Matter Wave Diffraction: The Beginnings of Quantum Theory

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The early twentieth century gave rise to the idea of quantized energy governing the behavior of radiation. This along with the exciting new theory of mass-energy equivalence led some physicists to question whether matter might also derive characteristic behaviors from quantized energy. This paper follows some of the earliest evidence that led to the birth of a more complete Quantum Mechanical Theory.

Early hints of Quantum Theory began in 1905 when Einstein proposed that photons carry a characteristic "quanta" of energy related to their frequency. This idea stems from his Photoelectric Effect Theory published in that same year. Einstein's bold statement was that photons can only be absorbed or produced entirely, hence the energy and wavelength of radiation are quantized. Other physicists like Max Planck had considered quantization mathematically, but Einstein was the first to accept quantization as a fundamental component of reality.

Once the idea of quantized energy entered the subject, physicists began to rewrite classical theory to encompass new experimental evidence, and the theory of quantized radiation was extremely successful in its predictions. The photon model was not without its own quirks, however. The model requires a photon to be a traveling yet localized phenomenon, part wave part particle. Though at first skeptical, the theorists began to accept that radiation was somehow both a wave and particle-like phenomenon. But there is far more to the universe than just radiation.

In 1924, Louis de Broglie boldly proposed that *matter* is also characterized by a quantized wavelength [1]. Many experimentalists began testing this new theory, which would eventually win de Broglie his Nobel Prize in 1929. In 1927, G. P. Thompson confirmed the de Broglie relationship by diffracting high-energy electrons. This experiment was one of the first examples of a matter particle being observed to diffract like a wave. Just like radiation, matter has wave-particle duality. Thompson's method produces a beautiful ring diffraction pattern with very sharp clarity [2]. This paper outlines the method of the G. P. Thompson experiment, its conformation of de Broglie's theory, and the implications of the experiment's results.

G.P Thompson's experiment is by no means a localized event, at least in a historical context that is. The lead-up to the experiment begins with Einstein. Not long after publishing, Einstein used his photon theory combined with Planck's law of black-body radiation to show that photons have momentum [2]:

$$p = E/c \tag{1}$$

Using this fact along with Einstein's original proposed theory that relates a photon's energy with a quantized wavelength one finds the following:

$$E = \frac{hc}{\lambda_{photon}} : E = pc \implies p = h/\lambda_{photon}$$
 (2)

Einstein suggests that the massless photon has a momentum related to its wavelength via Planck's constant. Classically momentum is only associated with massive objects, but radiation was already known not to behave in a classical manner, so this concept was not too much of a stretch. Then came 1924. Louis de Broglie hypothesized that if massless particles have momentum then maybe massive particles have a wavelength. By trading one non-intuitive result for another, de Broglie proposed his now-famous relationship that all matter has a characteristic wavelength associated with its momentum:

$$\lambda_{matter} = h/p \tag{3}$$

G. P. Thompson's experiment seeks to provide experimental evidence for the de Broglie relationship. The experiment draws inspiration from x-ray diffraction experiments. After all, if matter is governed by a similar equation to radiation then it should act in similar ways. In an x-ray powder diffraction experiment, a beam of x-ray photons is cast upon a powder sample of crystalline material. Under certain conditions, the photons will diffract in the powder, and form a constructive interference pattern. This pattern depends on the wavelength of the incident photons and the structure of the crystals in the powder. Thompson's experiment casts a beam of high-energy electrons through a thin foil of randomly oriented crystals which functionally behaves like a powder. If electrons are wave-particle dualistic as de Broglie proposed, then Thompson should expect to see a diffraction pattern similar to a photon experiment. FIG 1 shows a schematic of the experimental setup.

The experiment is conducted in a vacuum to avoid disturbances in the electron beam due to the air. Electrons are introduced into the test chamber via a cathode at the end of the tube depicted to the right of region A in FIG 1. An induction coil accelerates the electrons to the left at a known measurable voltage. Knowing the voltage allows one to calculate the momentum of each electron. Using the known momentum of the electrons and Planck's constant, one can use equation 3 to calculate the expected wavelength of the electrons in the beam.

