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Commentary

Celebrating the Birth Centenary of Quantum Mechanics: A Historical Perspective

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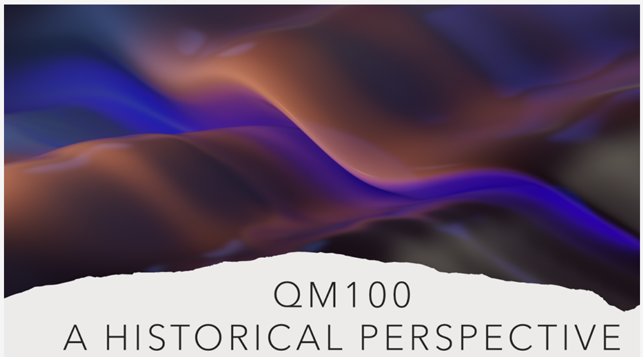

ABSTRACT: In July 1925, Werner Heisenberg submitted a paper to *Zeitschrift für Physik* entitled 'On quantum-theoretical reinterpretation of kinematic and mechanical relationships', thus giving birth to quantum mechanics. In the following year, building on de Broglie's wave-particle duality, Erwin Schrödinger developed wave mechanics, and soon, Max Born provided a probabilistic interpretation of the wave function. The theory was further enriched by the exclusion principle of Wolfgang Pauli and the uncertainty principle of Heisenberg, which ultimately led to the development of relativistic quantum mechanics by Dirac. The Copenhagen Interpretation created a probabilistic framework for understanding the theory. Over the past century, quantum mechanics has paved the way for advances in quantum field theory, computing, and modern technologies. This historical narrative provides insights into the complex discovery process that led to the development of quantum mechanics, which can potentially guide novel breakthroughs amid challenging conceptual struggles, as seen in the field of artificial intelligence today.

1. WHY IS THE HISTORY OF QUANTUM MECHANICS IMPORTANT?

This year, we mark a historic occasion: the centenary of the birth of quantum mechanics. A hundred years ago, the field of quantum mechanics emerged through the pioneering efforts of primarily Werner Heisenberg, Erwin Schrödinger, and Max Born.[1] Their groundbreaking contributions unraveled the mysteries of the atomic world, transforming our understanding of reality itself. Quantum mechanics stands as one of humanity's most profound intellectual achievements. Its founding principles—quantization, wave-particle duality, probability, uncertainty, and superposition— dramatically redefined our understanding of the universe. Jagdish Mehra, the authoritative chronicler of the history of quantum theory, declared:[1,2]

> *"The birth of quantum mechanics presents us with one of the most remarkable episodes in the history of science; it is as rich, complex, dramatic, and touching as any in the history of human thought."*

Quantum mechanics, with its further development as quantum field theory, is a magnificently beautiful theory, perhaps second only in its beauty to the general theory of relativity. But quantum mechanics is far more surprising than general relativity in its strangeness with concepts such as quantum entanglement – "spooky action-at-a-distance," as Einstein put it-, that whisper yet-to-be-revealed deeper secrets of reality that seem almost mystical.

In the July 1925 paper,[3] Heisenberg introduced matrix mechanics, marking the first comprehensive formulation of quantum theory that focused on observable quantities such as energy and spectral transitions. Between November 1925 and January 1926, Erwin Schrödinger developed wave mechanics, presenting the now-famous Schrödinger equation, which offered an alternative, yet equivalent, description of quantum systems. Soon, Max Born provided the probabilistic interpretation of the wave function, reshaping our notion of determinism and causality in physics.

These milestones were part of an extraordinary period of intellectual explosion, during which luminaries such as Niels Bohr, Paul Dirac, and Wolfgang Pauli contributed to the framework that continues to underpin modern physics.[1,2] This centennial is an opportunity to reflect on the profound human capacity for imagination and discovery. It is also an opportunity to marvel at "the unreasonable effectiveness of mathematics in the natural sciences," as Eugene Wigner wondered![4]

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This year, let us take a moment to appreciate and enjoy this crowning achievement of the human mind, which reveals the magnificent beauty of the hidden order of the cosmos. This paper is written with this objective in mind. Another important reason for studying the early history of quantum mechanics is that it is one of the rare occasions when a considerable wealth of first-hand accounts of momentous discoveries is available.[1] Fortunately, many of the original architects of quantum theory lived long lives and documented their discoveries in detail in papers, autobiographies, and interviews. These accounts offer valuable insights into the discovery process that can help guide novel discoveries during periods of profound conceptual difficulties and confusion, such as the current state of artificial intelligence.

Therefore, I will quote the original writings of the main protagonists wherever appropriate, as I am convinced that their own expressions lend authenticity and clarity to the very murky processes behind great conceptual discoveries. My hope is to give the reader a sense of what is involved in achieving major conceptual breakthroughs. As Max Planck said: "In the history of science, a new concept never springs up in its complete and final form, as in the ancient Greek myth, Pallas Athene sprang up from the head of Zeus." Heisenberg further elaborated:[5]

> *"The history of physics is not only a sequence of experimental discoveries and observations, followed by their mathematical description; it is also a history of concepts. For an understanding of the phenomena, the first condition is the introduction of adequate concepts.*
> *Only with the help of correct concepts can we really know what has been observed. When we enter a new field, very often, new concepts are needed. As a rule, new concepts come up in a rather unclear and undeveloped form. Later, they are modified, sometimes they are almost completely abandoned and are replaced by some better concepts, which then, finally, are clear and well-defined."*

In the remainder of this Commentary, I provide a historical perspective that highlights key breakthroughs. This perspective is meant for those unfamiliar with quantum mechanics or its historical development. It is not aimed at experts. The objective of this paper is not to teach readers quantum mechanics but only to expose them to the central ideas, their historical evolution, and the conceptual struggles, with a moderate amount of mathematics to illustrate these points. Given the scope of this perspective and its constraints, I will not discuss the mathematical details, referring the readers to more comprehensive sources.[1,6−10] Furthermore, this is a personal perspective that reflects what I consider important and interesting developments. However, I believe that most quantum experts agree with the observations made in this paper.

2. TWO CLOUDS IN THE HORIZON: THE "1900-MOMENT"

At the dawn of the 20th century, on April 27, 1900, Lord Kelvin delivered an important lecture at the Royal Institution in London,[11] summarizing the status of physics with the title "Nineteenth-Century Clouds Over the Dynamical Theory of Heat and Light." The "clouds" that bothered him were the two troublesome experiments that did not agree with the theoretical predictions: (i) the null result of the Michelson-Morley experiment, which could not detect the motion of the Earth through ether, and (ii) the *ultraviolet catastrophe* of blackbody radiation. Lord Kelvin correctly recognized the gravity of the situation and appreciated the profound uncertainty in the fundamentals of classical physics.

