

MATHEMATICAL HISTORY OF WAVE AND MATRIX QUANTUM MECHANICS

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Summary

The present chapter is a historical and pedagogical survey of the development of early quantum mechanics. As the title suggests, this work is about the history of the mathematical formalism of quantum mechanics in the short period between 1925/1926 (when wave and matrix mechanics were introduced) and 1932 when the first consistent proof of the equivalence between the two formalisms was given by J. von Neumann in his celebrated book *Mathematische Grundlagen der Quantenmechanik*.

In order to deal with atomic systems, Heisenberg developed matrix mechanics in 1925. Some time later, in the winter 25/26, Schrödinger established his wave mechanics. In the spring of 1926, quantum physicists had two theoretical models that allowed them to predict the same behavior for quantum systems, but both of them were very different. Schrödinger thought that the empirical equivalence could be explained by means of a proof of mathematical equivalence. The bulk of the present work revolves around this equivalence problem and is mainly dedicated to showing that the equivalence proofs, taken for granted in many books on history and foundations of quantum mechanics, were not conclusive. These proofs were presented by E. Schrödinger and independently by C. Eckart, more or less at the same time. The argument is that what made invalid the purported equivalence proofs were a great many imprecise points in them. The

contribution made by P. A. M. Dirac and P. Jordan to the same problem, regarding the introduction of the transformation theory, is also briefly discussed in the chapter, which finishes with the definitive solution to the mathematical equivalence given by Von Neumann. This chapter also gives a brief account of the aforementioned proof of equivalence between matrix mechanics and wave mechanics at a level accessible to physics students, teachers and researchers.

1. Introduction

Nowadays a classical mechanics course devotes a lot of time to various formulations of classical mechanics (Newtonian, Lagrangian, and Hamiltonian). However, most undergraduate and graduate level quantum mechanics courses present an amalgam of the wavefunction and matrix formulations, with an emphasis on the wavefunction side. They emphasize the wavefunction formulation almost to the exclusion of all variants. This fact implies that, for example, physics students do not take into account the important role that matrix theory played as a vehicle of discovery in quantum physics. The ever-popular wave mechanics was not the first quantum mechanics to be discovered. Moreover, as a matter of fact, physics students do not know one of the most interesting episodes of the history and philosophy of physics: the mathematical and empirical equivalence between matrix and wave mechanics. Heisenberg's mechanics and Schrödinger's mechanics differ dramatically in conceptual and epistemological overview, yet both make identical predictions for all experimental results and both of them are mathematically equivalent. The aim of this presentation is to give an account of the development of the mathematical equivalence of quantum mechanics at a level accessible to students. From Schrödinger's equivalence paper until Von Neumann's famous book, *Mathematical foundations of quantum mechanics*, passing through Dirac's work, all angles of approach are considered.

2. Old Quantum Theory

In order to deal with Nature, physicists postulate theoretical models as instruments intended to explain phenomena and to make testable predictions about the empirical domains they are concerned with. Every branch of theoretical physics: from cosmology to microphysics, and nearly every theoretical discipline, uses theoretical models. They are specially useful during the outset of emerging research fields. A theoretical model is a mathematical structure used to describe the behavior of a real system. The great strength of mathematics is that it enables physicists to describe abstract patterns that cannot be perceived by their own senses. Every algebraic, differential or integral equation or set of such equations defines a kind of pattern. The description of the pattern provided by the model is a tool which enables them to predict the manifestations that will appear under determined circumstances.

Starting in the seventeenth century, and continuing to the present day, physicists have developed a set of models that describe a lot about the world around us: the motion of a cannonball, the orbit of a planet, the working of an engine, etc. This body of ideas is called classical mechanics. In 1905, Albert Einstein realized that these ideas did not apply to objects moving at high speeds (that is, at speeds near the speed of light) and he developed an alternative set of models called relativistic mechanics. Classical

mechanics is wrong in principle, but it is a good approximation to relativistic mechanics when applied to objects moving at low speeds.

At about the same time, several experiments led physicists to realize that the classical models did not apply to very small objects, such as molecules and atoms, either. Over the period 1900-1932 a number of physicists (Planck, Bohr, Heisenberg, De Broglie, Schrödinger, and others) developed an alternative quantum mechanics. Classical mechanics is wrong in principle, but it is a good approximation to quantum mechanics when applied to large objects.

A full history of quantum mechanics would be a story full of serendipity, personal squabbles, opportunities missed and taken, and of luck both good and bad. It would have to discuss Schrödinger's many mistresses, Ehrenfest's suicide, and Heisenberg's involvement with Nazism (Cropper 1970). And it would have to treat the First World War's effect on the development of science (Forman 1971).

