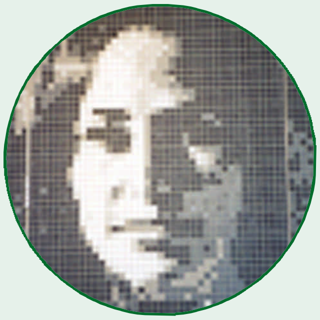
ELEGANT CONNECTIONS IN PHYSICS

A Pedestrian Approach to the Conceptual Foundations of Quantum Mechanics

by Dwight E. Neuenschwander



Tile Inset

— Photos by D. Neuenschwander

What Does Understanding the Quantum Really Mean?

It is often said that nobody "really" understands quantum mechanics.[0] We know how to *use* it, but one can argue that we don't understand deeply *why* it works. Be that as it may, in this article we review the conceptual foundations of quantum mechanics. This requires us to enter the minds of quantum mechanics' authors, as best we can from this distance.

This article is being written 100 years after Einstein's marvelous year, the five papers of 1905. Over the next 20 years Einstein was strongly influential, sometimes behind the scenes, in developing quantum mechanics. One of his celebrated 1905 papers kicked it off, when he asked a simple question about light: if we conceptualize matter as *discrete* atoms, on what grounds do we envision the electromagnetic field as *continuous*? (See The Quantum Tile sidebar.) Like most important questions, this one was loaded with not-so-simple answers. Here Einstein initiated wave-particle duality, the central concept of quantum mechanics. But he never liked the epistemology of quantum mechanics, and remained throughout his life one of its most perceptive skeptics.

Maxwell's equations (first published in 1862) are built on the assumption that electric and magnetic fields are continuous functions. An accelerated charged particle radiates waves in the field that move at the speed of light, *c*, an inherent velocity scale that emerges from Maxwell's theory unlike anything in Newtonian mechanics. These light waves carry the same frequency as the source particle's oscillations. The wave *model* of radiation forms one of the tremendous success stories of physics, with applications ranging from optics to radio to holograms.

But this wave model—which, like all models, is an *analogy*—can be pushed only so far. At the *microscopic* level—as in the interaction of light with a single electron bound to an atom—the wave picture breaks down. Such an electron does not behave like a Maxwellian antenna. This was glimpsed early, in experiments by Heinrich Hertz. By the 1880s he was generating electromagnetic waves artificially in the laboratory and confirming Maxwell. But along the way Hertz also noticed a glitch in his apparatus: when evacuated tubes containing alkali metals were hit with ultraviolet light, a current of electrons resulted. The details made no sense in terms of a wave model for light, where an electron would be released only after soaking up sufficient energy to overcome the binding energy. Even at ultra-low light intensities where that would take weeks, some electrons were liberated within nanoseconds, but *only* if the frequency exceeded a threshold value unique to that metal!

These facts remained enigmas until Einstein's 1905 paper,[1] when he accounted for them in terms of *collisions* between an electron and a *particle* of light! In Einstein's model light consists of little pellets of energy, the "quanta." The term "photon" appeared only in 1926[2], but was promptly adopted. For instance, the theme of the 1927 Fifth Solvay Conference was "electrons and photons."

The significance of Einstein's light quanta paper was far more fundamental than explaining the photoelectric effect. Einstein extended to *radiation* a hypothesis that Max Planck

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The Quantum Tile

Planck's constant h has the value 6.6×10^{-34} (kg m/s)(m), where the units written this way emphasize that h is a quantum of "Action," a product of momentum and displacement. A particle's momentum and position coordinates (p,x) describe "the state" of the particle as a point in "phase space." Both p and x are measured to within some uncertainties, $\pm\Delta p$ and $\pm\Delta x$. Heisenberg's Uncertainty Principle says that the product $\Delta p \Delta x$ must be no smaller than the quantum. The area of the smallest possible "tile" in phase space equals the quantum.

But at the scale of everyday phenomena, h cannot be distinguished from zero. So when we look at the macroscopic world, the quantum "tiles" are so small, compared to the everyday scale, that they lie below the threshold of resolution. The world then appears to be described by continuous functions, not discrete entities. An important fundamental question for us to ponder is this: where does the quantum-continuum transition occur?

This blending of many "quantum tiles," as we go from the quantum scale to the scale of classical fields, finds expression by analogy in these portraits. Close up (tile inset), we see each "quantized tile." Far away, the tiles spring to life in the form of the human face. This beautiful and interesting work of art, made in ceramic tiles, adorns an exterior wall of the Colorado Convention Center in Denver, CO.

had proposed for *mechanical oscillators* in 1900.[3] Back then Planck was the first person to successfully derive the spectrum of radiation in thermal equilibrium with matter. His breakthrough was to postulate that a charged *particle* oscillating at the frequency ν could, at any instant, vibrate with one and only one of the possible energies $nh\nu$, where $n = 0,1,2,3,...$ and h was a parameter to be fit to data. When in thermal equilibrium at temperature T, a population of oscillators would be distributed over these quantized states. The probability of an oscillator having energy $nh\nu$ would be proportional to the Boltzmann factor $\mathbf{e}^{-nh\nu/kT}$, where k denotes Boltzmann's constant. With this hypothesis and the usual machinery of statistical mechanics, Planck derived the energy density per frequency interval, $d\rho/d\nu$:

$$d\rho/d\nu = (8\pi h\,\nu^3/c^3)(\mathbf{e}^{h\nu/kT} - 1)^{-1}\ . \quad (1)$$

Planck's hypothetical spectrum fit the real spectrum if h was given the value

$$h = 6.6\times10^{-34}\ \text{J-s}\ . \quad (2)$$

Planck's strange hypothesis solved at first only this one problem. The greater reach of the quantum concept was impressed upon physicists five years later when Einstein had the temerity to ask why we should expect radiation to be *continuous* if matter was *discrete*. Einstein proceeded to quantize *radiation itself*. Restoring to h the status of a parameter of undetermined value, Einstein showed that if the entropy of radiation having frequency ν were set equal to the entropy of a gas of particles, these particles—particles of light—each carried energy $h\nu$. Einstein tested his photon concept by applying it to several problems in the interactions of light with matter, including the photoelectric effect. It went like this: Let an incoming photon impart all its energy to an electron bound in, say, a cesium atom. If it takes energy W to liberate the electron from the atom, leaving it with kinetic energy K, then conservation of energy in the photon-electron collision says

$$h\nu = K + W\ . \quad (3)$$

Because $K \geq 0$, the light's frequency must exceed a threshold value $\nu_o = W/h$. So an ejected electron's kinetic energy increases linearly with increasing light frequency when the threshold is exceeded:

$$K = h\,(\nu - \nu_o),\ \ \nu \geq \nu_o\ . \quad (4)$$

This linear plot of K vs. ν can be compared to data. As countless students have confirmed in physics labs ever since, it fits the data provided the value of h coincides with Planck's value of 1900! So h was *not* just a one-case fudge factor, but a fundamental constant! The quantum, and the particle model of light, had to be taken seriously.

Wave-particle duality was in 1905 a revolutionary concept. Einstein continued thinking hard about it. In 1909, he reflected that,

...It is my opinion that the next phase in the development of theoretical physics will bring us a theory of light that can be interpreted as a kind of fusion of the wave and emission theory...[4, 5]

Einstein's colleague and biographer Abraham Pais remarks,

...In 1909, at age thirty, [Einstein] was prepared for a fusion theory. He was alone in this. Planck certainly did not support this vision. Bohr had yet to arrive on the scene...[6]

Einstein originally conceptualized light as a quantum of *energy*. The photon must also be a quantum of *momentum*. Although the history of the ideas did not proceed as smoothly as suggested by the logic of hindsight to which we are privileged, that direct logical path says this: since photons *are* light they move of course at the speed of light, and must have zero mass. That means the energy-momentum relation of Special Relativity,

$$E^2 - (pc)^2 = (mc^2)^2\ , \quad (5)$$

can only *relate* the photon's energy and momentum through $E = pc$. The numerical *value* of a photon's energy and momentum must come from other information. This Einstein provided for energy with $E = h\nu$. Thanks to relativity, we automatically have for a photon's momentum $p = h\nu/c$. And because the frequency of light implies a wavelength λ by $c = \lambda\nu$, the photon's momentum may also be written $p = h/\lambda$.

To my knowledge Einstein first wrote an expression equivalent to $p = h\nu/c$ in 1909, when studying the fluctuations in the pressure on a surface immersed in radiation. There he noted,

...If the radiation were to consist of a very few extended complexes with energy hν which move independently through space and which are independently reflected...then as a consequence of fluctuations in the radiations pressure there would act on our plate only such momenta as are represented by the first term of our formula...

which was $h\nu/c$.[7] Later in that same year Johannes Stark wrote an equivalent expression in a discussion of *bremsstrahlung*.[8] Einstein revisited the issue in 1916, considering the Brownian motion of a molecule subject to radiation, and concluded that "if a bundle of radiation causes a molecule to emit or absorb an energy amount $h\nu$, then a momentum $h\nu/c$ is transferred to the molecule...."[9]

"SATURNIAN SYSTEMS"

In 1910–11 Ernest Rutherford and his students obtained the first empirical evidence for the mass and electric charge distributions of the atom through their discovery of the nucleus. The nucleus contained all the positive electric charge and almost all the mass, while the negatively charged electrons lived somehow outside the nucleus. Because of Coulomb attraction they could not just sit out there; presumably, Rutherford surmised, the electrons must orbit the nucleus, analogous to the ring particles in orbit about

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Saturn[10], or (as the analogy goes in today's pedagogy) like planets around the sun. But this could not be the whole story because it would be unstable. Orbiting electrons are accelerated electrons, which by Maxwell's equations must radiate away their energy and spiral into the nucleus. While spiraling in an electron would continuously emit light of ever-increasing frequency: IR to visible to UV to x-ray to gamma-ray, a rapid and spectacular collapse of the atom. But atoms are, in reality, quite stable on timescales comparable to the age of the universe! Clearly our conceptual framework was lacking some essential insight.