As we know, these two "clouds" revolutionized physics, indeed all science, over the following three decades.[12] The first "cloud" led to the birth of the theory of relativity, completely upending our understanding of space, time, gravity, and the cosmos itself. The second gave us quantum mechanics, opening the secret door to an almost "magical" realm that we did not even know existed all around us all of the time. In fact, quantum theory was born soon in the same year, 1900, when Max Planck presented his quantum hypothesis at a meeting of the German Physical Society on December 14th, initiating the dispersal of the second cloud.[13]

This scientific drama unfolded like a well-written suspense thriller full of plot twists, turns, and surprising conceptual leaps, except that it was written in the language of mathematics, namely, linear algebra, differential equations, and probability theory, echoing Galileo's declaration:[14]

> *"Philosophy is written in this grand book, I mean the universe, which stands continually open to our gaze, but it cannot be understood unless one first learns to comprehend the language in which it is written. It is written in the language of mathematics."*

In the annals of history, certain periods stand out as inflection points, times when scientific, technological, or social changes drastically altered the trajectory of our civilization. That moment in 1900, when Kelvin announced that all was not well in physics, was such a tipping point. The innovations that followed, both in theory and in practical applications, continue to transform our societies and economies profoundly. There is no other thirty-year period in history where our understanding of the universe was so dramatically upended as it was during 1900−1930.

3. ACT I: THE BIRTH OF QUANTUM THEORY (1900−1913)

Between 1900 and 1930, physicists were compelled to abandon classical mechanics in favor of quantum mechanics because the former could not predict or explain the atomic structure, spectral lines, and dual nature of matter and radiation as both waves and particles. This drama of frenetic intellectual activity occurred in four surprising breakthroughs. In the following sections, I provide an overview of these key advances.

3.1. Max Planck and Quantum Theory (1900). As noted, the roots of quantum mechanics can be traced to the "cloud" that Lord Kelvin worried about in the context of blackbody radiation. A blackbody is an idealized object that absorbs and emits electromagnetic radiation at all frequencies. Classical physics predicted the intensity of this radiation using the Rayleigh-Jeans law:

$$I(\lambda, T) = \frac{2ck_BT}{\lambda^4} \tag{1}$$

where $I(\lambda, T)$ is the radiation intensity, c is the speed of light, k_B is Boltzmann's constant, T is the temperature, and λ is the wavelength of the radiation. This equation worked well at long wavelengths but diverged to infinity at short wavelengths, as shown in Figure 1, known as the *ultraviolet catastrophe*, a term coined by Paul Ehrenfest in 1911.

Max Planck (Figure 2) got interested in this problem and, after a six-year struggle, introduced a revolutionary hypothesis: energy is not emitted continuously but in discrete packets.[16] Planck accomplished this in two critical steps, presented at the

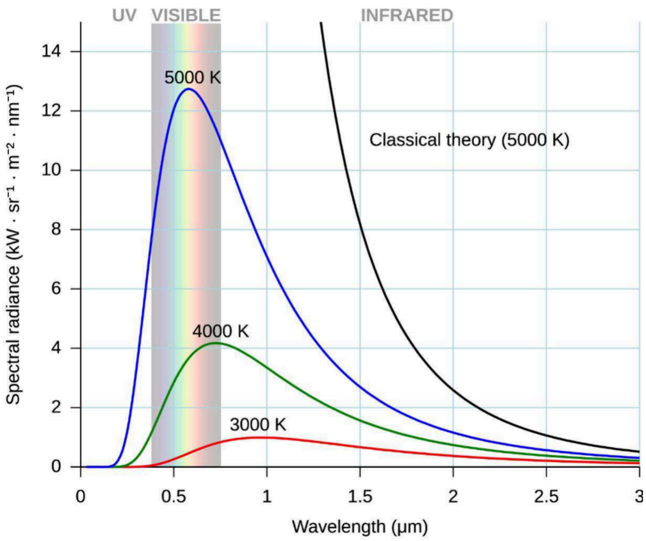

Figure 1. Ultraviolet catastrophe in classical Rayleigh-Jeans law. Reproduced with permission from ref 15. Copyright 2010 Darth Kule.

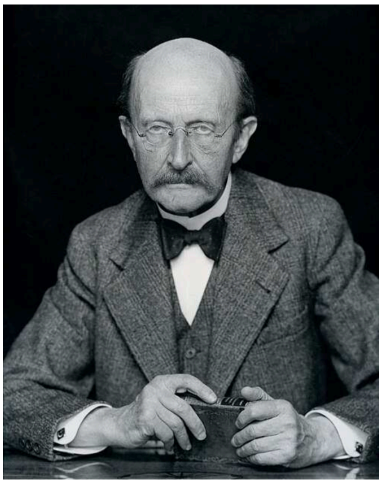

Figure 2. Max Planck. Reproduced with permission from ref 18. Copyright 1938 Hugo Erfurth.

German Physical Society meetings: (i) Discovering the correct radiation formula (on October 19, 1900) and (ii) Providing its conceptual justification via the *quantum hypothesis* (on December 14, 1900).

Let us hear about the first step from Planck himself from his scientific autobiography:[17]

"In fact, my previous studies of the Second Law of Thermodynamics came to stand me in good stead now, for at the very outset I hit upon the idea of correlating not the temperature but the entropy of the oscillator with its energy. It was an odd jest of fate that a circumstance which on former occasions I had found unpleasant, namely, the lack of interest of my colleagues in the direction taken by my investigations, now turned out to be an outright boon. While a host of outstanding physicists worked on the problem of spectral energy distribution, from both the experimental and theoretical aspects, every one of them directed his efforts solely toward exhibiting the dependence of the intensity of radiation on the temperature.

On the other hand, I suspected that the fundamental connection lies in the dependence of entropy upon energy. As the significance of the concept of entropy had not yet come to be fully appreciated, nobody paid any attention to the method adopted by me, and I could work out my calculations completely at my leisure, with absolute thoroughness, without fear of interference or competition ... In this way, a new radiation formula was obtained, and I submitted it for examination to the Berlin Physical Society, at the meeting on October 19, 1900."

Although Rudolf Clausius introduced the concept of entropy in 1864, it remained undervalued by the scientific community, surprisingly, for nearly three decades. This highlights the significant amount of time required for revolutionary concepts to gain widespread acceptance. Reflecting on this, Planck later remarked rather sardonically:[17]

"A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die out, and a new generation grows up that is familiar with it."

Planck's new radiation law is given by

$$I(\lambda, T) = \frac{2hc^2}{\lambda^5}\frac{1}{e^{hc/\lambda k_B T} - 1} \qquad (2)$$

(h is Planck's constant) correctly described experimental data at all wavelengths and resolved the ultraviolet catastrophe. However, Planck was unsatisfied with the clever guesswork that led to its discovery. He wanted to know its *conceptual* significance, and so he proceeded with the second step:[17]

"But even if the absolutely precise validity of the radiation formula is taken for granted, so long as it had merely the standing of a law disclosed by a lucky intuition, it could not be expected to possess more than a formal significance. For this reason, on the very day that I formulated this law, I began to devote myself to the task of investing it with a true physical meaning. This quest automatically led me to study the interrelation of entropy and probability—in other words, to pursue the line of thought inaugurated by Boltzmann.

Since the entropy S is an additive magnitude but the probability W is a multiplicative one, I simply postulated that S = k · log W, where k is a universal constant; and I investigated whether the formula for W, which is obtained when S is replaced by its value corresponding to the above radiation law, could be interpreted as a measure of probability ... It is, understandably, often called Boltzmann's constant. However, this calls for the comment that Boltzmann never introduced this constant, nor, to the best of my knowledge, did he ever think of investigating its numerical value."

