in figure 2 is in excellent agreement with the experimental diffraction patterns available in the literature [3].

The calculations [4] of the diffraction patterns were carried out in atomic units ($h = 2\pi$), so positions are given in a_0 and momenta in a_0^{-1}. The distance between adjacent scatters is 1.4 a_0 and their spatial dimension is 0.30 a_0 on a side.

In addition to showing the interference effects accompanying scattering from multiple positions, the figures also illustrate the uncertainty principle. Figure 1 shows no attenuation of the diffraction pattern at extreme values of momentum because the point scatterers sharply localize the particle being scattered in coordinate space, leading to a delocalized momentum distribution as required by the position–momentum uncertainty relation. By comparison the finite scatterers of figure (2) lead to some uncertainty in position and, therefore, less uncertainty in momentum. Therefore the diffraction pattern is attenuated at large values for both the x- and y-momentum components.

References

[1] Marcella T V 2002 *Eur. J. Phys.* **23** 615–21
[2] Bragg L 1944 *Nature* **154** 69–72
[3] Harburn G, Taylor C A and Welberry T R 1975 *Atlas of Optical Transforms* (Ithaca, NY: Cornell University Press) plates 4 and 5
[4] The Mathcad 5.0 files used to generate figures 1 and 2 are available for download at http://www.users.csbsju.edu/frioux/diffraction/hex-point.mcd and ~/hex-finite.mcd.