In 1913, Niels Bohr created a tentative solution by blending the quantum with Rutherford's planetary model of the atom. In so doing Bohr successfully predicted the size and spectrum of the simplest atom, hydrogen. The atomic size scale had been appreciated at least since Einstein's 1905 dissertation and paper on Brownian motion.[11] The frequencies of the spectral lines of hydrogen had been measured in the 19th century, and about 1885 were fit into a numerical pattern by the empirical Rydberg formula,

$$\nu = R(1/n_\ell^2 - 1/n_u^2) \qquad (6)$$

where $R = 3.290 \times 10^{15}$ Hz and n_ℓ and n_u denote "lower" and "upper" positive integers respectively, so that $n_\ell < n_u$. For instance, if $n_\ell = 2$ then $n_u = 3, 4, 5,...$ and the formula reproduces the "Balmer series" of visible lines. Before 1913 this equation *organized* the data but there was no *theory* beneath it. Bohr said, however, that when the Rydberg formula was shown to him, then the path before him lay clear.

Bohr arrived at Manchester in 1912, having come from Copenhagen to work in Rutherford's institute. At first Bohr experienced some difficulties in getting the senior scientists, including Rutherford, to listen to him. But eventually it was Rutherford himself who in 1913 sent to the *Philosophical Magazine* the manuscript of Bohr's paper, "On the Constitution of Atoms and Molecules."[12] Bohr's model of the hydrogen atom envisioned Rutherford's positive nucleus orbited by the negative electron, the electron bound to the nucleus by the Coulomb force (*see Figure 1a*). But Bohr asked his readers to exempt Maxwell's equations from this system, and said "Let us at first assume that there is no energy radiation. In this case the electron will describe stationary elliptical orbits." The orbit was assumed stationary and does not collapse. For this system Bohr wrote Newton's second law,

$$ke^2/r^2 = mV^2/r\,, \qquad (7)$$

and the mechanical energy of the electron,

$$E = \tfrac{1}{2}mV^2 - ke^2/r^2 \qquad (8)$$

where k denotes the Coulomb constant, m the electron mass, e the elementary charge, V the electron's speed, and r the orbit radius for circular orbits. So far, so Newtonian. Note that the magnitude of the potential energy equals twice the kinetic energy, $ke^2/r = mV^2$, so that,

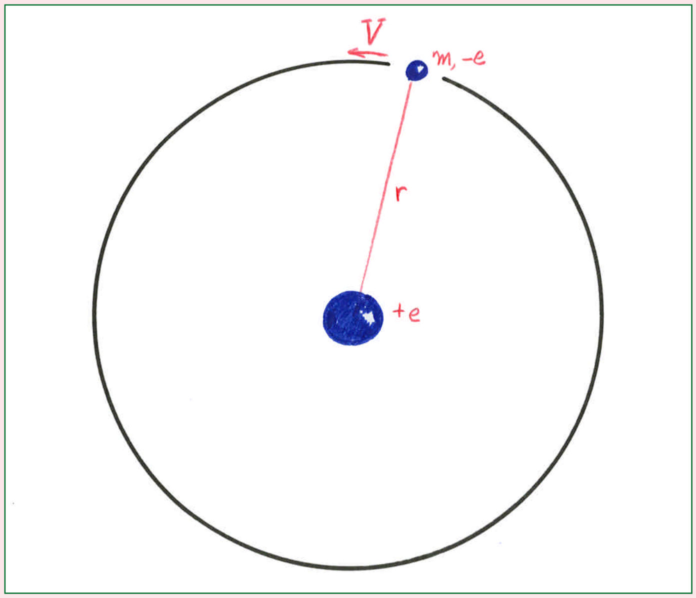

Fig. 1(a). The Rutherford-Bohr model of the hydrogen atom. The electron of mass m and charge –e orbits a nucleus of charge +e.

$$E = -\tfrac{1}{2}mV^2 = -ke^2/2r\,. \qquad (9)$$

Denote with Bohr $W = -E$ as the electron's binding energy, and put

$$\nu_{orb} = V/(2\pi r) \qquad (10)$$

as the frequency of the electron's orbit. According to Maxwell's equations, the orbiting electron should radiate light waves of this frequency, but Bohr has asked us to suspend Maxwell's equations here. From these Newtonian equations we derive with Bohr expressions, in terms of W, for the electron's orbital frequency and radius of a stationary orbit:

$$\nu_{orb} = (2W^3/\pi^2 m)^{1/2}(ke^2)^{-1} \qquad (11)$$

and

$$r = ke^2/2W\,. \qquad (12)$$

At this point Bohr observes, "We see that if the value of W is not given there will be no values of ν_{orb} and r characteristic for the system in question." He proceeds to create a postulate for W.

Bohr considers the assembly of a hydrogen atom from an isolated electron and bare nucleus. In the initial state the electron lies infinitely far away with "no sensible velocity" relative to the nucleus. For the final state, we "assume that the electron after the interaction has taken place has settled down in one of the stationary orbits around the nucleus." Since the electron's orbital frequency

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goes from zero to ν_{orb} during this atom-forming process, and, "If we assume that the radiation emitted is homogeneous," the average frequency of the electron is $\frac{1}{2}\nu_{orb}$. Bohr now invokes the Planck-Einstein hypothesis, and postulates that the electron's binding energy is proportional to a whole-number multiple of this frequency $\frac{1}{2}\nu_{orb}$, so that

$$W \equiv nh(\tfrac{1}{2}\nu_{orb}), \quad n = 1, 2, 3,... \tag{13}$$

Now Bohr can complete his calculation. Using contemporary values of e, m, and h, he finds for the n = 1 orbit a frequency of about 6×10^{15} Hz. The radius of the nth orbit turns out to be

$$r_n = n^2 (h^2/4\pi^2 mk^2e^2) \approx n^2 (\tfrac{1}{2}\text{Å}) ; \tag{14}$$

viz., in its n = 1 ground state the hydrogen atom is about 1Å wide. The ionization energies are,

$$W_n = (2\pi^2mk^4e^4/h^2)(1/n^2) \tag{15}$$

which gives about 13eV for the ground state. Bohr remarks that "these values are of the same order of magnitude as the linear dimensions of atoms, the optical frequencies, and the ionization-potentials."

Turning his attention to the hydrogen spectrum, Bohr assumed the electron radiates a photon only when it makes a *transition* from an upper orbit to a lower one.[13] The photon's energy would, of course, be given by $h\nu$, and conservation of energy yields for this transition (*see Figure 1b*),

$$h\nu = E_u - E_\ell . \tag{16}$$

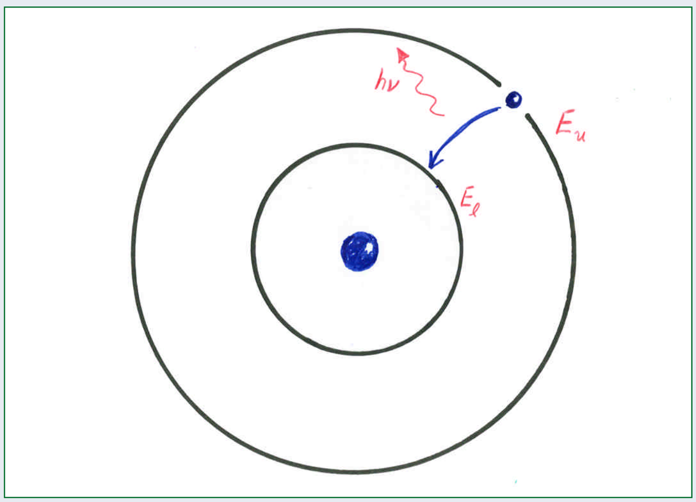

Fig. 1(b). When an electron makes a transition from an uppoer to a lower state, an emitted photon carries away the energy difference.

Using the expression for the quantized orbit energies, this predicts for the frequency of the emitted light,

$$\nu = (2\pi^2mk^4e^4/h^3)(1/n_\ell^2 - 1/n_u^2) . \tag{17}$$

The coefficient in front of the squared integers, as calculated by Bohr, has the value 3.1×10^{15} Hz, which agrees very closely with the empirical Rydberg constant R! At Bohr's hand the hydrogen atom's spectrum was successfully *predicted*.

As a consistency check on his postulate about W, Bohr applied a logic that would later be called the "correspondence principle." For very-large-n, the frequency of light emitted in the transition from state (n+1) to state n should match the electron's orbital frequency. Why should this be so? These large-n states lie very close together in energy, which means the quantum jumps between them are almost continuous. Thus the frequency of their emitted photons should agree with the continuous frequency ν_{orb} of the Maxwellian radiation emitted by a circulating electron. With Bohr let us see if they do. Noting that $R = 2\pi^2mk^4e^4/h^3$, Bohr's formula for the spectral line frequency, Eq. (17), becomes for large-n,

$$\nu = R\,[1/n^2 - 1/(n+1)^2] \approx 2R/n^3 . \tag{18}$$

In addition, Eq. (15) for W can be written,

$$W_n/hR = 1/n^2 \tag{19}$$

which turns Eq. (18) into

$$\nu = (2W_n^3/\pi^2m)^{1/2}\,(ke^2)^{-1} . \tag{20}$$

This coincides with the frequency of the light emitted by an orbiting electron in the Newtonian-Maxwellian paradigm, Eq. (11). Therefore Bohr's postulate for W agrees with established physics when deployed in the latter's domain of validity.

