

## Quantum Mechanics and the Fourier Transform Frank Rioux

Wave-particle duality as expressed by the de Broglie wave equation

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

is the seminal concept of quantum mechanics. On the left side we have the wave property, wavelength, and on the right in a reciprocal relationship mediated by the ubiquitous Planck's constant, we have the particle property, momentum.

Wave and particle are physically incompatible concepts because waves are spatially delocalized, while particles are spatially localized. In spite of this incongruity we find in quantum theory that they are necessary companions in the analysis of atomic and molecular phenomena. Both concepts are required for a complete examination of experiments at the nanoscale level.

This view can be summarized by saying that in quantum-level experiments we always detect particles, but we predict or interpret the experimental outcome by assuming wave-like behavior prior to particle detection. As Bragg once said, "Everything in the future is a wave, everything in the past is a particle." It has also been said that between release and detection particles behave like waves.

Wave-particle duality, a strange dichotomous co-dependency, was first recognized as a permanent feature of modern nanoscience when Niels Bohr proclaimed the complementarity principle as the corner stone of the Copenhagen interpretation of quantum theory. This scientific dogma states, among other things, that there will be no future resolution of the cognitive dissonance that results from analyses that require, at root level, the use of irreconcilable concepts such as wave and particle.

In what follows it will be shown that wave-particle duality leads naturally to other conjugate relationships between traditional physical variables such as position and momentum, and energy and time. The vehicle for this extension will turn out to be the Fourier transform.

To reason mathematically about wave behavior requires a wave function. The one-dimensional, time-independent plane wave expression for a free particle is suitable for this purpose.

$$\exp\left(i2\pi \frac{x}{\lambda}\right)$$

We see that this expression contains the basics of wave-particle duality;  $x$  represents position, a particle characteristic, and  $\lambda$  represents wave behavior. Substitution of the de

Broglie equation for  $\lambda$  yields one of the most important mathematical functions in quantum mechanics.

$$\exp\left(\frac{ipx}{\hbar}\right)$$

By convention this function is called the momentum eigenfunction in the coordinate representation. We express this in Dirac notation as follows (the normalization constant is ignored for the time being).

$$\langle x|p\rangle = \exp\left(\frac{ipx}{\hbar}\right)$$

Its complex conjugate is the position eigenfunction in the momentum representation.

$$\langle p|x\rangle = \langle x|p\rangle^* = \exp\left(\frac{-ipx}{\hbar}\right)$$

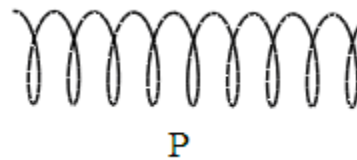
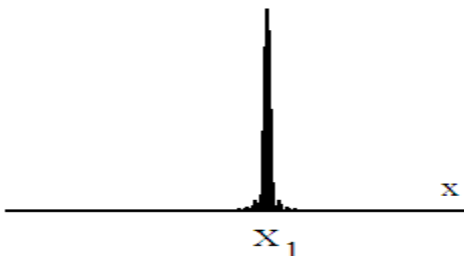
Both expressions are also simple examples of Fourier transforms. They are dictionaries for translating between two different languages or representations. A rudimentary graphical illustration of this ability to translate also provides a concise illustration of the uncertainty principle. (See *The Emperor's New Mind*, by Roger Penrose, page 246.)

A quon ("A quon is any entity, no matter how immense, that exhibits both wave and particle aspects in the peculiar quantum manner." *Quantum Reality* by Nick Herbert page 64.) with a precise position is represented by a Dirac delta function in coordinate space and a helix in momentum space. If the position is known exactly, the momentum is completely unknown because  $|\langle p|x_1\rangle|^2$  is a constant for all values of the momentum. All momentum values have the same probability of being observed.

A quon has position  $x_1$ :  $|x_1\rangle$

Coordinate space  $\Leftrightarrow$  Momentum space

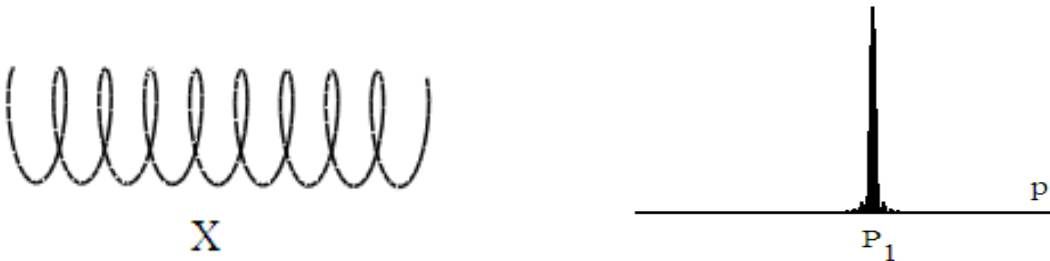
$$\langle x|x_1\rangle = \delta(x - x_1) \qquad \langle p|x_1\rangle = \exp\left(-\frac{ipx_1}{\hbar}\right)$$