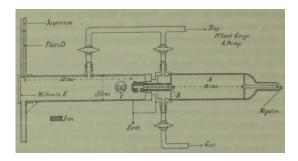


FIG. 1. Image taken from [3]. This original diagram was drawn by G.P. Thompson. The entire apparatus is inside a vacuum chamber to eliminate the effects of air on the beam of electrons. Region A contains an induction coil that produces high-energy electrons. The electrons are collimated into a beam by passing through the thin tube region B. B is shielded from magnetic effects due to an iron casing that surrounds it. The electron beam collides with the film/foil sample at position C where the diffraction will take place. D is the plate on which the diffraction pattern will appear. The voltage of the electron beam can be carefully measured using a spark gap which is not depicted here.

This wavelength will determine the diffraction pattern observed on the photographic plate similar to the way an x-ray wavelength determines the pattern for a powder diffraction experiment. For this reason, it is necessary to understand how a powder diffraction process works. The process is detailed, but the results are what make this experiment in particular so useful in testing the existence of matter waves.

Powder diffraction is the result of many randomly oriented single-crystal diffraction events combining to form a cumulative interference pattern [2]. For a single-crystal diffraction event to occur, the inter-atomic spacing between atomic planes in the crystal must be of comparable size to the wavelength of incident radiation. But there are a number of ways in which atomic planes can be constructed from a single crystal lattice, and each one will produce a different diffraction effect. To see that this is true, imagine a simple two-dimensional rectangular lattice as depicted in FIG 2.

It is clear to see from FIG 2 that the incident angle between different lattice plane families is unique unless the second family is described by an integer multiple of the first. The green arrows represent a perpendicular angle of incidence for the two families depicted. Notice how this coincides with the direction of the d-spacing vector. The two green arrows are obviously not parallel, which suggests geometrically that there is a difference in angle between one family of planes and another. It is also easy to see that the length of the d-spacing of each family is unique. To examine how this will affect diffraction, one must consider a reciprocal space.

A reciprocal lattice is constructed by inverting a lattice in real space. First, the d-spacing of a basis or primitive lattice plane family in a real space lattice is inverted into reciprocal space [5]. For example, the inverse of a vector

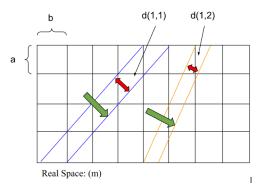


FIG. 2. Real space depiction of a rectangular two-dimensional lattice. Each intersection of a perpendicular black line represents the location of a lattice point or atom. The blue lines represent the [1x1] family and the orange lines represent the [1x2] family of lattice planes. The red arrows depict the interatomic spacing or d-spacing for that family of planes. The green arrows represent a vector perpendicular to the orientation of the plane families to highlight the difference in incident angle.

that represents the d-spacing of the [0x1] family in real space is the vector that describes the location of the [0x1] family in reciprocal space with respect to an origin point. That is, plotting a point in reciprocal space at the head of a vector originating from the origin with magnitude one over the real space d-spacing describes that family's location in reciprocal space. The planes will always be perpendicular to this vector. Linear combinations of that vector can be used to construct planes of an integer mul-

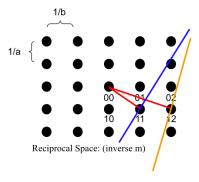


FIG. 3. Reciprocal space depiction of the lattice in FIG 2. Notice the spacing between the black points is now one over the original spacing. This is consistent with the inverse meter unit description below the image. Each point itself now represents the location of a family of lattice planes with respect to an origin point. The lines in the image are colored to match their respective lattice plane families from FIG 2. The red lines represent the reciprocal d-spacing of their respective plane families, which are still perpendicular to the direction of the planes. Notice that the blue [1x1] family d-spacing is longer than the orange [1x2] d-spacing in FIG 2, but here the inverse is true.

tiple value [5]. The process is repeated for each primitive family vector to form the reciprocal lattice as a whole. FIG 3 represents the result of performing this operation on FIG 2. It should come as no surprise that the reciprocal of a rectangular lattice is also rectangular, although the long and short sides of each cell now appear swapped. This example is relatively simple, but the method of its construction is the same for any lattice that has regular planes.