After deriving these results, Bohr remarked, "While there obviously can be no question of a mechanical foundation of the calculations given in this paper, it is, however, possible to give a very simple interpretation of the result...." The mechanical interpretation was the quantization of angular momentum. The postulated condition $W = \frac{1}{2}nh\nu_{orb}$ can be written,

$$\tfrac{1}{2}mV^2 = \tfrac{1}{2}\,nh\,(V/2\,\pi r) . \tag{21}$$

Several terms cancel, leaving

$$mVr = n(h/2\pi) . \tag{22}$$

This is the version of the Bohr quantization postulate usually presented in textbooks. In addition, we see the first emergence of the now-ubiquitous reduced Planck's constant "h-bar,"

$$\hbar \equiv h/2\pi \approx 1\times10^{-34}\ \text{J-s} . \tag{23}$$

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Bohr's model first came up for open discussion at a meeting of the British Association for the Advancement of Science, in September 1913 (the paper appeared in July). There Sir James Jeans, after outlining the problems of radiation, reported that, "Dr. Bohr has arrived at a most ingenious and suggesting, and I think we must add convincing, explanation of the laws of spectral lines." Some of the old guard were reticent. Lord Rayleigh, for instance, commented that it was inadvisable for people over 60 to pass judgment on modern ideas.[14] Arnold Sommerfeld and Peter Debye were enthusiastic, but Otto Stern and Max von Laue said that if Bohr were right, they would quit physics (he was; they did not). Bohr's close friend George Hevesy told Einstein about Bohr's work, and Einstein responded with enthusiasm. He mentioned that he had once had similar ideas but he did not dare pursue them.[15]

During the 1910s we had the quantized radiation of Einstein. The quantized mechanical systems included Planck's oscillators and Bohr's electron orbits. These latter results were generalized for periodic mechanical systems by the "Wilson-Sommerfeld quantization condition,"[16] the centerpiece of so-called "Old Quantum Theory."[17] The "action,"

$$\int \mathbf{p} \bullet d\mathbf{q}$$

was the quantity of choice for quantization. Here **q** denotes the vector of the particle's generalized coordinates, with **p** the momentum canonically conjugate to **q**. The action has not only the same dimensions as the quantum *h*, but it also plays a fundamental role in theoretical mechanics in many essential ways (e.g, relating the Lagrangian to the Hamiltonian). In addition, the action is an "adiabatic invariant": a quantity that, in periodic motion, is approximately conserved when external conditions change slowly on the timescale of one period.[18] Because periodic quantized mechanical systems such as harmonic oscillators and orbiting electrons have finite gaps between their possible energies, an adiabatic invariant seemed the natural choice as the object for quantization. For all these reasons, in Old Quantum Theory a particle's energy was quantized by the postulate of setting the action equal to a multiple of Planck's constant:

$$\oint \mathbf{p} \bullet d\mathbf{q} = nh, \qquad n = 1, 2, 3, \ldots \tag{24}$$

where the integral goes over one period of motion. When the particle moves along the x-axis subject to the potential energy $U(x)$, one writes $\boldsymbol{p} = \pm[2m(E-U)]^{1/2}$, evaluates the integral, and solves for E to find the particle's quantized energy levels in terms of nh and system parameters.

The Old Quantum Theory contained the spectra of Planck's oscillators and Bohr's hydrogen atom among its successes. But it could not predict the *rate* of transitions between energy states or the *size* and *shape* of quantized mechanical systems (for instance, the electron orbit trajectory had to be assumed from the outset). This formalism was a useful intermediate step, but was eclipsed in the 1920s by the wave mechanics of Louis de Broglie and Erwin Schrödinger and the matrix mechanics of Werner Heisenberg (which is methodically different but formally equivalent to wave mechanics). However, a remnant of Old Quantum Theory survives and is widely used even today in the so-called "semi-classical" or WKB approximation.[19] We will see below that Old Quantum Theory could have been used to *predict* the existence of the quantum mechanical wave function that was invented by Louis de Broglie using other methods.

THE PERSISTENCE OF PROBABILITY

As usual in science, the resolution of one puzzle creates new ones. No one could predict *when* an excited electron would make a spontaneous transition from an upper to a lower state, or predict in which *direction* the emitted photon would go. A decade earlier a similar puzzle arose in radioactive decay, where the *statistical* half-life was measurable but one could not predict when an *individual* atom would decay. All these atomic and nuclear decays, so far as anyone could tell, were described by *probability*. It was hoped, even presumed, that a deterministic mechanism would ultimately be found.

In 1917 Einstein wrote the paper on spontaneous and stimulated radiative emission that anticipated by 40 years the basic principles of the laser.[20] Here again the only predictions were statistical. This disturbed Einstein mightily. He pronounced this a "weakness of the theory...that it leaves time and direction of elementary processes to chance."[21]

Meanwhile, the photon as a relativistic particle of zero mass, energy $h\nu$, and directed momentum of magnitude $h\nu/c$ became convincing to holdouts in the community in 1922, when Arthur Compton and, independently, Peter Debye, published a quantitatively precise description of a photon scattering off a free electron.[22] From the conservation of momentum and energy applied to this collision, Compton predicted the photon wavelength shift in terms of scattering angle θ,

$$\Delta\lambda / \lambda = (h/mc)(1 - \cos\theta) \, . \tag{25}$$

He confirmed his own prediction with experimental data collected at three scattering angles. Einstein wrote in 1924, "The positive result of the Compton experiment proves that radiation behaves as if it consists of discrete energy projectiles, not only in regard to energy transfer but also in regard to momentum transfer."[23]

Within minor refinements, the foregoing features describe the state of quantum theory before the wave mechanics of Louis de Broglie and Erwin Schrödinger. Einstein also played an important role in facilitating the transition from Old Quantum Theory to Wave Mechanics.

DE BROGLIE'S MATTER WAVES

After a term in the army and some time spent studying history, Louis de Broglie began working in the laboratory of his older brother Maurice, where X-ray studies were a specialty. There Louis began to ponder the puzzles presented by light. The masslessness of the photon led immediately from $E = h\nu$ to $p = h/\lambda$. But in 1923 de Broglie stood these equations on their heads by proposing a beautiful symmetry argument. He suggested these relations hold true for

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all free particles, whatever their mass! At that moment there existed zero empirical evidence for this bold assertion. De Broglie was driven by the elegance of an *analogy*.[24]

To reinforce his weird hypothesis, de Broglie noted two pieces of circumstantial evidence.[25] First, both Newtonian mechanics and geometrical optics calculate *trajectories* that are derivable from minimization principles. The trajectory of a particle follows from Hamilton's Principle which for a particle in a potential energy field $U(\mathbf{r})$ gives Newton's Second Law in the form,

$$-\nabla U = md^2r/dt^2 \,, \tag{26}$$

where t denotes time. Similarly, the trajectory of a light ray interacting with a medium of refractive index $n(\mathbf{r})$ follows from Fermat's Principle, which yields a differential equation strikingly similar to Newton's,

$$\nabla\,(\tfrac{1}{2}n^2) = d^2\mathbf{r}/ds^2 \tag{27}$$

where s denotes arc length.[26] Change the names of the variables, and Newtonian mechanics and geometrical optics are the same subject! Geometrical optics is also the short-wavelength-limit of wave optics. Could Newtonian mechanics be the short-wavelength limit of some kind of "wave mechanics?"

The second piece of circumstantial evidence for the reciprocity of wave-particle duality came from the appearance of integers in Bohr's model of the hydrogen atom. The world's oldest quantum theory (but without h) dates not from 1900 or 1905 but from about 550 B.C.! I refer of course to the harmonic series of Pythagoras. A string of length L, clamped at both ends, has standing waves ("stationary states") of quantized frequencies that exhibit a harmonic series when L equals an integral number of half-wavelengths. De Broglie realized that if the Newtonian momentum for the electron mv could be set equal to h/λ, Bohr's angular momentum quantization condition, $mvr = n\hbar$, becomes, in wave language, the standing wave condition $2\pi r = n\lambda$. Bohr's "stationary orbits" were resonances of some kind of wave!

But de Broglie did not merely say, "Look, if $p = h/\lambda$ is good for photons, it must also be good for massive particles too," and let it go at that. He found a logical connection between p and h/λ that would make sense for *massive* particles. De Broglie's argument depends on Einstein's Special Theory of Relativity.[27] The essential features of his argument go as follows.