Conversely, a quon with a precise momentum is represented a helix in coordinate space and by a Dirac delta function in momentum space. If the momentum is known exactly, the position is completely unknown because  $|\langle x | p_1 \rangle|^2$  is a constant for all values of the position. All position values have the same probability of being observed.

A quon has momentum  $p_1$ :  $|p_1\rangle$

$$\begin{array}{ccc} \text{Coordinate space} & \Leftrightarrow & \text{Momentum space} \\ \langle x | p_1 \rangle = \exp\left(\frac{ip_1 x}{\hbar}\right) & & \langle p | p_1 \rangle = \delta(p - p_1) \end{array}$$



These rudimentary examples of the use of the Fourier transform in quantum mechanics involve infinitesimal points in coordinate and momentum space. To employ the Fourier transform for objects of finite dimensions requires integration over the spatial or momentum dimensions.

For example, suppose we ask what the pattern of diffracted light on a distant screen would look like if a light source illuminated a mask with a single small circular aperture. This, of course, yields the well-known Airy diffraction pattern, which is nothing more than the Fourier transform of the coordinate wave function (the circular aperture) into momentum space. The Airy pattern calculation is given in the following link, along with illustrations of how the radius of the hole illustrates the uncertainty principle.

<http://www.users.csbsju.edu/~frioux/diffraction/airy.pdf>

Thomas Young used the double-slit experiment to establish the wave nature of light. Richard Feynman used it to demonstrate the superposition principle as the paradigm of all quantum mechanical phenomena, illustrating wave-particle duality as stated above: between release and detection quons behave as waves.

However, just as with the circular aperture (Airy pattern) a single slit also yields a diffraction pattern when illuminated. Both are examples of the superposition principle because the photons that arrive at the detection screen can get there from any point within

the aperture or slit. So, in general, we calculate the diffraction pattern by a Fourier transform of the coordinate space geometry, slit or circle or something more complicated.

The following link explores single-slit diffraction and the uncertainty principle.

<http://www.users.csbsju.edu/~frioux/diffraction/1slit.pdf>

The next link shows how the methods used to examine these relatively simple cases can be expanded to more interesting geometries, including the DNA double helix.

<http://www.users.csbsju.edu/~frioux/diffraction/910012fr.pdf>

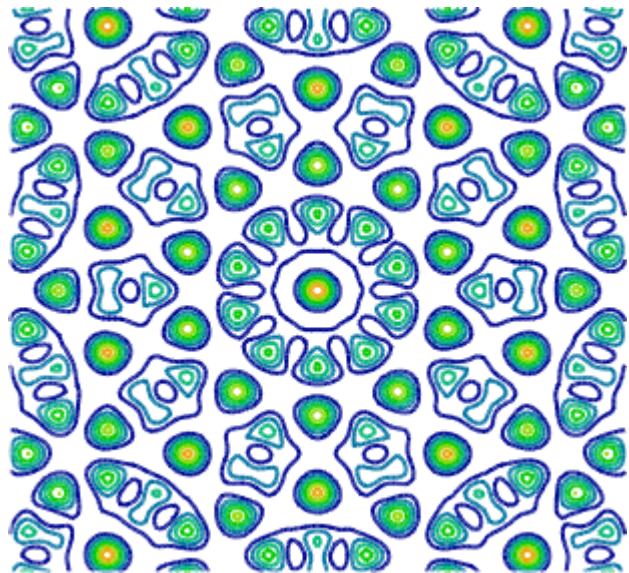
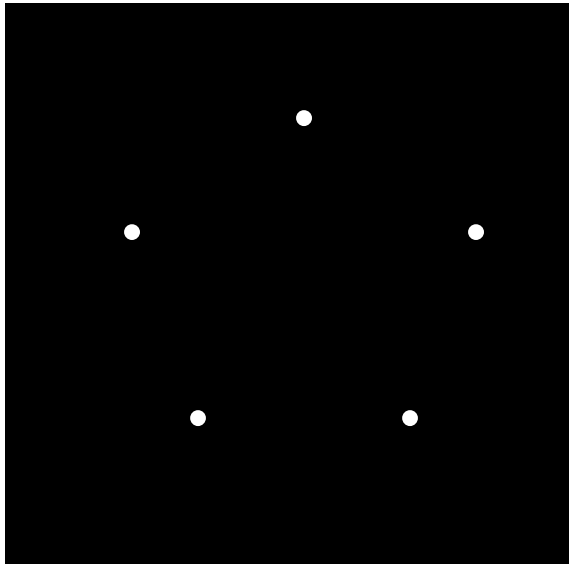
The following link provides details regarding a simple simulation of the DNA diffraction pattern.