Interestingly, the famous equation $S = k \log W$, which is inscribed on Boltzmann's tomb in Vienna, was not stated in this form by Boltzmann. It was Planck who expressed the Boltzmann result in this now familiar form.[16]

Applying Boltzmann's reasoning about entropy from his 1877 paper[19] to blackbody radiation, Planck was led to the concept of discrete packets of energy, which he termed *quanta*.[13,20] He was, however, uncomfortable with this idea as he was aware that he was violating the continuity principle,[21] a fundamental principle that dates back to Leibnitz, who famously said:[22] "*Natura non facit saltus*" (Latin for "nature does not make jumps"). This

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principle also serves as the foundation for differential and integral calculus.

Planck alerts us to this crucial feature of his theory in his December 14, 1900, paper:[13]

"If E [the total energy] is considered to be a continuous divisible quantity, this distribution is possible in infinitely many ways. We consider, however — this is the most essential point of the whole calculation — E to be composed of a well defined number of equal parts [of magnitude ϵ] and use thereto the constant of nature $h = 6.55 \times 10^{-27}$ erg sec [setting $\epsilon = h\nu$]."

About his break with classical physics tradition and his embracing of Boltzmann's "atomistic" ideas, which he had been critical of for many years, Planck would later recall:

"Briefly summarized, what I did can be described as simply an act of desperation. By nature, I am peacefully inclined and reject all doubtful adventures. But by then I had been wrestling unsuccessfully for six years (since 1894) with the problem of equilibrium between radiation and matter, and I knew that this problem was of fundamental importance to physics; I also knew the formula that expresses the energy distribution in normal spectra. A theoretical interpretation therefore had to be found at any cost, no matter how high. It was clear to me that classical physics could offer no solution to this problem and would have meant that all of the energy would eventually transfer from matter into radiation. In order to prevent this, a new constant is required to ensure that energy does not disintegrate. But the only way to recognize how this can be done is to start from a definite point of view. This approach was opened to me by maintaining the laws of thermodynamics. The two laws, it seems to me, must be upheld under all circumstances. For the rest, I was ready to sacrifice every one of my previous convictions about physical laws."

Although historians continue to debate how much Planck realized the significance of his quantum hypothesis,[13,20,21] Erwin Planck later recalled what his father told him soon after his discovery:[20]

"Either what I have found out now is complete nonsense or it might be one of the greatest discoveries in physics since Newton."

Planck proposed that the energy of a radiation mode is quantized and proportional to its frequency:

$$E = nh\nu \qquad n = 1, 2, 3, ... \tag{3}$$

where h is Planck's constant and ν is the frequency of the radiation. This assumption prevented infinite energy at short wavelengths and correctly described blackbody radiation. Using energy quantization, Planck derived the formula presented above, now expressed in terms of frequency ν:

$$I(\nu, T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_BT} - 1} \tag{4}$$

Max Planck was awarded the 1918 Physics Nobel Prize for his discovery. Although Planck gave birth to quantum theory, he remained a reluctant revolutionary for a long time, viewing quantization only as a "mathematical trick" rather than as a fundamental law of nature. After all, he was very much a part of the old guard and therefore was hesitant to abandon the "sacred" principle of continuity. It was only much later that he came around to accepting the new reality.

3.2. Albert Einstein and the Photoelectric Effect (1905). On the other hand, the Young Turk who followed Planck next in this exciting drama was a rebellious iconoclast who was rearing to upend the very foundations of physics, not just radiation theory. Enter Albert Einstein (Figure 3), a 26-year-old unknown clerk at the Swiss Patent Office in Bern. While Planck saw quantization as just a "mathematical trick", not a feature of physical nature, Einstein took it more seriously as a fundamental property of nature. He was open to such radical rethinking as he was, at the same time, busy overthrowing the Newtonian concepts of space and time in his new theory of special relativity, which dispersed the first "cloud" that Lord Kelvin worried about.

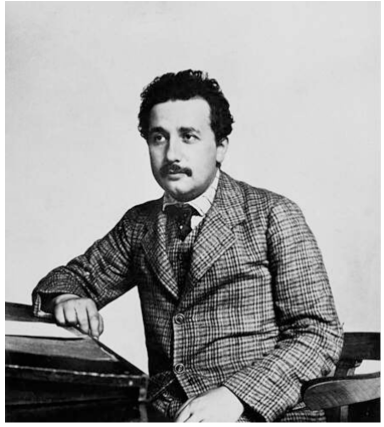

Figure 3. Albert Einstein. Reproduced with permission from ref 23. Copyright 1905 Lucien Chavan.

In his *Annus Mirabilis*, 1905, Einstein extended Planck's idea and proposed that light itself consists of quantized particles called *photons*, each carrying energy $E = h\nu$, to solve a puzzling result in the *photoelectric effect*, where light incident on a metal surface ejects electrons. The classical wave theory of light predicted that increasing the light intensity should increase the electron energy. However, experiments showed that no electrons are emitted below a threshold frequency, regardless of intensity. They further showed that the electron energy depends on the frequency, not the intensity. The higher light intensity increased the number of emitted electrons, but not their individual energy.

Einstein's theory treats the photoelectric effect as a one-to-one interaction between a photon and an electron. The energy balance equation is

$$h\nu = W + E_k \tag{5}$$

where $h\nu$ is the energy of the incoming photon, W (or work function) is the minimum energy required to free an electron from the metal, and E_k is the maximum kinetic energy of the emitted electron. This equation explained all of the experimental results. Reflecting on his groundbreaking papers from 1905, which included his first two on relativity, he regarded only the light-quanta paper as genuinely revolutionary. Einstein was awarded the Nobel Prize in Physics in 1921 for this discovery. It is interesting to note that the prize was not for his work on relativity.

From the perspective of the evolution of quantum theory, Einstein's theory confirmed the particle nature of light, supporting the idea that light exhibits both wave and particle properties, i.e., wave-particle duality. This paved the way for the acts that followed next.

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3.3. Niels Bohr and the Hydrogen Atom (1913). In 1897, J. J. Thomson at Cambridge discovered the electron in cathode-ray tube experiments. Ernest Rutherford, who had trained under Thomson, showed in his gold foil experiment at Manchester in 1911 that the atom is mostly an empty space with a tiny, dense, positively charged nucleus with orbiting electrons. However, classical electrodynamics predicted that electrons should spiral into the nucleus due to radiation loss. Furthermore, the atomic spectra of hydrogen showed discrete spectral lines, contradicting classical physics, which predicted a continuous spectrum.

In 1911, Niels Bohr (Figure 4) arrived in England to study the atomic structure under Thomson first and with Rutherford later in Manchester. In 1913, in a series of three papers, Bohr proposed an atomic model that resolved the contradictions. While Einstein extended Planck's quantum hypothesis to photons, Bohr further extended it to electrons by introducing quantized orbits for electrons. Bohr's atomic model introduced three key quantum postulates:[25]

Figure 4. Niels Bohr. Reproduced with permission from ref 24. Copyright 1922 AB Lagrelius & Westphal.

(i) Electrons move in fixed circular orbits around the nucleus, where their *angular momentum* is quantized:

$$L = n\hbar = n\frac{h}{2\pi}, \quad n = 1, 2, 3, ... \tag{6}$$

where L is the electron's angular momentum, $\hbar = h/2\pi$ is the reduced Planck constant, and n is the principal quantum number specifying the allowed orbits. This assumption prevented electrons from spiraling into the nucleus, ensuring atomic stability.