Let a *particle* of mass m move freely along the x-axis with velocity u. According to Special Relativity, this particle has energy E and momentum p given by,

$$E = mc^2\gamma \quad\text{and}\quad p = mu\gamma \tag{28}$$

where $\gamma \equiv (1 - u^2/c^2)^{-1/2}$. From these follow the well-known relations between the free particle's energy and momentum,

$$E^2 - (pc)^2 = (mc^2)^2 \tag{29}$$

and

$$u = pc^2/E \,. \tag{30}$$

Its velocity is $u = dx/dt$, so that $dt = dx/u$, or by Eq. (30),

$$t = \int (E/pc^2)\, dx \,. \tag{31}$$

By differentiating the energy-momentum condition, Eq. (29), we may write $E/p = c^2\, dp/dE$, so that

$$t = \int (dp/dE)\, dx = d/dE \int p\, dx \,. \tag{32}$$

So far there is nothing wave-like here. In 1929, de Broglie recalled:

> *Now a purely corpuscular theory contains nothing that enables us to define a frequency....On the other hand, determination of the stable motion of electrons in the atom introduces integers; and up to this point the only phenomena involving integers in physics were those of interference and the normal modes of vibration. This fact suggested to me the idea that electrons too could not be considered simply as corpuscles; but that periodicity must be assigned to them also.*[28]

He "defines a frequency" for this moving particle by *imposing* the Planck-Einstein relation $E = h\nu$ so that,

$$\nu = mc^2\gamma/h \,. \tag{33}$$

To this frequency de Broglie attaches a harmonic (sinusoidal) wave,[29]

$$\psi_E(t) \sim \cos(2\pi\nu t) = \cos(Et/\hbar) \,. \tag{34}$$

Introducing $\phi(x,E)$ as the spatial contribution to the phase of the wave function, de Broglie's wave takes the form,

$$\psi_E(x,t) = A\cos[\phi(x,E) - Et/\hbar] \,. \tag{35}$$

This wave function, corresponding somehow to the free particle, is *defined* to be harmonic in *time*, its frequency set by the particle's *energy*. With de Broglie we do not impose at the outset that the wave function be harmonic in *space*; that will be determined.

Indeed, because a *particle* by definition happens to be localized, any *wave* that is approximately localized *cannot* be a *pure* harmonic, but must be a superposition of harmonics,

$$\psi(x,t) = \int A(E)\cos[\phi(x,E) - Et/\hbar]\, dE \,, \tag{36}$$

where the amplitudes per energy $A(E)$ are sharply peaked about some central value (presumably $mc^2\gamma$). For the wave packet to hang together, and represent a particle for a finite time, the harmonics having energies within the peak of $A(E)$ must stay in phase so they continue to add constructively. This requires[30]

$$d[\phi(x,E) - Et/\hbar]/dE = 0 \,, \tag{37}$$

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or

$$t = \hbar\, d\phi/dE\ . \qquad (38)$$

Comparing our particle and wave expressions for t, Eqs. (32) and (38), we find the spatial part of the phase resembles the action used in Old Quantum Theory:

$$\phi = \int p\, dx/\hbar\ . \qquad (39)$$

For a free particle the momentum does not depend on x, therefore Eq. (39) integrates to,

$$\phi_{\text{free}} = px/\hbar + \delta \qquad (40)$$

where δ denotes an integration constant. Now the wave packet of Eq. (36) becomes,

$$\psi_{\text{free}}(x,t) = \int A(E) \cos[(px - Et)/\hbar + \delta]\, dE\ , \qquad (41)$$

and one of its harmonic components corresponding to the particle having *precisely* the energy E is,

$$\psi_{\text{E, free}}(x,t) = A \cos[(px - Et)/\hbar + \delta]\ . \qquad (42)$$

A harmonic *wave* of wavelength λ and frequency ν that moves to the right has phase $2\pi(x/\lambda - \nu t)$ or $(kx - \omega t)$ where $k = 2\pi/\lambda$ denotes the wavenumber and $\omega = 2\pi\nu$ the angular frequency. The phase velocity is the ratio of the coefficients of x and t in the phase, as in the familiar expression

$$V_{\text{phase}} = \lambda\nu\ . \qquad (43)$$

But for the de Broglie wave of Eq. (42), we also have

$$V_{\text{phase}} = E/p\ . \qquad (44)$$

Therefore,

$$\lambda\nu = E/p\ . \qquad (45)$$

Because $E = h\nu$ by hypothesis, this becomes

$$p = h/\lambda = \hbar k\ . \qquad (46)$$

◆ **COMMENT:** The phase velocity of a harmonic is $\lambda\nu = \omega/k$, which for our de Broglie wave becomes in particle language $E/p = c^2/u \geq c$. But the superluminal propagation of any *harmonic* wave does not imply the superluminal propagation of *information* or signals, because a harmonic wave looks everywhere the same. The *group velocity* $d\omega/dk$ carries the *information* of a de Broglie wave, for $d\omega/dk = dE/dp = u \leq c$: the de Broglie's *group* velocity equals the *particle's* velocity.[31] ◆

Before continuing with the historical development of wave-particle duality, it's interesting to see how de Broglie's hypothesis *could* have been anticipated from Old Quantum Theory. As a preliminary step consider a beam of x-rays, modeled here as waves of wavelength λ, and undergoing specular reflection on the layers of atoms of a crystal. Let adjacent parallel planes of atoms lie the distance D apart. Let the x-rays approach the planes at the angle θ above the planes (*see Fig. 2*). This situation leads to thin film interference. Two rays of reflected x-rays can enter a detector after traveling paths that differ in length by $2D \sin\theta$; and if this path difference equals an integral number of wavelengths, we obtain the constructive interference condition for Bragg scattering,

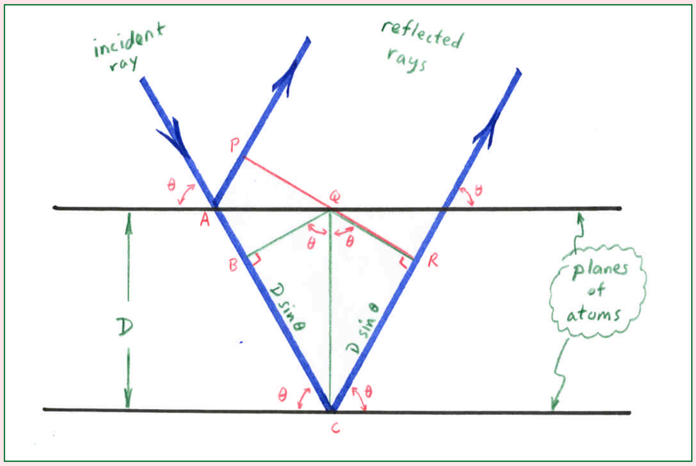

Fig. 2. The reflection of x-rays from adjacent planes of atoms. If the two reflected waves at P and R are in phase, they will arrive in phase at a distant detector. Point Q lies halfway between P and R. For the waves at P and R to be in phase, the path difference ACR – AP = 2Dsinθ must equal a whole number of wavelengths. When the x-rays are replaced by an electron beam, the electron's momentum vectors are co-linear with the ray lines, and CQ defines the z-axis.

$$2D\sin\theta = n\,\lambda\ . \qquad (47)$$

Now consider an electron approaching the planes of atoms along the same path of the previous rays. Let the z-axis be perpendicular to the planes, and let the electron's momentum be $\mathbf{p}$. Because the planes of atoms form a periodic array the Wilson-Sommerfeld quantization condition applies, and gives $p_z D = nh$. If an electron reflects off a plane, and suffers the momentum change $2p \sin\theta$, this impulse corresponds to the difference in the quantum conditions of two states, so that

$$2pD \sin\theta = \Delta n\, h\ . \qquad (48)$$

But a difference in integers Δn is just another integer n'; hence

$$2D \sin\theta = n'\, h/p\ . \qquad (49)$$

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Comparing the Bragg scattering formula (Eq. 47), to this prediction of Old Quantum Theory (Eq. 49), we see that one could have anticipated the relation $\lambda = h/p$ any time after the Wilson-Sommerfeld rules had been formulated in 1915–16. This approach to the de Broglie wavelength *was* derived, but in 1923 by W. Duane and Compton after de Broglie had already done his work.[32]

De Broglie published preliminary thoughts along these lines in 1923 and 1924, which he also developed into his doctoral dissertation in 1924.[33] His examination committee was chaired by Jean Perrin and his thesis advisor was Paul Langevin. The latter sent a copy of his students' thesis to his old friend Albert Einstein. One of de Broglie's biographers writes that,

De Broglie's ideas found a sympathetic reception with Einstein, as he himself had gone through an extended struggle to convince his colleagues of the wave-particle duality of photons. Einstein had a liking for symmetry arguments in physics, and de Broglie's theory established such a symmetry for material particles.[34]

It is interesting to reflect how Einstein and de Broglie were led to their revolutionary hypotheses through reciprocal symmetry arguments. Einstein said, Why shouldn't radiation, like matter, be particle-like? De Broglie said, Why shouldn't matter, like radiation, be wave-like?

Einstein was hard at work developing a theory of the monatomic gas when he heard of de Broglie's work. He immediately began applying some of de Broglie's ideas in 1925, citing the dissertation as "a very noteworthy paper." Not a bad day for a graduate student! De Broglie, incidentally, passed his doctoral examinations, despite his risky hypothesis.

Einstein's enthusiasm for matter waves influenced other physicists, notably Erwin Schrödinger, who had also been urged by Langevin to study de Broglie's thesis. Schrödinger later acknowledged that he was influenced on the subject by the thesis and "by short but truly visionary remarks by A. Einstein."[35] In a letter to Einstein of 23 April 1926, Schrödinger recounted how "the whole [wave mechanics] would not have been created and perhaps never (I mean, by myself) if your second paper on the gas degeneracy had not pushed my nose into the importance of de Broglie's ideas."[36] Schrödinger developed the equation from which one finds the *wave* function, given the *particle's* interactions.

At the time of de Broglie's dissertation defense there was not a shred of empirical evidence for or against the idea. De Broglie had made a shot in the dark, on the elegance of an analogy.