A reciprocal lattice can also be constructed on a lattice point by lattice point basis. Mathematically, this can be described using a Fourier transform whose periodicity coincides with the location of lattice points in a real space lattice. Fourier analysis selects reciprocal lattice vectors that preserve the geometry of the crystal during the transformation from real to reciprocal space [4]. For the purposes of this paper, it is only important to understand the following: For a real space crystal, any linear translation or rotation does not affect the physical properties of the crystal, and the same is true for the reciprocal lattice [4]. This fact will be important in a later argument. For now, a reciprocal space will aid in understanding how an interference pattern is formed from incident waves. This key concept is what makes the results of this experiment so versatile to work with. For a single crystal one can imagine a reciprocal lattice with an incident beam of constant wavelength as in FIG 4:

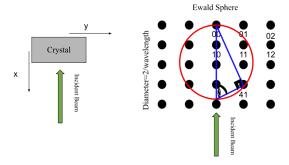


FIG. 4. Left: Two-dimensional crystal oriented along x and y. A beam of constant wavelength is incident upon the crystal. Right: Orientation preserving reciprocal lattice of crystal seen on the left. An Ewald sphere (circle) of diameter 2λ is drawn on the reciprocal lattice. This sphere intersects a [4x1] family point. Inside the sphere is a right triangle which demonstrates the Bragg diffraction equation for constructive interference. The intersection of the reciprocal point and the triangle suggests that diffracted waves at angle theta will cause constructive interference.

The Bragg equation for constructive interference states that for lattice planes with d-spacing d, constructive interference will occur at $n\lambda=2d\sin\theta$ [2]. The design of the triangle in FIG 4 is such that the hypotenuse is equal to $2/\lambda$ and the leg opposite the angle θ is 1/d-spacing for the [4x1] family of planes. The adjacent leg lies in the lattice plane [4x1], which is (as always) perpendicular to the d-spacing leg. Simple trigonometry reveals the Bragg equation:

$$\sin \theta = \frac{1/d_{4,1}}{2/\lambda} \implies \lambda = 2d_{4,1} \sin \theta \tag{4}$$

The circle in FIG 4 represents an Ewald Sphere in two dimensions. Any point on the sphere can be described by a triangle like the one depicted. But as equation 4 suggests, whenever the leg opposite the angle θ lands on a reciprocal point the conditions are met for constructive interference. If one were to fix the Ewald sphere and incident beam while rotating the reciprocal lattice about the origin, reciprocal points would occasionally intersect the sphere and therefore satisfy the conditions for constructive interference. FIG 5 shows this effect.

The triangle and subsequent angle θ used to describe the location on the sphere is unique for each primitive reciprocal point. The diffracted constructive interference wave will point along the vector exactly 2θ degrees away from the incident beam. A powder of many randomly oriented crystals can be thought of as a collection of many single crystals all at slightly different orientations. In order to represent a single crystal in every possible orientation in the x-y-plane one can rotate a crystal that lies in the plane through all angles. As mentioned earlier, this will not affect the physical properties of the crystal other than its orientation in relation to the beam. For a single crystal rotated about the origin as in FIG 5, one would expect an array of diffraction spots spaced along a horizontal line like in FIG 6.

A powder of crystals will contain single crystals of all orientations in the x-y-plane, but these crystals will also have random orientations with respect to the z-axis. To understand how this affects the interference pattern one can consider a crystal that is orientated level with the x-y-plane, and rotate the plane through all angles with

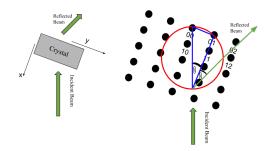


FIG. 5. As the crystal is rotated reciprocal points will sometimes intersect the Ewald sphere. The construction of the sphere always satisfies the constructive interference condition, so whenever a reciprocal point intersects the sphere the unique angle θ represents the angle of incidence for the incoming beam. The leg adjacent to the angle θ lies in the lattice plane that is responsible for the reflection. This means that a reflected beam will leave at an angle of exactly θ degrees in the opposite direction or 2θ degrees from the incident beam in the depicted orientation. The thinner green arrow shows this direction.