<http://www.users.csbsju.edu/~frioux/diffraction/dna.pdf>

A brief discussion of the impact of rotational symmetry in determining diffraction patterns and the concept of the quasi-crystal can be found at the following link.

<http://www.users.csbsju.edu/~frioux/diffraction/crystal-rot.pdf>

The striking diffraction pattern created by a pentagon of point scatterers is shown below.



In these recent examples we have been Fourier transforming from coordinate space to momentum space because the momentum distribution function is the diffraction pattern, and our experiments are set up in coordinate space. In quantum mechanics an experiment requires two steps: state preparation followed by a measurement. State preparation occurs

at the slit screen and measurement at the detection screen. The following link shows how to go from the coordinate representation to the momentum representation and back again.

<http://www.users.csbsju.edu/~frioux/q-intro/1slit-uncertainty.pdf>

Quantum chemists work almost exclusively in coordinate space because they need wave functions that will help them understand molecular structure and chemical reactivity. They need the location of the nuclear centers and electron density maps. Consequently undergraduate physical chemistry texts examine all the traditional model problems (particle in a box, rigid rotor, harmonic oscillator, hydrogen atom, hydrogen molecule ion, hydrogen molecule, etc.) using spatial wave functions. Students learn how to interpret graphical representations of the various wave functions. If knowledge is required about electron momentum, for example, expectation values are calculated using the coordinate wave function.

For the model systems listed above, it is a simple matter to carry out a Fourier transform into momentum space. This allows the same kind of visualization in momentum space that is available in the coordinate representation. The value of this capability in presenting a graphical illustration of the uncertainty principle for the particle-in-the-box (PIB) problem is illustrated in the following link.

<http://www.users.csbsju.edu/~frioux/sho/heisenberg.pdf>

We use the particle-in-the-box example to introduce students to almost all of the fundamental quantum mechanical concepts. When we come to spectroscopy and the chemical bond, we initially model the chemical bond as a harmonic oscillator. Here there are two physical parameters, force constant and effective mass. The following link shows how the coordinate and momentum wave functions can be used to illustrate the uncertainty principle for various values of  $k$  and  $\mu$ .

<http://www.users.csbsju.edu/~frioux/sho/Uncertainty-SHO.pdf>

It is easy to derive the angular position, angular momentum uncertainty relationship for a particle on a ring using the position-momentum uncertainty equation and the classical definition of angular momentum. Visualization is provided by the next link.

<http://www.users.csbsju.edu/~frioux/sho/AngularUncertaintyPrinciple.pdf>

Moving on to the hydrogen atom, we can use the spatial and momentum wave functions for the 1s, 2s and 3s energy states to again illustrate visually the uncertainty principle.

<http://www.users.csbsju.edu/~frioux/sho/MomentumHatom.pdf>

In addition to the coordinate and momentum representation, there is also the phase space approach to quantum mechanics, which physicist in particular find useful. It combines the coordinate and momentum approaches and requires a phase-space distribution function

such as the Wigner function. The following tutorial illustrates the computational consistency of the three approaches to quantum mechanics.

<http://www.users.csbsju.edu/~frioux/wigner/CoordMomPhase.pdf>

Two related tutorials dealing with quantum mechanical tunneling and the repackaging of quantum weirdness are also available.

<http://www.users.csbsju.edu/~frioux/wigner/Tunneling.pdf>

<http://www.users.csbsju.edu/~frioux/wigner/PhaseSpaceQM.pdf>

Finally, I would like to point out that the elementary Fourier transforms that we started with,  $\langle x | p \rangle$  and  $\langle p | x \rangle$ , can also be used to derive the mathematical form of quantum mechanical operators. This is shown in some detail in *An Approach to Quantum Mechanics*.

<http://www.users.csbsju.edu/~frioux/q-intro/INTRO-QM-DIRAC.pdf>