The early experiments that affirmed the wave-like behavior of electrons came from several laboratories. In 1923, Clinton Davisson and Charles Kunsman performed electron scattering experiments that graduate student Walter Elsasser interpreted as diffraction maxima and minima in de Broglie's matter waves.[37] George Thompson confirmed electrons to be wave-like in 1927 with diffraction evidence. He fired electrons through a thin metallic foil, whose atoms provided the diffraction grating. (Ironically, George was the son of J. J. Thompson, whose cathode ray experiments of 1895 showed electrons to be particle-like.) Then in 1929, Davisson and Lester Germer scattered electrons off a nickel crystal. The planes of nickel atoms behaved like a "thin film" for the "electron waves," and the interference maxima and minima that resulted from the electron scattering were the same as one would expect for waves with wavelength h/p. Thompson and Davisson shared the 1937 Nobel Prize for this work in electron wave optics.

◆ **COMMENT:** I highly recommend the paper by Jönsson, Brandt, & Hirschi, "Electron Diffraction at Multiple Slits," *Am. J. Phys.* **42**, 4–11 (1974). In 1961 these experimenters made multiple slits about 0.3 microns wide, spaced about 1 micron apart. This technical feat anticipated the mask-and-etch techniques used in the semiconductor industry. Radiating their slits with beams of electrons, these experimenters recorded interference and diffraction patterns identical to what one would expect for waves. This work was first published in *Zeitschrift für Physik* in 1961 and reprinted by the *American Journal of Physics* in 1974. ◆

THE WAVE EQUATION FOR DE BROGLIE WAVES

Any harmonic wave as a function of position x and time t may be written

$$A\cos(kx \pm \omega t)\ . \tag{50}$$

Thanks to Euler's formula,

$$e^{i\theta} = \cos\theta + i\sin\theta\ , \tag{51}$$

a harmonic wave function may be represented as

$$A\exp[\,i(kx \pm \omega t)] \tag{52}$$

(no additive phase shift is necessary in the following discussion). In acoustics or optics one understands the real part of this complex number represents the physical wave function, with the imaginary part ignored as an unphysical redundancy.

Taken together, the Planck-Einstein and de Broglie hypotheses form the foundational ideas of quantum mechanics. They say:

Corresponding to the motion of any free particle having precisely the energy E and momentum p, there exists a harmonic wave with angular frequency $\omega = 2\pi\nu$ and wavenumber $k = 2\pi/\lambda$, where

$$E = \hbar\omega = h\nu \tag{53}$$

and

$$p = \hbar k = h/\lambda\ . \tag{54}$$

By virtue of these postulates, corresponding to the free particle of energy E and momentum p there exists the harmonic wave ψ_E,

$$\psi_E(x,t) = A\exp[\,i(px - Et)/\hbar] \tag{55}$$

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(for motion to the right) where $E^2 - (pc)^2 = (mc^2)^2$, which reduces non-relativistically to

$$E = p^2/2m \; . \tag{56}$$

If de Broglie waves exist, they must be the solutions of a wave equation! What is the wave equation for de Broglie waves? The answer, for non-relativistic particles, was provided by Erwin Schrödinger in 1926.[38] Recall that Bohr's postulates for the hydrogen atom, later generalized in the Wilson-Sommerfeld rule, *postulated* integer multiples of Planck's constant. At the beginning of Schrödinger's paper he wrote,

In this communication I wish to show, first for the simplest case of the non-relativistic and unperturbed hydrogen atom, that the rules of quantization can be replaced by another postulate, in which there occurs no mention of whole numbers. Instead, the introduction of integers arises in the same natural way as, for example, in a vibrating string, for which the number of nodes is integral. The new conception can be generalized, and I believe that it penetrates deeply into the nature of the quantum rules.

Let us review the usual linear wave equation that describes, for example, waves on vibrating strings. Written here for the wave propagating with speed u along the x-axis, all such cases take the form,

$$\partial^2 \psi/\partial x^2 = (1/u^2)\, \partial^2 \psi/\partial t^2 \tag{57}$$

so that a change in x is compensated with a change in ut, and thus $x \pm ut$ forms the only independent variable of the disturbance. Because the wave equation is linear in ψ, any sum of solutions is also a solution; and because of the orthogonality of the harmonic waves any wave can be written as a superposition of harmonics, denoted schematically here as

$$\psi = \sum_\omega A_\omega \psi_\omega \tag{58}$$

where ψ_ω denotes the harmonic with angular frequency ω and wavenumber k, and A_ω its amplitude. Therefore to know how the *harmonics* behave is to know how *any* wave behaves, so long as the wave equation is linear.

In the case of the wave on a string, the example to which Schrödinger refers, one sees integers emerge for the standing waves as follows. Seek a solution where all points on the string vibrate with a common frequency ω. That means

$$\psi_\omega = f_\omega(x)\, e^{-i\omega t}, \tag{59}$$

turning the wave equation into an equation for f,

$$d^2 f_k/dx^2 + k^2 f_k = 0 \tag{60}$$

where $k = \omega/u$. For a wave on a string of length L, where both endpoints are nodes (as on a stringed instrument), $f(0) = 0$ says $f \sim \sin kx$, and $f(L) = 0$ says $kL = n\pi$ where $n = 1, 2, 3,...$ Integers *emerge* in the solution; they do not have to be postulated! This "quantization" condition can be written in terms of wavelength as $L = n\lambda/2$, or in terms of frequency $\nu = nu/2L$. If something similar could be derived for a de Broglie *wave*, one would have the quantized energies and momenta of the *particle*. This Schrödinger set out to do.

No doubt he was tempted at first to try the standard wave equation, Eq. (57), but even for the free particle, and thus the harmonic de Broglie wave, this would not work. For when we plug $\psi \sim \exp[i(px - Et)/\hbar]$ into the cookie-cutter wave equation, the derivatives pull down p and E twice, giving $p^2\, \psi = (E/u)^2\, \psi$, which says,

$$E/p = \pm\, u \tag{61}$$

which is not correct either classically or relativistically, except in the latter case for massless particles. Therefore, the de Broglie wave equation could not in general be the "usual" wave equation. Schrödinger had to try something else, especially for non-relativistic particles. (Relativistic wave equations were developed later, but as this article already exceeds all reasonable limits of length, their story will have to be told some other time.) Here of course, he was being led not by logic alone but by a craftsman's sense of what's *good*. "Your search for what's *true* is guided by your sense of what's *good*."[24]

Let us now motivate the Schrödinger equation, whose solutions will tell us the *wave* function when we know the *particle's* interactions. Recall that a *free* particle moving along the x-axis is described, according to the basic postulates, by the harmonic wave function,

$$\psi(x,t) = A\, exp[\, i(px - Et)/\hbar] \; . \tag{62}$$

On the other hand, for the wave function ψ' at an infinitesimally near point $x + \Delta x$, we would write

$$\begin{aligned}\psi'(x+\Delta x,t) &= A\, exp\{i[p(x+\Delta x) - Et)/\hbar]\} \\ &= exp(ip\, \Delta x/\hbar)\psi(x,t) \; .\end{aligned} \tag{63}$$

Because Δx is small, we can use the Taylor series expansion of the exponent, $e^{i\theta} \approx 1 + i\theta$, so that to first order in Δx,

$$\psi' \approx [1 + ip\Delta x/\hbar]\psi \; . \tag{64}$$

and thus

$$\Delta\psi/\Delta x = (ip/\hbar)\psi \tag{65}$$

where $\Delta\psi \equiv \psi' - \psi$. In the limit that $\Delta x \to 0$, we have a curious result:

$$(\hbar/i)\, \partial\psi/\partial x = p\psi \; . \tag{66}$$

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What shall we make of this? It says that multiplying the wave function by the momentum is the *same as taking its derivative with respect to x* (holding t fixed) and multiplying by $\hbar/i$. This means that $p\psi$ is not, in general, merely the product of a *number p* and a function ψ; rather, $p\psi$ is *another function* distinct from ψ itself. This has consequences, as we shall see.

Let us consider next an infinitesimal elapse of time (at fixed x). Then,

$$\psi'(x,t+\Delta t) = A\, exp\{i[px - E(t+\Delta t)/\hbar]\}. \tag{67}$$

Through arguments similar to those used above, we derive[39]

$$(-\hbar\,/i)\,\partial\psi/\partial t = E\psi\,. \tag{68}$$

To measure the particle's energy corresponds mathematically to evaluating the wave function's *derivative with respect to time* (holding x fixed).

Now at last we are ready to propose a wave equation for de Broglie waves. Let us begin in particle language: imagine a nonrelativistic particle, *not necessarily free*, interacting with the world through a potential energy function $U(x)$. The particle's total energy E now includes both kinetic and potential energies:[39, 40]

$$p^2/2m + U(x) = E\,. \tag{69}$$

Introduce wave language by multiplying Eq. (69) on the right with ψ:

$$[p^2/2m + U(x)]\psi = E\psi\,, \tag{70}$$

and use our rules of "quantum mechanics," Eqs. (66) and (68). We *assume* those rules, which were derived for a free particle, continue to apply *even when the particle is not free, but interacting*. On what ground would we make any *other* assumption? In the creation of a scientific theory you are pulled along by arguments of elegance and simplicity, and see how far they take you; keep them until events force you to think otherwise! This assumption now turns Eq. (70) into the Schrödinger equation

$$-(\hbar^2/2m)\partial^2\psi/\partial x^2 + U(x)\psi = -(\hbar/i)\partial\psi/\partial t\,. \tag{71}$$

If I tell you the particle's potential energy and the boundary conditions, then you can solve the Schrödinger equation for the wave function $\psi(x,t)$. This Schrödinger did, in a breathless series of papers in 1926, finding the de Broglie wave functions and the quantized energies for the harmonic oscillator, rigid rotator, the hydrogen atom, and perturbations on the hydrogen atom applied to the Stark effect (the atom placed in an external electric field).