But this chapter does not contain a social but a mathematical history of quantum mechanics. In the sequel, the author is going to spend some space on the old atomic models, which will be explained now, because quantum physics grew out from attempts to understand the behavior of atomic systems. The strange quantum world and the need for new mathematics have their origin in this research.

2.1 From Planck to Bohr

The heroic origin of quantum theory dates from December 14th, 1900. In this date, during the meeting of the German Physical Society, Max Planck read a paper titled 'On the Law of Distribution of Energy in the Normal Spectrum'. The date of its presentation is considered the birth date of quantum physics, even though it was not until a quarter of a century later that Heisenberg, Schrödinger and others developed modern quantum mechanics. The *dramatis personae* of the prehistory of quantum theory (1900-1924) includes the names of Max Planck, Albert Einstein and Niels Bohr, among others.

In 1900, Planck reported his investigations on the law of black-body radiation. He had discovered a discontinuous phenomenon totally unknown to classical physics. The energy of vibrating systems could not change continuously, but only in such a way that it always remained equal to an integral number of so-called *energy-quanta*. The proportionality factor had to be regarded as a new universal constant, known as Planck's constant h (from the German *Hilfsmittel*, auxiliary) since then. All this implied a rupture, because energy could not be treated any longer as a continuous variable. Planck introduced an intrinsic discontinuity: the *quantum discontinuity*.

A few years later, in the years 1905-1907, Albert Einstein emphasized another consequence of Planck's results, namely, that radiant energy could only be emitted or absorbed by an oscillating particle in so-called *quanta of radiation*, the magnitude of each was equal to Planck's constant h multiplied by the frequency of radiation ν . The hypothesis of *light-quanta* led Einstein to his well-known theory of the photoelectric effect, which was well supported by R. Millikan's experiments. These experiments always gave the same value of Planck's constant h .

The knowledge of atomic structure was reached through the discovery of the electron, due to J. J. Thomson, and through the discovery of the atomic nucleus, which we owe to E. Rutherford, by studying radioactive substances and working with α - and β -particles. Towards 1910, experimental evidence existed that atoms were made up of electrons. Given that atoms were neutral, they had to contain a positive charge equal in magnitude to the negative charge provided by their electrons. Thomson proposed a tentative model, whereby the negatively charged electrons were found inside a positively charged distribution. In 1911, Rutherford demonstrated that the positive charge was not distributed throughout the atom, but on the contrary, was concentrated in a very small area that could be considered the atomic nucleus. An atom was built up of a nucleus that had a positive electrical charge, together with a number of electrons which had a negative charge and move around the nucleus. This picture had a resemblance to a planetary system.

However, this conception did not provide a better explanation for the spectra of the atoms. It was impossible to understand why atomic spectra consisted of sharp lines at all. Moreover, according to classical electrodynamic theory, electrons had to fall onto the nucleus because their motion would emit a continuous radiation of energy from the atom. Who could explain the data of the spectroscopy and the amazing stability of atoms? A genius called Niels Bohr, a Dane (age 28) who had recently worked in Rutherford's laboratory. He avoided these difficulties by introducing concepts borrowed from quantum theory. Bohr exploited the quantum discontinuity in his first atomic theory.

Bohr's leading role in the development of atomic theory began in 1913 with a fundamental memoir, 'On the constitution of atoms and molecules', published in three parts in the *Philosophical Magazine*. Bohr's atomic theory emerged from an endeavor to explain the properties of chemical elements on the basis of Rutherford's planetary model of atoms. While the most obvious property expected from real atoms was their stability with respect to external perturbations, Bohr found that Rutherford's model was unstable, both mechanically and electro-dynamically. Not discouraged by this conflict, he proposed a quantum notion of stability that was embodied in his concept of *stationary state*. In the first part of his trilogy, Bohr introduced this concept. The stability of atoms transcended classical mechanical explanation. The essential motivation for the introduction of this bold hypothesis was the impossibility of adapting the mechanical stability arguments of Thomson's atom to the new planetary models.

The atomic model of Bohr solved the riddle by means of two postulates. The first one accounted for the stability of the atom and it stated that an atomic system cannot exist in all mechanically possible states, forming a continuum, but in series of discrete stationary states. The second postulate accounted for the line-spectra. It claimed that the difference in energy in a transition from one stationary state to another was emitted or absorbed as a light quantum $h\nu$. By definition the stationary states were subject to the following assumptions, which were mostly suggested by the quantum theory of Planck and Einstein, and the simple regularities of the hydrogen spectrum:

I. An atomic system can, and can only, exist permanently in a certain series of

states corresponding to a discontinuous series of values for its energy, and that consequently any change of the energy of the system, including emission and absorption of electromagnetic radiation, must take place by a complete transition between two such states. These states will be denoted as the ‘stationary states’ of the system.