(ii) The total energy of an electron in orbit is also quantized and given by

$$E_n = -\frac{13.6\text{eV}}{n^2} \tag{7}$$

where E_n is the energy of an electron in orbit n, and -13.6 eV is the ground-state energy of hydrogen (energy levels are negative, meaning that electrons are bound to the nucleus). This quantization explains why the atoms do not radiate continuously.

(iii) Electrons can transition between orbits, i.e., perform quantum jumps, by absorbing or emitting a photon of energy:

$$E_{\text{photon}} = h\nu = E_i - E_f \tag{8}$$

where ν is the frequency of emitted/absorbed light and E_i and E_f are the initial and final energy levels. This correctly explained hydrogen's spectral lines, known as the Balmer series, given by

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \tag{9}$$

where R_H is the Rydberg constant.

Thus, the Bohr model successfully explained the atomic stability and correctly predicted hydrogen spectral lines.[26] Most importantly, Bohr had conceptually generalized Planck's "mathematical trick" and made quantization a fundamental feature of nature. Bohr was awarded the Nobel Prize in Physics in 1922. With this, the first act ends, and the stage is set for even more surprising twists and turns.

4. ACT II: DE BROGLIE AND WAVE-PARTICLE DUALITY (1923–1924)

About ten years after Bohr, the next crucial conceptual breakthrough came in the form of further generalization of the wave-particle duality of light. In 1923, Prince Louis de Broglie (Figure 5) introduced the shocking concept of matter waves, which impressed Einstein so much that he remarked:[27] "He has lifted a corner of the great veil." Put simply, de Broglie asked himself: If light, which was thought of as a wave, can exhibit particle-like behavior (as photons), why cannot particles like electrons exhibit wave-like behavior? He defended this idea in his Ph.D. thesis on 25 November 1924, in Paris.[28] In this thesis, he proposed wave-particle duality for matter, suggesting that "matter waves" obey the equation

Figure 5. Louis de Broglie. Reproduced with permission from ref 29. Copyright 1929 University of Maryland

$$\lambda = \frac{h}{p} \tag{10}$$

where λ is the de Broglie wavelength and p is momentum. In 1927, Davisson and Germer, and independently Thomson and Reid, confirmed this idea in electron diffraction experiments. de Broglie received his Nobel Prize in Physics in 1929, a mere five years after his Ph.D. defense. Davisson and Thomson received theirs in 1937.

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One question physicists and historians have puzzled over for many years is why de Broglie, who discovered matter waves, did not proceed to discover Schrödinger's wave equation. Although we cannot be certain, experts have identified several reasons after conducting careful studies. Here, I quote Olivier Darrigol:[27]

"A first element of the answer is that, notwithstanding with his grand analogy between dynamics and optics, he (de Broglie) was shy in adventuring beyond the approximation of geometrical optics. He focused on retrieving results of the received quantum theory, such as the Bohr–Sommerfeld conditions, and he underplayed the more disturbing consequences of his concept of matter waves.

Another possible obstacle to his developing a wave theory of matter was his conviction that both light and matter had a dual nature, implying the synchronous motion of waves and particles. This duality focused on the interplay between waves and particles rather than on the search for a new wave equation.

Third and most importantly, de Broglie believed that the analogy between light and matter implied the electromagnetic nature of his matter waves. Consequently, he also believed that matter waves obeyed the d'Alembertian equation of electromagnetism. Direct evidence of this conviction is found in a note of 1925 in which he describes the intrinsic oscillation of an electron in its rest frame as the stationary superposition of the retarded and advanced solutions of the d'Alembertian equation.

The same heuristic principle, the analogy between matter and light, led de Broglie to the matter waves and prevented him from seeking a specific equation for these waves!"

Therein lies a very important lesson in the use of analogies to discover new conceptual breakthroughs. One should not take it too literally or expect an exact analogy of the new phenomenon in every detail. Although de Broglie was correct in reasoning that the wave-particle duality of light implied a similar duality for electrons (matter, in general), he took this analogy too far to reason that matter waves would also be electromagnetic in nature. This is where the analogy broke down. Fortunately, Schrödinger did not make this mistake!

5. ACT III: THE BIRTH OF QUANTUM MECHANICS (1925–1927)

Finally, we arrive at the main event, the birth of quantum mechanics. The key characters are Werner Heisenberg, Erwin Schrödinger, Max Born, Paul Dirac, and Wolfgang Pauli. Even a decade after the Bohr atom, atomic phenomena have remained largely unexplained, with many disturbing fundamental questions. There was no coherent mathematical theory yet, only a collection of seemingly ad hoc rules of quantum behavior. The transition from classical mechanics to quantum mechanics remained an elusive goal before 1925.

5.1. Heisenberg and Born: Matrix Mechanics. The first major breakthrough in resolving this impasse was initiated by 23-year-old Heisenberg (Figure 6) in his historic 1925 paper noted earlier,[3] marking the birth of quantum mechanics. Heisenberg's innovative idea, guided by Bohr's Correspondence Principle, was to retain classical mechanics equations but replace the classical position coordinate with a quantum-theoretical quantity. The new position quantity contains information about the measurable line spectrum of an atom rather than the unobservable orbital of the electron. He devised a special kinematical rule for multiplying position quantities. Mehra gives a vivid description of this momentous discovery:[2]

Figure 6. Werner Heisenberg. Reproduced with permission from ref 31. Copyright 1933 German Federal Archives.

"With the coming of spring in 1925, Heisenberg had developed a case of severe hay fever, which would just not leave him, and he decided to take a week or ten days off in June 1925 at the rocky island of Helgoland in the North Sea. At Helgoland, not only did he cure his hay fever but wiped the nose clean of the chronic colds of erstwhile problems of atomic mechanics ...

At Helgoland, Heisenberg divided his time in taking long walks, reading Goethe's West-Ostlicher Divan, and seeking to give his vague ideas on quantum mechanics a more definite shape. There he solved two problems ...

The example of the anharmonic oscillator showed him that a dynamical problem in quantum theory could be solved with the help of his scheme.

As he (Heisenberg) recalled:[30] 'It was almost three o'clock in the morning before the final result of my computations lay before me. The energy principle had held for all of the terms, and I could no longer doubt the mathematical consistency and coherence of the kind of quantum mechanics to which my calculations pointed. At first, I was deeply alarmed. I had the feeling that, through the surface of atomic phenomena, I was looking at a strangely beautiful interior and felt almost giddy at the thought that I now had to probe this wealth of mathematical structures nature had so generously spread out before me. I was far too excited to sleep, and so, as a new day dawned, I made a trip to the southern tip of the island, where I had been longing to climb a rock jutting out into the sea. I now did so without too much trouble, and waited for the sun to rise.'"