For instance, in three spatial dimensions, as relevant to the hydrogen atom, the Schrödinger equation becomes,

$$-(\hbar^2/2m)\nabla^2\,\psi - (ke^2/r)\psi = -(\hbar/i)\partial\psi/\partial t\,. \tag{72}$$

Seeking stationary states with simple harmonic time dependence but a position-dependent amplitude, Schrödinger wrote,

$$\psi_E = f_E(\mathbf{r})\, e^{-i\omega t}\,, \tag{73}$$

where of course $E = \hbar\omega$ (where this E is a *number*). This turned Eq. (72) into an equation for the amplitude,

$$-(\hbar^2/2m)\nabla^2 f_E - (ke^2/r)\, f_E = E\, f_E\,. \tag{74}$$

Unlike the waves on the string, the solutions here are Laguerre polynomials and spherical harmonics instead of sines; but the idea is the same. The boundary conditions (developed in all the textbooks) gave the same energy values for the electrons in their "stationary states" as Bohr had derived 13 years earlier! But this time "the introduction of integers arose in a natural way."

When Schrödinger developed his equation for the de Broglie wave function in 1926, for some time nobody was sure *what* exactly was waving! A poem circulated for awhile went like this:

Erwin with his ψ can do
Calculations quite a few.
But one thing has not been seen:
Just what does ψ really mean.[41]

Schrödinger first suggested $e|\psi|^2$ might represent the electric charge density of the electron, which would have meant the electron became a smeared-out field. But when an electron hits the screen of the oscilloscope or television picture tube, the entire electron charge is encountered, not 15 percent or 63 percent of it (charge is *quantized*!).

Max Born provided the interpretation that is most widely used today: the square of the de Broglie wave equals the *probability density* of locating the electron.[42]

The basis of the entire quantum theory is Planck's relation between energy and frequency... In this 'quantum postulate,' however, there is an absurdity. For the concept of energy clearly refers to a single particle,...that is, to something of small extent; the concept of frequency, however, belongs to a wave, which must necessarily occupy a large region of space, and indeed, strictly speaking, the whole of space: if a segment of a purely periodic wave-train is removed, it is no longer periodic. The equating of the energy of a particle and the frequency of a wave is this in itself quite irrational. It can, however, be made rational, if a principle is renounced which was previously always accepted in physics, namely, that of determinism....

Let us therefore not ask where exactly a particle is, but be satisfied to know that it is in a definite, though fairly large, region of space. The contradiction between the wave and corpuscular theories then disappears. This is most easily seen if we allot to the wave the function of determining the probability that a particle will appear...[43]

More specifically, according to Born, at time t the probability $P(a,b)$ of finding the particle between $x = a$ and $x = b$ may be calculated by evaluating the integral,

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$$P(a,b) = \int_a^b |\psi(x,t)|^2 \, dx \,. \qquad (75)$$

This is the *interpretation* of the wave function's meaning. We recall that Einstein first envisioned a fusion of wave and particle concepts. When this hybrid concept got rolling in the mid-1920s, Einstein felt that by being able *only* to calculate probabilities, quantum mechanics was, at best, merely a working tool, not a description of ultimate reality. Einstein recognized here a fundamental epistemological shift in the direction physics was going. For if quantum theory was firmly correct, then some aspects of Nature were, in a deterministic sense, unknowable. Einstein saw this as a crisis for physics and tried, unsuccessfully, to see how quantum uncertainty could be undermined. His criticisms over the years of this aspect of quantum theory forced its proponents to think more clearly than they might have done otherwise.

To *test* a probabilistic prediction one must arrange an ensemble of particles under conditions as identical as possible, make the necessary measurement for each particle, collect statistics, and analyze the results. A prediction that 57 percent of the particles lie between a and b, for instance, means that out of every 100 particles examined, about 57 of them should lie between a and b. That is how you compare quantum predictions to experimental data. To say, "the particle is in the state ψ where $P(a,b) = 0.57$," means the particle is a member of such an ensemble.

As long as the particle exists, the probability of it being *somewhere* on the x-axis, from $x = -\infty$ to $x = +\infty$, must be 1. Then the wave function must be "normalized." Herein lies an intriguing consequence: we know that a pure harmonic wave, as the sine or cosine of $kx \pm \omega t$, extends to infinity without damping out. So the probability of finding the particle between $x = 0$ and $x = a$ is the same as finding it between, say, $x = 100a$ and $x = 101a$. We don't have a clue where a *truly* free particle may be located, at any time! A *pure harmonic* wave is not normalizable!

Of course, no particle is ever *truly* free, and *pure* harmonic waves don't really exist in nature either, because any physically realistic wave eventually damps out. But a wave of finite length can be represented as a *sum of harmonics*. The harmonics in such a sum carry a *range* of frequencies and wavelengths. So, switching back to particle language, the particle will have a *range of possible momentum and energy values*! As Born continued,

...If the region of space is considered large, and the wave-train consequently almost unperturbed and purely periodic, there corresponds to it a precise frequency, and a precisely defined particle energy; but the point where the particles appear in this region of space are quite indefinite. If it is desired to determine the position of the particles more exactly, the region of space in which the process is observed must be diminished; by do doing, however, a segment of the wave is removed, and its purely periodic character is destroyed; such a non-periodic disturbance, nevertheless, can be analyzed into a greater or lesser number of purely periodic oscillations; to each of the various frequencies of this mixture, there then corresponds a different energy of the observed particles. Thus an exact determination of position destroys the determination of the energy, and vice versa.[44]

Here we encounter in quantum mechanics an expression of the bandwidth theorems of wave physics. Applied to de Broglie's matter waves, they have important implications for the epistemology of particles.

The bandwidth theorems of ordinary wave physics reveal a fundamental limitation, based on a matter of *principle*, on how accurately one can measure a supposedly harmonic signal's wavelength and frequency. Suppose I take a tuning fork of frequency ν_o, and let its period, $1/\nu_o$, *define* the unit of time. The question I want to raise is this: if I bring up another tuning fork whose frequency is ν, *to how many decimal places can I measure* ν? One way to approach this problem is to sound my second tuning fork and the standard one together, and listen for beats. Because ν_o is given *exactly by definition*, I only need to measure the beat frequency, which is the difference between the two signals' frequencies, $\nu_{beat} = |\nu - \nu_o| \equiv \Delta\nu$. To hear at least one beat, I must listen for a time interval Δt at least as great as one beat period, $\Delta t \geq 1/\Delta\nu$, or

$$\Delta t \Delta \nu \geq 1. \qquad (76)$$

If it is claimed $\nu = \nu_o$, and I listen for, say, 10^6 seconds and hear no beats, I can conclude only that the difference between ν and ν_o lies beyond the sixth decimal place. If I listen for 10^{18} seconds (a time on the order of the age of the universe, or some faculty committee meetings) and hear no beats, I only know that difference between ν and ν_o lies beyond the eighteenth decial place. *Since we cannot listen an infinite time, we can never know the frequency of the second signal to an infinite number of decimal places.*

In terms of spatial variables, the bandwidth theorem says,

$$\Delta k \Delta x \geq 2\pi \,. \qquad (77)$$

In the context of quantum mechanics, these bandwidth theorems become the Uncertainty Principle, made quantitatively precise by Werner Heisenberg in 1927.[45] By merging the bandwidth theorems with the Planck-Einstein hypothesis $E = h\nu$ and the de Broglie hypotheses $p = \hbar k$, we find that Eqs. (76) and (77) give respectively,

$$\Delta t \Delta E \geq h \,. \qquad (78)$$

and

$$\Delta x \Delta p \geq h \,. \qquad (79)$$

Heisenberg's famous "Uncertainty Principle" is essentially a bandwidth theorem. Heisenberg made it precise by specifying the limits to which *pairs* of variables can be simultaneously measured. Born continues,

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The law of restricted measurability discovered by Heisenberg has been confirmed in every case. For every extensive quantity (such as determinations of position and time), there is an intensive quantity (such as velocity and energy), such that, the more exactly one is determined, the less accurately can the other be determined, and it is found that the product of the ranges to within which two such associated quantities are known is exactly Planck's constant. That is the true significance of this hitherto mysterious constant of nature; it is the absolute limit of accuracy of all measurements. Only its extreme smallness is responsible for the fact that its existence was not discovered earlier.[46]

Born's last comment can be illustrated like this: Suppose you have a 1 kg ball "at rest," located "right here." *How precisely can you actually measure its velocity and location?* Got the location nailed to within an atomic diameter? Then $\Delta x \sim 10^{-10}$m. In one year of watching, the ball rolls less than an atomic diameter, you say? That means $\Delta p \sim$ (1kg) (10^{-10}m)/(32×10^6 s) ~ 3×10^{-18} kgm/s. So $\Delta x\Delta p \sim 3\times10^{-28}$ kgm^2/s, three million times bigger than $\hbar$!

DE BROGLIE WAVES AND COMPLEX NUMBERS

We used complex variables to describe the wave function. People do that in acoustics and optics too, strictly for convenience, because the real and imaginary parts are redundant. If you write,

$$\psi = \phi + i\zeta \qquad (80)$$

and plug it into the "usual" wave equation (Eq. 57), you find that both ϕ and ζ satisfy the *same* equation. But try that with the Schrödinger equation: in the real and imaginary parts you find a pair of equations in which ϕ and ζ are *coupled*. Each depends on the other. This happens mathematically, of course, because the Schrödinger equation is second-order in space derivatives but first-order in the time derivative. Thus the Schrödinger equation is also like a diffusion equation. The upshot is that the wave function of quantum mechanics is *necessarily* complex; it's not just for convenience that we use complex numbers in quantum theory.[48] A *physical* reason can be given as follows.