II. The radiation absorbed or emitted during a transition between two stationary states is ‘unifrequent’ and possesses a frequency ν , given by the relation

$$E' - E'' = h\nu \quad (1)$$

where h is Planck’s constant and where E' and E'' are the values of the energy in the two states under consideration. (Van der Waerden 1968, 97-98.)

The strange conception of atoms as systems which were only able to assume discrete energy changes was a masterpiece because it gave an explanation of the Balmer formula and the Rydberg constant. Bohr’s theory was remarkably successful in explaining the colours emitted by hydrogen glowing in a discharge tube, and the Periodic System of the elements. Moreover, it sparked enormous interest in developing and extending the old quantum theory.

This development was hindered but not halted completely by the start of the First World War in 1914. During the war Arnold Sommerfeld made progress on the implications of quantization. He extended the circular orbits of Bohr to elliptical orbits, and he refined his atomic model by introducing several quantum numbers in order to explain the fine structure shown by the hydrogen spectrum when it was observed with a spectroscope of high resolving power.

With the coming of the armistice in 1918, work in quantum mechanics expanded rapidly. Many theories were suggested and many experiments performed. To cite just one example, in 1922 O. Stern and his graduate student W. Gerlach performed their important experiment on the deflection of particles, often used to illustrate the basic principles of quantum physics. They demonstrated the space quantization rule, that is, the magnetic moment of the silver atoms could take only two positions, not a continuum one. At the turn of the year from 1922 to 1923, physicists looked forward with enormous enthusiasm towards detailed solutions of the outstanding problems, such as the helium problem and the anomalous Zeeman Effect (the split lines in a magnetic field). However, within less than a year, the investigation of these problems revealed an almost complete failure of Bohr’s atomic theory. Bohr’s model, which was perfected by Sommerfeld’s quantization rules, worked when applied to the spectrum of the hydrogen atom, even solving the relativistic fine-structure and the split lines in an electric field (the Stark Effect). Nevertheless, there was a great difficulty: it was not possible to use the Bohr-Sommerfeld quantization rules for the anomalous Zeeman Effect and for the helium atom, whose electrons rotate around the nucleus, because the three-body problem, of difficult mathematical treatment, is encountered. The anomalous Zeeman Effect and the helium spectrum were the two stumbling blocks in the old quantum theory.

3. Early Quantum Mechanics

Old quantum physics was a house built on sand. Each problem had to be solved first within the classical physics realm, and only then the solution could be translated by means of diverse computation rules – for instance, the correspondence principle of Bohr, i.e. the view of classical mechanics as a limit case of quantum theory – into a meaningful statement in quantum physics. Bohr's principle of correspondence transferred a number of conclusions formulated in classical mechanics to quantum theory. This consisted in the obvious requirement that ordinary classical mechanics had to hold to a high degree of approximation in the limiting case where the numbers of the stationary states, the so-called *quantum numbers*, were very large. The correspondence principle acted as a code book for translating a classical relation into its quantum counterpart. It was a daring fusion of old and new. But these rules revealed a dismaying state of affairs in 1924. In words of Bohr, Kramers and Slater, 1924:

'At the present state of science it does not seem possible to avoid the formal character of the quantum theory which is shown by the fact that the interpretation of atomic phenomena does not involve a description of the mechanism of the discontinuous processes, which in the quantum theory of spectra are designated as transitions between stationary states of the atom.' (Van der Waerden 1968, 159.)

Quantum physicists became more and more convinced that a radical change on the foundations of physics was necessary, that is to say: a new kind of mechanics which they called *quantum mechanics*. To tell the truth, the name was coined by Max Born in a 1924 paper. Werner Heisenberg, who at that time was Born's assistant, had to come into the scene. Beginning with Heisenberg's inspired bout of hay fever of 1925, we follow the development of matrix mechanics and Schrödinger's wave mechanics, and end the tour with the comparison of both formalisms.

3.1 Matrix Mechanics

In June 1925 Werner Heisenberg cut the Gordian knot and developed matrix mechanics in his historic paper '*Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen*', although he did not even know what a matrix was, as he confessed and Max Born and Pascual Jordan pointed out.

Heisenberg aimed at constructing a quantum-mechanical formalism corresponding as closely as possible to that of classical mechanics. Thus he considered the classical equation of motion

$$\ddot{x} = f(x) \tag{2}$$

where he substituted \ddot{x} and $f(x)$ by their quantum analogues. The classical position q and momentum p (and their operations $q^2, p^2, pq...$) were assigned the quantum position Q and the quantum moment P (and, respectively, their operations $Q^2, P^2, PQ...$), where Q and P were sets of numbers completely determined by the intensity and frequency of the emitted or absorbed atomic radiation. The new kinematic

quantities contained information about the measurable line spectrum of an atom rather than the unobservable orbit of the electron.