After he returned from Helgoland, Heisenberg gave his paper to Max Born (Figure 7) in early July for his opinion. Heisenberg was working as Born's research assistant at the University of Göttingen at that time. Born had been keenly aware of the difficulties in quantum theory for some time as he wrote:[32] "It becomes increasingly probable that not only new assumptions will be needed in the sense of physical hypotheses, but that the entire system of concepts of physics must be rebuilt from the ground up." So, when he saw Heisenberg's new mathematical

Figure 7. Max Born. Reproduced with permission from ref 33. Copyright 1954 German Federal Archives.

formulation of kinematics of quantum systems, Born immediately recognized its importance, as he recalls:[2]

> *"I began to ponder about his symbolic multiplication and was soon involved in it. I thought the whole day and could hardly sleep at night ... In the morning I suddenly saw the light: Heisenberg's symbolic multiplication was nothing but the matrix calculus, well-known to me since my student days from the lectures of Rosanes in Breslau."*

A few days later, on July 19, 1925, Born traveled from Göttingen to Hanover to attend a meeting of the German Physical Society, where he informed Wolfgang Pauli about the matrices. Pauli was critical:[2]

> *"Yes, I know that you are fond of a tedious and complicated formalism. You are only going to spoil Heisenberg's physical ideas by your futile mathematics."*

To a modern physicist, it is astonishing that Heisenberg did not know about matrices when he made his great discovery, as he admits:[5]

> *"At that time I must confess I did not know what a matrix was and did not know the rules of matrix multiplication."*

As Fedak and Prentis describe,[34] it was Born who recognized that the next step was to formalize Heisenberg's theory using the language of matrices, which he did with his student Pascual Jordan[35] after Pauli turned him down.[2] This was followed by another paper by Born, Heisenberg, and Jordan.[36] It was also Born who coined the name *Quantum Mechanics* for the new field.[34,37] Born expressed Heisenberg's results in a more elegant form using the matrix notation. If Q and P are the position and momentum matrices, they satisfy

$$[P, Q] = PQ - QP = (h/2\pi i)I \tag{11}$$

where I is the identity matrix, and the quantity $[P, Q]$ is known as the *commutator*. It is important to note that using matrices is not just a matter of mathematical elegance. What Heisenberg had discovered inadvertently was one of the fundamental aspects of quantum reality: its dynamic variables are represented by operators (and hence matrices), unlike classical variables, which are represented by scalars. This critical feature was also independently recognized by Paul Dirac around the same time[38] (more on this below). These papers introduced a novel approach to atomic Hamiltonian mechanics using noncommutative quantum methods. This marked the beginning of a new phase in theoretical physics, characterized by the use of Hermitian matrices, commutators, and eigenvalue problems as key mathematical tools in atomic theory.

This noncommutativity of position and momentum matrices led to a major breakthrough two years later, in 1927, while Heisenberg was visiting the Niels Bohr Institute in Copenhagen. He describes what happened one late evening as he took a stroll through *Faelledparken*, the lovely park behind the institute:[30]

> *"It must have been one evening after midnight when I suddenly remembered my conversation with Einstein and particularly his statement, 'It is the theory which decides what we can observe.' I was immediately convinced that the key to the gate that had been closed for so long must be sought right here. I decided to go on a nocturnal walk through Faelled Park and to think further about the matter. We had always said so glibly that the path of the electron in the cloud chamber could be observed. But perhaps what we really observed was something much less. Perhaps we merely saw a series of discrete and ill-defined spots through which the electron had passed. In fact, all we do see in the cloud chamber are individual water droplets, which must certainly be much larger than the electron. The right question should therefore be: Can quantum mechanics represent the fact that an electron finds itself approximately in a given place and that it moves approximately with a given velocity, and can we make these approximations so close that they do not cause experimental difficulties?*
>
> *A brief calculation after my return to the Institute showed that one could indeed represent such situations mathematically and that the approximations are governed by what would later be called the uncertainty principle of quantum mechanics: the product of the uncertainties in the measured values of the position and momentum (i.e., the product of mass and velocity) cannot be smaller than Planck's constant. This formulation, I felt, established the much-needed bridge between cloud chamber observations and the mathematics of quantum mechanics. True, it had still to be proved that any experiment whatsoever was bound to set up situations satisfying the uncertainty principle, but this struck me as plausible a priori since the processes involved in the experiment or the observation had necessarily to satisfy the laws of quantum mechanics. On this presupposition, experiments are unlikely to produce situations that do not accord with quantum mechanics. 'It is the theory which decides what we can observe.' I resolved to prove this by calculations based on simple experiments during the next few days."*

The uncertainty principle states that there is an intrinsic limit to how precisely we can simultaneously measure the position q and the momentum p of a particle. Heisenberg derived the following inequality:

$$\Delta q \cdot \Delta p \geq \frac{\hbar}{2} \tag{12}$$

where Δq is the standard deviation of position and Δp is the standard deviation of momentum. If we try to measure a particle's position very precisely (Δq small), the uncertainty in momentum Δp increases. Conversely, if we measure the momentum precisely, the uncertainty in the position grows. This principle is not due to measurement errors but rather an inherent property of quantum systems.

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Given this history of the uncertainty principle and its close association with the Niels Bohr Institute, I found it so fitting, in a lighter vein, to see this cartoon (Figure 8) displayed on a door of the Institute during my visit in August of 2022.

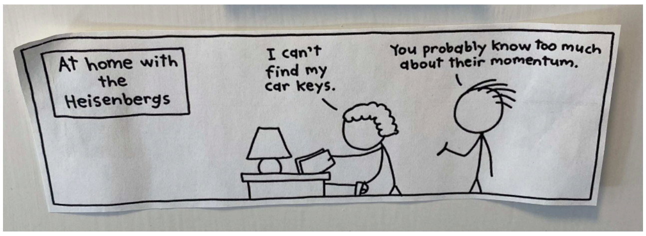

Figure 8. Cartoon on a wall of the Niels Bohr Institute. Photo by the author in 2022. Artist unknown.

There are serious implications captured by this fundamental property of nature. (i) Observer's interference: the very act of measurement disturbs the system. (ii) Wave-particle duality: position and momentum cannot be simultaneously well-defined. (iii) Limits of classical concepts: the classical idea of a trajectory does not hold in the quantum realm.

Heisenberg would later speak in sheer awe of the startling simplicity and beauty of the new theory:[30]

"If nature leads us to mathematical forms of great simplicity and beauty — by forms, I am referring to coherent systems of hypotheses, axioms, etc. — to forms that no one has previously encountered, we cannot help thinking that they are 'true,' that they reveal a genuine feature of nature ... You must have felt this too: the almost frightening simplicity and wholeness of the relationships which nature suddenly spreads out before us and for which none of us was in the least prepared."

Heisenberg was awarded the 1932 Nobel Prize in Physics. Given Born and Jordan's pivotal role in the discovery of quantum mechanics, it is natural to wonder why they were left out. In 1933, Heisenberg wrote Born saying:[39]

"The fact that I am to receive the Nobel Prize alone, for work done in Göttingen in collaboration—you, Jordan, and I—this fact depresses me, and I hardly know what to write to you. I am, of course, glad that our common efforts are now appreciated and I enjoy the recollection of the beautiful time of collaboration. I also believe that all good physicists know how great was your and Jordan's contribution to the structure of quantum mechanics—and this remains unchanged by a wrong decision from outside. Yet I myself can do nothing but thank you again for all the fine collaboration and feel a little ashamed."

Fortunately, Born was awarded the Nobel Prize in Physics in 1954 for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wave function (as discussed below). Engraved on Max Born's tombstone in Göttingen is a one-line epitaph: $pq - qp = h/2\pi i$.

5.2. Schrödinger's Wave Mechanics (1926). 1925 was already an amazing year, but the quantum mechanics revolution was not yet finished for the year. Following a line of attack that is different from the matrix mechanics formalism, Erwin Schrödinger (Figure 9) was developing something very interesting. Inspired by de Broglie's matter waves, he introduced *wave mechanics*, and the fundamental equation governing quantum evolution, the Schrödinger equation:

Figure 9. Erwin Schrödinger. Reproduced with permission from ref 40. Copyright 1930 Nobel Foundation.