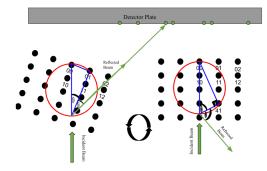


FIG. 6. The basic diffraction pattern. Left: A reciprocal lattice of a crystal oriented such that the [0x1] family of planes satisfies the constructive interference condition. The incident beam is diffracted in the crystal, and the outgoing constructive interference ray is shown creating a diffraction spot on the detector/photographic plate. Right: The crystal has now been rotated so that the [4x1] family of planes satisfy the constructive interference condition. Again the outgoing ray points in the direction of the reflected wave. Notice this ray does not intersect the detector plate. This suggests only small angles of reflection will produce a visible pattern on the plate. Also notice that between the two cases presented other diffraction spots are formed as the crystal is rotated and the Ewald sphere aligns itself with planar families.

respect to the z-axis. FIG 7 represents this operation for a single diffraction spot. As the figure demonstrates, a single spot is drawn into a ring as the crystal is rotated around that particular planar axis. One can imagine then the array of diffraction spots would simply trace a collection of concentric rings whose radial spacing is equal to the linear spacing of the original horizontal array. These rings are known as Debye-Scherrer Rings [2]. This argument assumes a two-dimensional crystal, but a similar argument in three dimensions leads to an identical result.

Debye-Scherrer rings are the constructive interference pattern for powder diffraction. A detailed understanding of the inner workings of powder diffraction highlights the genius of G.P. Thompson's experimental design. Thompson's foils and respective diffraction patterns are formed in the same manner as powder diffraction. The foils are collections of randomly oriented crystals whose combined constructive interference patterns form rings. The experiment relies on the known atomic crystal structure and inter-atomic spacing of several foil materials as well as equation 3 to calculate the expected diffraction pattern of electrons with known momentum [3]. Performing all of these calculations before revealing the big results makes the interpretation of the data a simple and rewarding process.

One begins by calculating the momentum of an electron accelerated through the potential difference in the tube. Equation 5 describes how to calculate the momentum of an electron accelerated through a potential difference.

$$K = \frac{1}{2}mv^2 \implies p = \sqrt{2mK}$$
 (5)
$$K = eV \implies p = \sqrt{2m_{e^-}eV}$$

The kinetic energy of an electron in the beam is equal to the charge of the electron times the value of the potential difference that supplied its motion. Substituting this value into the non-relativistic momentum equation for kinetic energy yields equation 5. This momentum is used to calculate the de Broglie wavelength of the electron by applying equation 3 from earlier.

$$\lambda = \frac{h}{\sqrt{2m_{e^{-}}eV}} \tag{6}$$

The de Broglie wavelength along with the known dspacings of the atomic plane families can be used to calculate the angle of each diffraction cone like the ones shown in FIG 7. This angle will satisfy the Bragg equation for constructive interference 4. The detector plate intersects these cones at a known distance away from the sample creating a cross-section. The cross-section of the cones will appear as rings. Finally, simple trigonometry can be used to calculate the expected diameter of each ring. FIG 8 shows the basic orientation of two diffraction cones. The radius of their respective rings on the detector can be described as the far-side leg of a right triangle. That makes their diameters $D_1 = 2 \tan(\theta) L$ and $D_2 = 2 \tan{(\phi)} L$ respectively. Finally, the results are simply a manner of measuring these diameters and comparing the values with expected results.