Consider the interaction of a particle with an energy barrier. Let the particle move freely with zero potential energy everywhere along the x axis, *except* from $x = 0$ to $x = L$, where $U = U_o = const.$ (*see Fig. 3*).

Let the particle's energy be $E < U_o$. According to Newtonian mechanics, the particle lacks sufficient energy to get over the barrier, and must be reflected *every single time* we attempt the experiment. But this is *not always* the actual outcome! *In an ensemble of experiments, some fraction of the particles that we send with energy $E < U_o$ actually get past the barrier.* The *fraction* of the particles that get through, and thus the *probability* of any one particle getting through, diminishes exponentially with barrier height and thickness. It's *as though* the particle "tunnels" through the barrier when it lacks sufficient energy to climb over it! Does this *really* happen? Yes, indeed: every time you turn on a computer or cell phone or any other device that uses semiconductors, you have switched on the

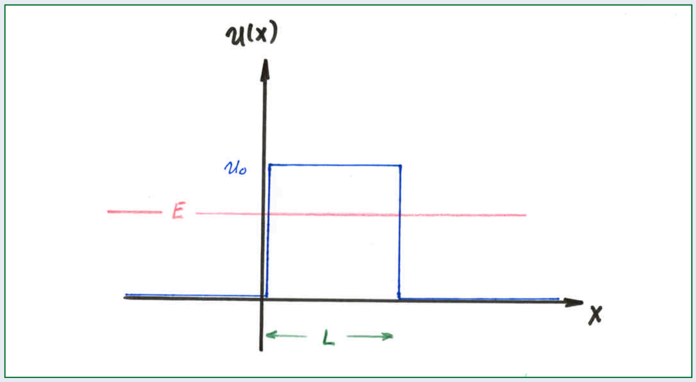

Fig. 3. The situation illustrating the "tunnel effect." The incoming particle of energy E encounters a potential energy barrier of height $U_o > E$.

tunnel effect. The tunnel effect has become part of our global economy! Let us see how the tunnel effect happens according to quantum mechanics.

Outside the barrier, a particle moving to the right carries momentum $p = \sqrt{(2mE)}$. But *inside* this barrier the momentum would be the *imaginary* number,

$$p = \sqrt{[2m(E - U_o)]}\ , \qquad (81)$$

which is imaginary because $E < U_o$. Let's factor out an i explicitly, by writing (81) as,

$$p = i\,p' \qquad (82)$$

where $p' = \sqrt{[2m(U_o - E)]}$ is a positive real number. In Newtonian theory, imaginary momentum would be ridiculous; the only physical interpretation of such a result in a calculation would be the prediction that the process in question cannot happen! However, the *reality* of the tunnel effect suggests that the *complex* wave function of Eq. (55) falls readily to hand as just the tool we *need*, not merely a trick of convenience; for inside the barrier, where the momentum is ip', the wave function of Eq. (55) exhibits an *exponentially damped amplitude*:

$$\psi(x,t) = A\,exp[-p'x/\hbar]\,exp[-iEt/\hbar]\ . \qquad (83)$$

So now the probability density for a particle to emerge out the other side of the barrier—which it is classically forbidden to do—is not *zero*, but *exponentially damped*:

$$|\psi(L,t)|^2 = A^2\,e^{-2p'L/\hbar}\ . \qquad (84)$$

How might this happen physically? When we say that a "particle has energy E," what do we really *know*? We cannot know E to an *infinite* number of decimal places. With the claimed energy value E comes an uncertainty, ΔE. So the horizontal line showing the particle's energy in the sketch above should really be drawn as a fuzzy

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band of some indefinite width. It is like the chalk lines drawn on a football field: the rule book says that the goal lines are 100 yards apart. But not every single particle of chalk dust lies on opposite lines that are *exactly* 100 yards apart. It is not *wrong* to say the lines are 100 yards apart; that is just an *average* value with a small but nonzero spread around the average. Likewise, when we create an ensemble of particles to run our tunneling experiment, and we claim to give each of them 9.5 eV of energy, we must recognize that we don't know it to be 9.50000...eV to an infinite number of significant figures. In particle energies, as in chalk lines, there's going to be a *distribution about a central value.* The particles that make it through the barrier are the few that happen to be on the high side of that distribution. The same "fuzziness" applies to U_o as well.

Conversely, if we send the particle with energy $E > U_o$ towards the barrier, some of them will be reflected backwards, even though, classically, not one of them should reflect!

So the weird stuff that you hear about in quantum mechanics happens because there are observables that cannot, in principle, be measured with infinite precision. There are always distributions about the "classical" values of any observable. Heisenberg's Uncertainty Principle puts limits on how precisely a *pair* of observables can be *simultaneously* measured, limited only by matters of principle.

OPERATORS

Normally in statistics, if you have some distribution function $f(x)$ and want to calculate the average value (or "expectation value") $\langle x\rangle$ you evaluate the integral,

$$\langle x\rangle = \int_{-\infty}^{+\infty} x\, f(x)\, dx\,. \tag{85}$$

Similarly, for measuring the expectation value of a particle's location, in quantum mechanics you would evaluate

$$\langle x\rangle = \int_{-\infty}^{+\infty} \psi^* \, x\, \psi\, dx\,. \tag{86}$$

because the distribution function is $|\psi|^2 = \psi^*\psi$. We could have written the integrand as $x\,|\psi|^2$ in this case. But you can *not* write $p|\psi|^2$ when calculating the expectation value of the particle's momentum, $\langle p\rangle$. Analogous to Eq. (86), in quantum mechanics you form the integral,

$$\langle p\rangle = \int_{-\infty}^{+\infty} \psi^* \, p\, \psi\, dx\,. \tag{87}$$

which you evaluate according to our derivative rule,

$$\langle p\rangle = (\hbar/i) \int_{-\infty}^{+\infty} \psi^* \,(\partial\psi/\partial x)\, dx\,. \tag{88}$$

Why is quantum mechanics done this way? This *must* be done because $p\psi$ is a *different state* from a rescaled ψ. When the particle's state is ψ and you measure its momentum, then the act of measuring the momentum puts the particle into the state $p\psi = (\hbar/i)(\partial\psi/\partial x)$. One says that p "operates" on the state; it's an "operator." An operator in general "does something to" the state besides merely rescaling the state by scalar multiplication.

Any time you have two states ψ and ξ, then the "overlap," a kind of scalar product between them, takes the form,

$$\int_{-\infty}^{+\infty} \psi^* \, \xi\, dx\,. \tag{89}$$

Hence the expectation value of momentum is the "overlap" of $p\psi$ with ψ.

Of special interest are the "eigenstates" of an operator. For these special states, the operator *only* rescales them. In symbols, if the operator N happens to merely rescale some wave function ϕ, so that $N\phi = \eta\phi$ where η is just a scalar, then ϕ is said to be an "eigenfunction of N with eigenvalue η".

If you think of wave functions as "vectors" in some abstract "state space," then the operator, in general, rotates and possibly rescales a vector. It turns one vector into another one, with a different "magnitude" and "direction" in this abstract space of all possible states. But if the state happens to be an eigenfunction of the operator, then the operator can only rescale it; the operator does not "rotate" one of its eigenstates. For example, $x\psi(x,t)$ only "rescales" the state $\psi(x,t)$, but in contrast $p\psi(x,t)$ rescales *and* "changes the direction" of $\psi(x,t)$ in the abstract state space. The momentum operator p operates as a derivative, and the derivative of a vector lies in the "tangent space" to the original vector.

For an example, which we include because of its importance, we turn to the Schrödinger equation. Here to be technically correct we must make the distinction between the particle's energy E as a *number*, and energy as an *operator*, the Hamiltonian, H. In terms of this vocabulary, Eq. (68) "really" says,

$$H\psi = (-\hbar/i)\, \partial\psi/\partial t\,. \tag{90}$$

This *is* the Schrödinger equation when we recall from classical physics the Hamiltonian for a nonrelativistic particle,

$$H = p^2/2m + U\,. \tag{91}$$

So when Eq. (91) is put in for the left-hand side of Eq. (90), and Eq. (66) used, we have the time-dependent Schrödinger *differential* equation, Eq. (71). To seek the *eigenfunctions* of the Hamiltonian—in this case the "standing de Broglie waves"—we seek a set of functions $\{\psi_E\}$ for which, instead of Eq. (90) we would have

$$H\psi_E = E\psi_E \tag{92}$$

(continued on next page)

where E now denotes the particle's energy, a number, the eigenvalue of H. As a matter of technique we *find* these eigenfunctions and their eigenvalues by separating the time-dependent Schrödinger equation according to

$$\psi_E = f_E(\mathbf{r})\, e^{-i\omega t} \tag{93}$$

where $\omega = E/\hbar$, and leads to Eq. (92).

The physical act of probing the system with a measurement changes the system's state, represented mathematically by an operator doing its thing to the original state. That means the *order* in which two measurements are made really does matter! For instance, suppose you want to measure the position *and* the momentum of an electron. Start with the electron in state ψ. If you measure the electron's position, you generate some state $\psi' = x\psi$. Now measure the electron's momentum, to get the state $\psi'' = p\psi' = px\psi$. Will you get the same result if you measure "p then x" instead of "x then p?" Definitely not! The issue is discussed in terms of the "commutator" of p and x, defined by

$$(p,x) \equiv px - xp\ . \tag{94}$$

What we're talking about here is expressed in the outcome of evaluating $(p,x)\psi$:

$$\begin{aligned}(p,x)\psi &= px\psi - xp\psi \\ &= (\hbar/i)[\partial(x\psi)/\partial x - x\partial\psi/\partial x] \\ &= (\hbar/i)\psi\ . \end{aligned} \tag{95}$$

Whenever two operators do not commute, then a state cannot be *simultaneously* an eigenstate of both of these operators.