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi \tag{13}$$

where $\hat{H}$ is the Hamiltonian operator and ψ is the wave function. The time-independent version,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{14}$$

explains energy quantization and atomic structure. Schrödinger showed that wave mechanics is mathematically equivalent to matrix mechanics.

Just as he proposed the matrix formalism to clarify Heisenberg's quantum mechanics, Max Born once again stepped up and clarified the meaning of the wave function in wave mechanics in 1926.[41] Born interpreted the wave function $\psi(x, t)$ as a probability amplitude. The probability of finding a particle at position x is given by:

$$P(x) = |\psi(x)|^2 \tag{15}$$

This marked a fundamental conceptual shift from a deterministic perspective of the universe in classical mechanics to a probabilistic view of quantum mechanics. It is indeed quite remarkable that such a fundamental interpretation that completely revolutionized our view of the universe was mentioned in a mere footnote of Born's 1926 paper.[41] In fact, there is a fascinating backstory to this. In a paper written on the occasion of the birth centenary of Born in 1982, Abraham Pais observed:[42]

"Then, Born declares: 'ϕ_{mn} (i.e. the wavefunction, $\psi(x)$) determines the probability for the scattering of the electron from the z-direction into the direction $[\theta, \phi]$.'
At best, this statement is vague. Born added a footnote in proof to his evidently hastily written paper: 'A more precise consideration shows that the probability is proportional to the square of ϕ_{mn}.' He should have said 'absolute square.' But he clearly had got the point, and so the correct expression for the transition probability concept entered physics via a footnote.

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I shall return shortly to the significant fact that Born originally associated probability with ϕ_{mn} rather than with $|\phi_{mn}|^2$. As I learned from recent private discussions, Dirac had the very same idea at that time. So did Wigner, who told me that some sort of probability interpretation was then on the minds of several people, and that he, too, had thought of identifying ϕ_{mn} or $|\phi_{mn}|$ with a probability. When Born's paper came out and $|\phi_{mn}|^2$ turned out to be the relevant quantity, 'I was at first taken aback but soon realized that Born was right,' Wigner said."

It is absolutely incredible and deeply instructive that such a fundamental feature of quantum mechanics, namely, its probabilistic nature, was initially guessed wrong even by giants like Born, Dirac, and Wigner, and was subsequently corrected in a footnote only during the proof stage of the manuscript. Again, this teaches us valuable lessons about the nature of the discovery process, particularly fundamental concepts.

Over the years, many have wondered why Schrödinger, of all theoretical physicists, took up de Broglie's ideas and developed them into wave mechanics.[43] We briefly saw above why de Broglie himself did not do it. Raman and Forman provide an interesting account[43] that de Broglie was not taken seriously by the quantum establishment:

"Thus in Copenhagen and in Gottingen, where atomic physics was pursued in the Copenhagen spirit, de Broglie would certainly have had the reputation of a renegade, if not exactly a crank, who stuck obstinately to his own ill-conceived theories ... Thus among the central European physicists deeply involved in the problems of theoretical spectroscopy, and this was indeed the great majority of those seriously concerned with the quantum theory, de Broglie must have had a very bad reputation."

On the other hand, Schrödinger had no such biases against de Broglie and so took his work seriously. There is a well-known anecdote due to Dirac[44] that the first wave equation Schrödinger guessed later became known as the relativistic Klein-Gordon equation. When this equation, applied to the hydrogen atom, did not yield the familiar results, Schrödinger abandoned this equation, searched again for a better candidate, and discovered the famous Schrödinger equation.

Felix Bloch, the 1952 Nobel laureate in Physics, who was a student at ETH-Zurich at that time, provides additional details[45] on the events when Schrödinger participated in their physics colloquium run by Peter Debye (Nobel Prize in Chemistry, 1936). Bloch recalls Schrödinger's seminar in early November 1925:

"Once at the end of a colloquium I heard Debye saying something like: 'Schrödinger, you are not working right now on very important problems anyway. Why don't you tell us some time about that thesis of de Broglie, which seems to have attracted some attention.'

So, in one of the next colloquia, Schrödinger gave a beautifully clear account of how de Broglie associated a wave with a particle and how he could obtain the quantization rules of Niels Bohr and Sommerfeld by demanding that an integer number of waves should be fitted along a stationary orbit. When he had finished, Debye casually remarked that he thought that this way of talking was rather childish. As a student of Sommerfeld he had learned that, to deal properly with waves, one had to have a wave equation ... Just a few weeks later he (Schrödinger) gave another talk in the colloquium which he started by saying: 'My colleague Debye suggested that one should have a wave equation; well, I have found one!'"

Prompted by Debye, Schrödinger discovered his famous equation in about three months, between November 1925 and January 1926, and published a series of four papers on wave mechanics entitled *Quantization as an eigenvalue Problem*.[46−48]

It is understandable that the members of the "Copenhagen Establishment" did not discover the wave equation, as they did not take de Broglie seriously. But I have often wondered why Einstein or Debye did not discover the wave equation themselves. I believe that while Einstein understood the importance of de Broglie's matter wave concept, he was too preoccupied with his search for the unified field theory, which he worked on for the rest of his life. As for Debye, it appears that he had some regrets, as narrated again by Bloch:[45]

"Many years later, I reminded Debye of his remark about the wave equation; interestingly enough he claimed that he had forgotten about it, and I am not quite sure whether this was not the subconscious suppression of his regret that he had not done it himself. In any event, he turned to me with a broad smile and said: 'Well, wasn't I right?'" "

Initially, Heisenberg's matrix mechanics and Schrödinger's wave mechanics appeared to be very different from each other, and an acrimonious debate ensued over which one was correct. In a footnote to a 1926 paper, Schrödinger wrote: "I was discouraged, if not repelled, by what appeared to me rather difficult method of transcendental algebra, defying any visualization." Meanwhile, Heisenberg complained to Pauli: "The more I think about the physical part of Schrödinger theory, the more detestable I find it." Fortunately, the debate was resolved in 1926. Schrödinger, along with Carl Eckert, working independently, demonstrated that the two new mechanics, although superficially very different, were mathematically equivalent to each other.

Schrödinger was awarded the Nobel Prize in Physics in 1933, which he shared with Paul Dirac, discussed next, for their contributions to quantum mechanics.

5.3. Commutator and the Poisson Brackets: Dirac's Discovery (1928−1930). Right before the paper by Born, Heisenberg, and Jordan was published in January 1926, another paper outlining the whole framework of quantum mechanics was published in the Proceedings of the Royal Society by Paul Dirac (Figure 10), then a research student of R. H. Fowler's in Cambridge. Reflecting on Heisenberg's paper, Dirac recalled:[49]

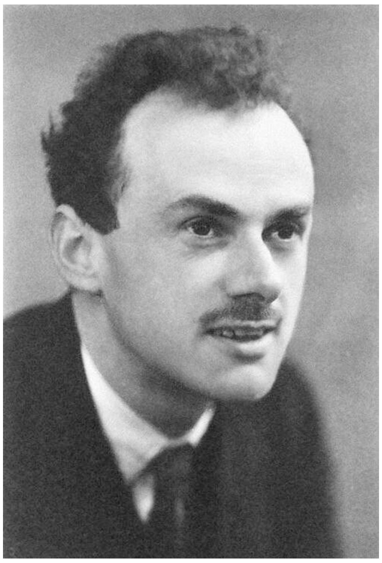

Figure 10. Paul Dirac. Reproduced with permission from ref 50. Copyright 1933 Nobel Foundation.