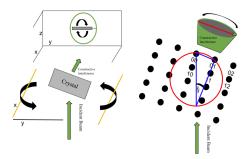


FIG. 7. A crystal that satisfies the constructive interference condition for the [0x1] planar family is oriented level with the x-y-plane. Left: The entire plane is then rotated about the axis of the incident beam. The diffraction spot becomes a ring as the constructive interference ray vector traces itself on the detector through the rotation. Right: The reciprocal lattice representation of the same operation. This time a cone is drawn to represent the path of the constructive interference ray. The red line in the cone represents a side-on view of the Ewald sphere, which maps the point on its surface to the rim of the cone as it rotates.

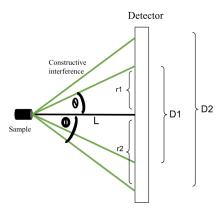


FIG. 8. Two-Dimensional side view of the space between the sample and the detector plate. (Space between region C and region D in FIG 1) The distance between the sample and the detector is L. One diffraction cone makes an angle θ with the horizontal plane, while another diffraction cone makes an angle ϕ . Each angle produces a different diameter ring on the detector plate: θ makes diameter one and ϕ makes diameter two. These diameters depend on the angles and distance from the sample.

What makes this experiment stand out amongst others is its design. The concepts of many detailed fields of study combine to form simple and immediately attainable results. First, G.P Thompson used x-rays of a known wavelength to determine the d-spacing of the crystals in his foils. Then he could send electrons through the same foil and perform the opposite calculation to find their wavelengths. But that is not all. He could also use the de Broglie relationship to calculate the electrons' wavelength before sending them through and predict the diffraction pattern he expected to see. The design is so accomplished that the data of the experiment requires no refinement. There is simply no need to manipulate data to produce a curve or plot when the ring patterns speak for themselves. Measuring the diameter of the rings tells one everything about the wavelength that created them. Or conversely, calculating the wavelength tells one exactly what diameter of rings to expect.

Just as de Broglie had predicted, the momentum of the electrons and Planck's constant determines their wavelength. Matter is governed by quantization. FIG 9 shows a side-by-side comparison of x-ray and electron diffraction patterns. The existence of these patterns stands as

simple visual proof that radiation and matter both exhibit quantized wave-like behavior.

The results of Thompson's experiment speak to something deeply fundamental about the universe. Again, radiation and matter both demonstrate quantized behavior. Beneath the seamless appearance of the universe on a human scale lies a quantized picture. Thompson's experiment only cemented the need for a complete theory of radiation and matter at this scale. Inevitably this new understanding led physicists to draft a complete quantum model of matter and radiation. Quantum Mechanical Theory is necessary for operating in the realm of subatomic particles.

Max Planck's early inception of the idea of quantizing energy as a mathematical trick has grown into a modern theory that describes a fundamental reality of the universe. The lesson behind this narrative in time is that experiment and theory are inseparable. Experimentation necessitates theory to cement its findings, and theory necessitates experiment to cement its concepts. Thompson's experiment combines a complex piece of Solid-State Physics and a small piece of early Quantum Theory into one simple measurement of distance. These small measurements simultaneously confirmed de Broglie's theory, and in part ushered in the beginning of the modern Quantum Mechanical Theory that exists today.

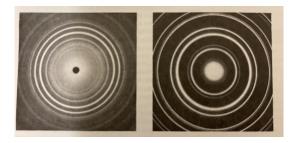


FIG. 9. Image taken form [2]. Left: Debye-Scherrer pattern for x-ray diffraction. Right: Debye-Scherrer pattern for electron diffraction. Notice the clarity of the electron diffraction image. G.P. Thompson's use of high-energy electrons (below relativist speeds, however) all them to penetrate deep into the crystals. In this way, hundreds of atomic planes are contributing to the diffraction pattern, which is what gives it such a sharp and defined appearance. The blur of the x-ray image is a result of having less energy than the electron image.

^[1] Louis de Broglie Biography, https://www.nobelprize.org/prizes/physics/1929/broglie/biographical/

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^[5] Patrick Shamberger, Intro to diffraction pt 3 Reciprocal Space. https://youtu.be/cdN6OgwH8Bg