This is the fancy mathematics behind the simple reality that if you observe the diffraction of an electron beam that passes through a double slit, then you try to see through which slit an electron goes, the act of probing the electron's *location* jolts its *momentum*, and therefore destroys the coherent phase differences that led to the wave interference in the first place!

Heisenberg made the Uncertainty Principle precise, by giving a precise prescription for what the "Δ" means in the bandwidth theorems. Consider two operators A and B. From statistics we recall the variance ΔA (square of standard deviation) as measured for some operator A:

$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2\ . \tag{96}$$

Heisenberg was able to show that pairs of canonically conjugate variables respect this inequality, given in terms of their commutator:[47]

$$(\Delta A)^2\,(\Delta B)^2 \;\geq\; \tfrac{1}{4}\,|\langle (A,B)\rangle|^2 \tag{97}$$

For example, when A and B are replaced with position and momentum, we obtain

$$\Delta p \Delta x \geq \tfrac{1}{2}\hbar\ . \tag{98}$$

DO WE REALLY UNDERSTAND QUANTUM MECHANICS?

Quantum mechanics requires *two* mental pictures of waves and particles. "Waves" and "particles" are complementary *models*; they are *conceptual representations* of real systems. The necessity of wave-particle *dualism* means that we have exhausted our store of analogies that can be based on a single mental picture. Such hybrid mixing of both languages is necessary to understand light or electrons, because neither language *by itself* captures all they can do.

The Uncertainty Principle sometimes seems a great mystery, but the existence of the *inequality*, of itself, poses no mystery: it is just the old bandwidth theorem that also applies to acoustics or Internet connections! The real "mystery" of quantum mechanics lies in the *reason* for the success of the basic quantum postulates: *why* are the Planck-Einstein and de Broglie hypotheses so incredibly successful? This, I think, is what people mean when they say "nobody really understands quantum mechanics." Nobody has yet found a deeper principle in terms of which these hybrid wave-particle equations arise as consequences.

That's enough introduction to the main ideas of quantum mechanics for today. Enough to get us started anyway. The relativistic wave equations will have to wait for another day. In the meantime, we must still ponder why

$$E = \hbar\omega \tag{99}$$

and

$$p = \hbar k \tag{100}$$

are so successful. When someone—perhaps you—discovers a deeper principle that *predicts* these links between the particle and wave models, then you will have made an important stride towards helping the rest of us truly understand quantum mechanics!
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Also, to search the photo collection on the Emilio Segrè Visual Archives, go to **www.aip.org/history/esva**/

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[1] A. Einstein, "On a Heuristic Point of View Concerning the Production and Transformation of Light," *Annalen der Physik,* **17**, 132–148 (1905). See the translation in *Einstein's Miraculous Year: Five Papers that Changed the Face of Physics,* J. Stachel, Ed., Princeton Univ. Pr. (1998). See the discussion of this paper in "Elegant Connections in Physics: Einstein's Quanta, Entropy, and the Photoelectric Effect," *SPS Observer*, Fall 2004, pp. 10–14.
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[3] M. Planck, *Ann. d. Phys.* **4**, 553 (1901).
[4] A. Pais, 'Subtle is the Lord...' *The Science and the Life of Albert Einstein*, Oxford Univ. Pr. (1982), p. 404.
[5] E. Segrè, *From X-Rays to Quarks: Modern Physicists and Their Discoveries*, Freeman (1980), p. 89.
[6] Pais, ref. 4, p. 404.
[7] ibid., p. 409.
[8] ibid., p. 409.
[9] ibid., p. 410.
[10] A mass distribution similar to Saturn and its rings was proposed for by the Japanese physicist H. Nagaoka in 1904. The mental picture of a "Saturnian system" was taken up by others; a brief history is provided in the forword by L. Rosenfeld in *On the Constitution of Atoms and Molecules* by N. Bohr, reprints by Munksgaard Ltd. of Copenhagen (Benjamin, 1963), of Bohr's 1913 papers from the *Philosophical Magazine*.
[11] Einstein's dissertation (PhD, University of Zurich, 30 April 1905) was called "A New Determination of Molecular Dimensions." The Brownian motion paper, "On the Motion of Small Particles Suspended in Liquids at Rest Required by the Molecular Kinetic Theory of Heat" was published in *Annalen der Physik* **17** (1905), 549–560. Both papers are reprinted in Stachel, Ref. 1. Einstein's dissertation is summarized and annotated in "Elegant Connections in Physics: Albert Einstein's Dissertation," *SPS Observer*, Spring 2005, pp. 10–14; the Brownian motion paper is touched upon in "Elegant Connections in Physics: Brownian Motion and the Fluctuation-Dissipation Theorem," *SPS Observer*, Winter 2004, pp. 10–14.
[12] N. Bohr, *Phil. Mag.* **26** (1913), reproduced in ref. 10. The first page of the paper bears the footnote, "Communicated by Prof. E. Rutherford, F. R. S."
[13] The electron gets kicked into the upper orbit in the first place by absorbing an incoming photon of the right energy, a partial photoelectric effect; or by collisions (as in the Frank-Hertz experiment) where the appropriate amount of energy gets exchanged in collisions between atoms.
[14] Ref. 10, quoted and cited in Rosenfeld's preface, p. *xlix*.
[15] Segrè, ref. 5, pp. 128–129.
[16] W. Wilson, *Phil. Mag.* **29**, 795 (1915); A. Sommerfeld, *Ann. d. Phys.* **51**, 1 (1916). This rule is sometimes called the Bohr-Sommerfeld quantization condition.
[17] See L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill, 1935), Ch. 2, for a splendid discussion of Old Quantum Theory, with detailed examples of its use.
[18] For discussions of adiabatic invariance, see e.g., M. Born, *Atomic Physics*, pp. 109–110 (Hafner, 1946, an English translation of Born's 1933 *Moderne Physik*); M. Jammer, *The Conceptual Development of Quantum Mechanics* (McGraw-Hill, 1966), pp. 89–109; D. Bohm, *Quantum Theory* (Prentice-Hall, 1951), pp. 41–48.
[19] The Wilson-Sommerfeld rules find modern expression in the "WKB approximation," or "semi-classical approximation," discussed in all the quantum mechanics textbooks as an important method approximating the wave functiion. "WKB" stands for Wentzel, Kramers, and Brillouin (sometimes JWKB including Jeffreys) who developed the method. The Wilson-Sommerfeld rules were refined by Einstein, Brillouin, and Keller into a form still used today (to account for zero-point energies as exhibited by the simple harmonic oscillator). See "Use of the Einstein-Brillouin-Keller action quantization" by Lorenzo Curtis and David Ellis, *Am. J. Phys.* **72** (9), 1-3 (2004) for discussion and references to the original EBK papers.
[20] A. Einstein, *Phys. Zeitschr*. **18**, 121 (1917), discussed in "Elegant Connections in Physics: Lasers in 1917—The Stimulated Emission of Radiation," *Radiations*, Spring 2004, pp. 18-21.
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[24] Robert Pirsig, *Zen and the Art of Motorcycle Maintenance: An Inquiry Into Values*, Morrow-Quill (1974).
[25] De Broglie's thoughts along these lines in his own words can be found in L. de Broglie, *Physics and Microphysics* (Grosset & Dunlap, 1955), pp. 147–148.
[26] This analogy is further developed by B. Turner, "A Hamiltonian for Geometrical Optics," *J. of Undergraduate Research in Physics,* 10, 23 (1991).
[27] One wonders how far nonrelativistic quantum mechanics would have progressed without the Special Theory of Relativity.
[28] Segrè, ref. 5, p. 151, a quote from de Broglie's Nobel Lecture.
[29] See H. A. Medicus, "Fifty Years of Matter Waves," *Physics Today*, Feb. 1974, pp. 38–45.
[30] E. Merzbacher, *Quantum Mechanics*, Second Ed. (Wiley, 1970), pp. 29–32.
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[32] The comparison of x-ray and electron scattering is discussed in Pauling and Wilson, ref. 17, pp. 34–35, and cite W. Duane, *Proc. Nat. Acad. Sci.* **9**, 158 (1923); and A. H. Compton, *ibid*., **9**, 359 (1923).
[33] Ref. 29 gives a comprehensive list of de Broglie's 1923–1924 papers and his 1924 dissertation, including the latter's 1963 reprinting.
[34] Ref. 29, p. 41.
[35] *ibid*., p. 41.
[36] *ibid*., p. 42.
[37] *ibid*., p. 42.
[38] E. Schrödinger, *Ann. d. Phys*. 79, 361 (1926). A series of papers followed this one, applying the wave equation to various systems that are familiar to students of any quantum textbook.
[39] Strictly, I should make a distinction between the Hamiltonian and the energy here. This will be done shortly.
[40] We can of course accommodate time-dependent interactions via $U = U(x,t)$. This leads to non-conservation of probability and need not concern us for now.
[41] Poem composed by Walter Hückel, translated by Felix Bloch, found in Segrè, Ref. 5, p. 164.
[42] M. Born, *Zeit. f. Phys*., **37**, 803 (1926).
[43] M. Born, *Physics in My Generation* (Springer-Verlag, 1969), pp. 26–27.
[44] *ibid*.
[45] W. Heisenberg, *Zeit. f. Phys*., **43**, 172 (1927).
[46] Born, Ref. 43.
[47] The approach outlined here begins with the Schwarz Inequality.

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