> *"During a long walk on a Sunday it occurred to me that the commutator might be the analogue of the Poisson bracket, but I did not know very well then what a Poisson bracket was. I had just read a bit about it and forgotten most of what I had read. I wanted to check up on this idea, but I could not do so because I did not have any book at home that gave Poisson brackets, and all the libraries were closed. So I had just to wait impatiently until Monday morning when the libraries were open to check on what Poisson bracket really was. Then I found that they would fit, but I had one impatient night of waiting."*

By recognizing the link between these two brackets, Dirac effectively clarified the connection between Heisenberg's variables and classical variables, giving the formulation a more classical appearance. Meanwhile, it neatly highlighted the precise point where the reformulation diverged from the classical theory.

Dirac was one of the most brilliant theoretical physicists of the twentieth century, making profound contributions to quantum mechanics, quantum field theory, and relativistic quantum mechanics. His work introduced the Dirac equation, predicted the existence of antimatter, and laid the mathematical foundation for quantum electrodynamics (QED). Dirac shared his Nobel in 1933 with Schrödinger.

5.4. Pauli Exclusion Principle (1925). As I wrap up this period of frenetic activity, I would be remiss if I did not mention the contributions of Wolfgang Pauli (Figure 11), particularly his exclusion principle. Pauli made fundamental contributions to quantum mechanics and quantum field theory, significantly shaping modern physics. His most famous work includes the Pauli exclusion principle, his contributions to spin theory, the theory of quantum electrodynamics (QED), and the prediction of the neutrino.

In 1925, Pauli formulated the exclusion principle, stating that no two identical fermions can occupy the same quantum state simultaneously. Mathematically, this means that for a system of two electrons, the wave function Ψ must be antisymmetric under particle exchange: $\Psi(1, 2) = -\Psi(2, 1)$. This ensures that if two electrons were in the same quantum state, then the wave function would be zero, prohibiting such configurations.

Figure 11. Wolfgang Pauli. Reproduced with permission from ref 51. Copyright 1945 Nobel Foundation.

The Pauli exclusion principle explains: (i) electron shell structure of atoms, (ii) periodic table organization and why different elements have distinct chemical properties, and (iii) stability of matter, as it prevents electrons from collapsing into the lowest energy state. For his contributions to the development of quantum mechanics, Pauli was awarded the Nobel Prize in Physics in 1945.

6. ACT IV: THE COPENHAGEN INTERPRETATION (1927−1930)

Starting with Heisenberg's matrix mechanics in 1925 and concluding with Dirac's relativistic quantum theory in 1930, in a short span of five years, a coherent mathematical formalism of quantum mechanics emerged. However, its conceptual implications seriously bothered several leading physicists, including those who contributed to its development, such as Einstein, Schrödinger, and others. Objecting to the probabilistic foundations of quantum mechanics, Einstein was perhaps the most vocal, famously saying:[52] "God does not play dice with the universe." On quantum entanglement,[52] he called it "spooky action at a distance." Schrödinger devised the famous Schrödinger's cat paradox to highlight the interpretational issues of quantum mechanics.

Despite such objections, physicists converged around a set of principles advocated by Bohr and Heisenberg in 1927, known as the *Copenhagen Interpretation*, which has remained the most widely accepted view of quantum mechanics for a century. The key tenets of this view are: (i) Nature at the quantum level is intrinsically probabilistic, and the square of the wave function $|\psi(x, t)|^2$ gives the probability of finding a particle at (x, t). (ii) A quantum system exists in a superposition until measured, at which point it collapses into a definite state. (iii) The act of measurement affects the system. (iv) Key quantities such as energy, momentum, spin, etc. are quantized.

There are some fundamental concerns with this interpretation of quantum mechanics, particularly with respect to the wave function collapse, which we shall not go into.[53−56] The fact that the predictions of quantum mechanics have been fantastically accurate, as verified by countless experiments over the decades, although its conceptual foundations are somewhat murky, prompted N. David Mermin, the physics professor who taught

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me quantum mechanics at Cornell, to summarize the Copenhagen Interpretation as "Shut up and calculate!" This quote is often misattributed to Richard Feynman.[57]

7. IMPACT OF QUANTUM MECHANICS IN CHEMICAL ENGINEERING

Although the objective of this paper is not on the application of quantum mechanics, I would like to briefly mention its profound impact on chemical engineering and materials science.[58,59] From reaction kinetics to materials design, quantum mechanics provides the fundamental principles that govern atomic interactions, electronic structure, chemical bonding, computational chemistry, catalysis, nanotechnology, and quantum computing, among other areas. Quantum mechanics provides insights into (i) molecular interactions and reaction mechanisms, (ii) electronic structures governing chemical and material properties, and (iii) energy levels that define molecular and solid-state behaviors. Using such information, chemical engineers optimize catalysts, polymers, drug molecules, and nanomaterials, improving efficiency and sustainability.

For example, the Schrödinger equation is routinely used to determine molecular structures and properties, such as bond lengths and angles, reaction energy barriers for kinetic analysis, and molecular orbitals and charge distributions. The Density Functional Theory is widely used to design catalysts, semiconductors, polymers, and nanomaterials. Quantum dots are yet another application for designing nanoscale semiconductors with tunable electronic properties used in LED displays and photovoltaics. Quantum confinement is utilized, for example, in the design of graphene-based sensors and supercapacitors for energy storage. As quantum technology advances, chemical engineering and materials science will continue to leverage its principles for sustainable industrial processes, advanced materials, and novel pharmaceuticals, driving innovation in the 21st century.

8. IS AI AT A "1900-MOMENT"?

From its origins in abstract thought to its applications in materials science and quantum computing, quantum mechanics is a testament to the power of the human intellect to unlock nature's most closely guarded secrets. Quantum mechanics revolutionized physics by fundamentally altering our understanding of nature on the atomic scale. As Bohr remarked: "If quantum mechanics has not profoundly shocked you, you haven't understood it yet."

The key conceptual breakthroughs, summarized in Table 1, reveal an interesting finding. It appears that even the pioneers missed the next conceptual step. For example, Planck considered his quantum hypothesis merely a "mathematical trick," not a fundamental law of nature, and, therefore, missed the connection with the photoelectric effect. Einstein understood this connection, but surprisingly, he did not realize its broader implications for other kinds of matter when he applied the hypothesis to photons. It was Bohr who connected it to electrons and their atomic orbitals, yet he, too, failed to grasp its generality. de Broglie was the one who perceived the universal nature of the wave-particle duality. However, his excessive reliance on electromagnetic wave analogies prevented him from discovering the wave equation, a feat accomplished by Schrödinger. Again, Schrödinger did not quite understand the conceptual significance of the wave function, which Born later interpreted probabilistically. Dirac accomplished the next conceptual step.

