Single-Slit Diffraction and the Uncertainty Principle

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Muiño has used single-slit diffraction to provide an introduction to the uncertainty principle suitable for an undergraduate physical chemistry course *(1)*. His article provided both a theoretical analysis of single-slit diffraction and a lecture demonstration of the phenomenon using readily-available equipment. In the current research literature Nairz and colleagues have confirmed the uncertainty principle in a single-slit diffraction experiment with a beam of C_{70} molecules *(2)*. And, quite recently, a research team led by Marcus Arndt and Anton Zeilinger performed multi-slit experiments demonstrating wave-particle behavior for tetraphenylporphyrin and a fluorinated fullerene, $C_{60}F_{48}$ *(3)*. The significance of these results is that tetraphenylporphyrin is an important biomolecule and $C_{60}F_{48}$ is the most massive particle to demonstrate wavelike properties to date.

The purpose of this short article is to provide an alternative theoretical analysis of single-slit diffraction based on the Fourier transform between coordinate and momentum space. This approach was recently used by Marcella *(4)* to analyze single- and double-slit diffraction and has been extended by the author to more complicated slit geometries *(5)*.

Quantum experiments have three parts: (i) state preparation; (ii) subsequent measurement of an observable; and (iii) theoretical interpretation of experimental results. In diffraction experiments, passage through the slit screen represents a position measurement that establishes the state of the system in coordinate space. The coordinate-space wave function for a photon or massive particle that has passed a screen with a slit of width w centered at $x = 0$ is

$$\Psi(x,w) = \begin{cases} 0 & \text{for} \quad x < -\dfrac{w}{2} \\ \dfrac{1}{\sqrt{w}} & \text{for} \quad -\dfrac{w}{2} \le x \le \dfrac{w}{2} \\ 0 & \text{for} \quad x > \dfrac{w}{2} \end{cases} \tag{1}$$

The quantum mechanical interpretation of diffraction is that the physical property recorded at the detection screen is the momentum distribution of the diffracted particle.

A Fourier transform of $\Psi(x, w)$ into the momentum representation yields the momentum-space wave function

$$\Phi(p_x, w) = \int_{-\frac{w}{2}}^{\frac{w}{2}} \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-\frac{ip_x x}{\hbar}\right) \frac{1}{\sqrt{w}}\, dx$$

$$= \sqrt{\frac{2\hbar}{\pi w}}\, \frac{\sin\left(\dfrac{p_x w}{2\hbar}\right)}{p_x} \tag{2}$$

where p_x is the x-direction momentum. Thus, according to quantum mechanics, the diffraction pattern observed is the square of the absolute magnitude of the momentum wave function, $|\Phi(p_x, w)|^2$. This is shown in Figure 1 for two slit widths.

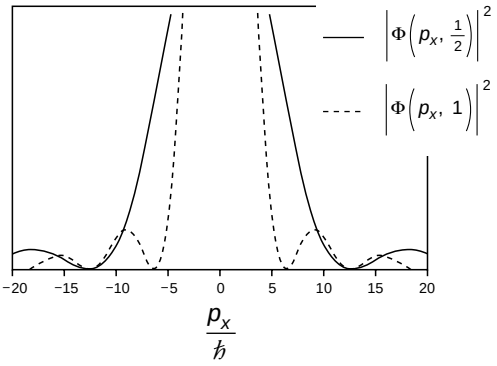

Figure 1. Momentum distribution at the slit screen for slit widths of 0.5 and 1.0 a_0 (1 a_0 = 52.9 pm).

The uncertainty principle is clearly revealed—the narrow slit produces a broader momentum distribution. In other words, localization in coordinate space leads to delocalization in momentum space. However, we can also treat this effect in a more quantitative manner.

Following Muiño we will assume that the uncertainty in position is the slit width, w. The uncertainty in momentum is defined as half the width of the momentum distribution of the central diffraction band *(2)*. As the momentum distribution is zero for

$$\frac{p_x w}{2\hbar} = \pm n\pi \tag{3}$$

it is easy to show that using this criterion the uncertainty in momentum is $2\pi\hbar/w$. Therefore, the product of the uncertainty in position and momentum is greater than $\hbar/2$ as required by the uncertainty principle.

$$\Delta x\, \Delta p_x = w\frac{2\pi\hbar}{w} = 2\pi\hbar \tag{4}$$

The Fourier transform connecting complementary observables is ubiquitous in quantum theory (and, of course, in our laboratory instruments). Here the transform between position and momentum has been used to illuminate the intimate relationship between single-slit diffraction and the uncertainty principle.

Literature Cited

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