Table 1. Key Developments in Quantum Mechanics (1900–1930)

Year	Development
1900	Following Boltzmann's reasoning, Planck proposes his quantum hypothesis: Energy is quantized in discrete packets (quanta, $E = h\nu$).
1905	Einstein's photoelectric effect: Light behaves as particles (photons) with energy ($E = h\nu$).
1913	Bohr's atomic model: Electrons exist in quantized orbits, explaining hydrogen spectra.
1924	de Broglie's wave-particle duality: Matter exhibits both wave-like and particle-like properties.
1925	Heisenberg's matrix mechanics: The first mathematical formulation of quantum mechanics.
1925	Pauli Exclusion Principle: No two identical fermions (e.g., electrons) can occupy the same quantum state simultaneously, explaining the structure of electron shells in atoms.
1926	Schrödinger's wave equation: Describes quantum states using wave functions.
1926	Born's probabilistic interpretation: The absolute square of the wave function represents probability amplitudes, introducing the statistical nature of quantum mechanics.
1927	Heisenberg's uncertainty principle: Position and momentum cannot be precisely known simultaneously.
1927	The Copenhagen Interpretation: Quantum mechanics is fundamentally probabilistic. The wave function collapses upon measurement, and complementarity dictates that quantum objects exhibit either particle or wave-like behavior depending on observation.
1927	Confirmation of wave-particle duality in electron diffraction experiments by Davisson-Germer and Thomson-Reid.
1928	Dirac's relativistic quantum theory: Introduced the Dirac equation and predicted antimatter.
1930	Dirac's quantum field theory: Established the foundation of quantum electrodynamics (QED).

This analysis teaches us how hard conceptual discoveries are. As Heisenberg remarked: "As a rule, new concepts come up in a rather unclear and undeveloped form." This sequence of missed opportunities reminds us of how, in the technology space, IBM missed Microsoft (i.e., creating a software giant), Microsoft missed Apple (i.e., Apple products), Apple missed Google, Google missed Facebook, and all of them missed OpenAI. All were gigantic missed opportunities. I wonder what else lies ahead that we are missing now!

The early history of quantum mechanics illustrates how messy the discovery process really is. The textbooks and courses often gloss over this aspect, presenting the final equations as if they were reached clearly, smoothly, and logically. This is rarely the case. They are often discovered through clever guesswork. Even the most beautiful Einstein field equations of gravity were discovered in this manner.[60] I am reminded of a remark by Henri Poincare:[61] "Guessing before proving! Need I remind you that it is so that all important discoveries have been made?"

Our analysis also reveals that the key challenges were conceptual rather than mathematical. Planck's revolutionary quantum hypothesis is mathematically trivial: $\epsilon = h\nu$. Einstein's Nobel-winning equation is so simple that a high school student can understand: $h\nu = W + E_k$. Even Heisenberg-Born's matrix formulation or Schrödinger's equation is not tricky mathematically. Mathematical sophistication first emerged through Dirac's relativistic quantum mechanics and later in quantum field theory. Furthermore, the mathematical tools were already available and ready to be applied once the conceptual difficulties were resolved. For example, matrices, probability theory, and partial differential equations—the main tools of quantum mechanics—have been around for a long time. Similarly, for

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the theory of relativity. The mathematics of special theory is just elementary high school algebra, but the conceptual breakthroughs about space and time were colossal. The general theory required more sophisticated mathematics, to be sure, but it was readily available, thanks to Riemann.[60]

The only instance in the history of physics where the mathematical framework was also lacking, along with the need for a conceptual breakthrough, was the discovery of the theory of gravitation. In addition to the conceptual breakthrough of universal gravitation, Newton also had to develop the mathematical tool needed, namely, the calculus. However, this is the only exception that I am aware of.

This analysis suggests another valuable lesson for the present time. Like the 1900s clouds, I believe we have a large cloud now on the horizon: the lack of a theory for deep neural networks and large language models. By theory, I mean fundamental organizing principles that can predict important system-wide properties, such as the structure and behavior of LLMs, from token-level properties.[62,63] To be sure, significant progress has been made in the last three decades in neural network training, including the development of the backpropagation algorithm, various regularization techniques, reinforcement learning, and transformer architecture, among others. However, these are merely recipes for training; they do not provide a comprehensive theory of deep neural networks or large language models (LLMs). This is the central conceptual challenge facing AI today.

In 1972, physics Nobel laureate Philip Anderson published an influential paper entitled "More is Different".[64] He observed:

> *"The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity, entirely new properties appear, and the understanding of the new behaviors requires research that we think is as fundamental in its nature as any other ... At each stage, entirely new laws, concepts, and generalizations are necessary, requiring inspiration and creativity to just as great a degree as in the previous one. Psychology is not applied biology, nor is biology applied chemistry."*

In this sense, invoking another physics analogy, Newtonian mechanics and $F = ma$ can explain the dynamics of a few particles. However, when we have Avogadro's number (6.02×10^{23}) of molecules dynamically interacting in a gas, the collective behavior cannot be explained by applying Newton's law 10^{23} times! To be sure, $F = ma$ is going on at the *molecular* level, but much more happens at the *system* level that cannot be understood by Newton's Second Law alone.

To explain macroscopic phenomena, we need entirely new concepts, such as temperature, free energy, entropy, and chemical potential, to predict and explain the behavior of a gas. These concepts are absent at the individual particle level in Newtonian mechanics. We require an entirely new conceptual and mathematical framework, known as statistical mechanics, to address this new physics. It turns out that we need the Second Law of Thermodynamics and not the Second Law of Newton. This dichotomy between classical and statistical mechanics is like the proverbial "seeing trees but not the forest". The $F = ma$ perspective is "seeing the trees," and $S = k \ln W$ is "seeing the forest."

Likewise, large language models are not mere stochastic autocomplete engines. They have new emergent capabilities that require creating a new conceptual framework similar to the transformation from Newtonian to statistical mechanics or from classical to quantum mechanics. The LLMs may not have developed a human-like understanding of their domain, but they seem to have acquired a different kind of understanding and intelligence. Although it is difficult to say without any uncertainty that AI is at a "1900-moment," the signs are compelling. For millennia, we have taken for granted the meanings of words such as "understanding" and "intelligence" without much introspection. With the advent of LLMs, we are compelled to reevaluate our understanding of such concepts. LLMs raise profound philosophical questions about consciousness, free will, and the nature of creativity and intelligence, conceptual questions with which we are only beginning to grapple.

So, what would a mathematical theory of LLMs look like? As noted, I believe mathematical tools are already available: linear algebra, probability theory, statistical mechanics, game theory, graph theory, group theory, and topology. The challenge lies in discovering new concepts necessary for this problem. As discussed, quantum theory was born from the analysis of the energy distribution in blackbody radiation. Classical physics-based theories could not explain this distribution, which compelled Planck to propose a quantum hypothesis. Similarly, in well-trained deep neural networks, the connection weights are distributed lognormally. Neither the Hopfield nor the Boltzmann Machine model, which were recognized with the 2024 Nobel Prize in Physics, can predict or explain the lognormal outcome. Recently, a new conceptual framework,[63] called *statistical teleodynamics*, which combines game theory and statistical mechanics, has been proposed to predict this outcome as a first step toward a mathematical theory of LLMs. Borrowing from physics, the Hopfield and Boltzmann machine models employ *energy minimization*, whereas the new framework uses *effective-utility maximization* from economics as its organizing principle.

The ultimate theory of LLMs can potentially upend our views of cognition and sentience, much like the "1900-moment" did in physics a century ago. Thus, as Planck and Heisenberg remarked about how new concepts are born amid profound confusion, understanding the historical evolution of the quantum mechanical concepts could be helpful in a similar situation to that we face in artificial intelligence.

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Notes

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