Fourier's orbital components

$$f_n(t) = \sum_k f(n, k) = \sum_k x(n, k) \exp\{2\pi i v(n, k)t\} \quad (3)$$

were substituted by the respective radiation elements

$$f_n(t) = \sum_k x_{n,n-k} \exp\{2\pi i v_{n,n-k}t\}, \quad (4)$$

where $x_{n,n-k}$ and $v_{n,n-k}$ were the amplitude and the frequency of the transition radiation between two stationary states n and $n-k$. In Heisenberg's theory, therefore, the places of the particle coordinates q or p were taken by sets Q and P of numbers corresponding to the Fourier coefficients of classical motion.

Inspired in Einstein's theory of relativity, Heisenberg had eliminated these representations that did not correspond to experimentally observable facts. To put it another way, the old picture of electronic orbits. Given that an electron trajectory inside an atom was not observable, it was necessary to drop such a concept and the concepts associated to it, like those of position and velocity. Only intensities, frequencies, and amplitudes of radiation were observable, because they could be determined by spectral lines. The new theory replaced the electron orbits by square arrays that represented emitted or absorbed radiation. That is, for instance,

$$\left\{ x_{n,n-k} \exp(2\pi i v_{n,n-k}t) \right\}_{n,k}. \quad (5)$$

Those square arrays Q and P were matrices, as Born and Jordan (1925) indicated. Heisenberg did not really arrange his quantum-theoretical quantities into a table or array. He began to deal with sets of allowed physical quantities. But Born looked at these sets of numbers and he suddenly saw that they could be interpreted as mathematical matrices. Furthermore, Born could not take his mind off Heisenberg's symbolic rule for multiplying kinematic quantities, and after a time of intensive thought and trial he suddenly remembered an algebraic theory which he had learned from his teacher, Professor Rosanes, in Breslau. In 1925, matrix calculus was an advanced abstract technique, well known to Born from his student days from the lectures of Rosanes in Breslau, but Heisenberg struggled with it. Born realized that Heisenberg's multiplication rule was nothing but to the mathematical rule for multiplying matrices. In fact, if

$$A = \left\{ x_{n,n-k} \exp(2\pi i v_{n,n-k}t) \right\}_{n,k} \quad (6)$$

and

$$B = \left\{ y_{n,n-k} \exp(2\pi i v_{n,n-k} t) \right\}_{n,k}, \quad (7)$$

then

$$A \cdot B = \left\{ z_{n,n-k} \exp(2\pi i v_{n,n-k} t) \right\}_{n,k} \quad (8)$$

where

$$z_{n,n-k} = \sum_j x_{n,n-j} y_{n-j,n-k}. \quad (9)$$

This led to the puzzling result that the commutation law was no longer necessarily valid. That is, A times B does not necessarily equal B times A in quantum mechanics. This was particularly important when Born and Jordan obtained the quantum mechanical expression corresponding to the quantum conditions in the old quantum theory.

Some days later Born met Pauli in a train from Göttingen to Hannover and asked him to collaborate on the matrix program but he impertinently declined the invitation, on the grounds that Göttingen's futile mathematics would spoil Heisenberg's physical ideas. Pauli vilified 'Göttinger formalen Gelehrsamkeitsschwall' (Göttingen's torrent of erudite formalism). This rejection failed to demoralize Born, who immediately set out to work with a more benevolent collaborator, his pupil Pascual Jordan, who overheard Born discussing matrix theory with Pauli on the train. The next step was to formalize Heisenberg's theory using the language of matrices. The mathematical method of treatment inherent in the new quantum mechanics was characterized by the use of matrix calculus in place of the usual number analysis.

Born and Jordan (1925) proved that the matrices P and Q satisfied the so-called *exact quantum condition*:

$$PQ - QP = \frac{h}{2\pi i} I. \quad (10)$$

In fact, if $Q = (q_{m,n} \exp(2\pi i v_{m,n} t))_{m,n}$, $P = (p_{m,n} \exp(2\pi i v_{m,n} t))_{m,n}$, and $D = PQ - QP = (d_{m,n} \exp(2\pi i v_{m,n} t))_{m,n}$, then, using the *old quantum condition* $J = nh$ and the Born rule $k \frac{\partial \Phi(n)}{\partial n} = \Phi(n) - \Phi(n-k)$ to transform continuous functions in discrete functions, the diagonal elements are:

$$d_{n,n} = \sum_k (p_{n,k} q_{k,n} - q_{n,k} p_{k,n})$$

$$\begin{aligned}
 &= \sum_k (p_{n,n-k} q_{n-k,n} - q_{n,n+k} p_{n+k,n}) = -\sum_k k \frac{\partial}{\partial n} [p(n,k) q(n,-k)] \\
 &= \frac{1}{2\pi i} \frac{\partial}{\partial n} \sum_k -2\pi i k p(n,k) q(n,-k) = \frac{1}{2\pi i} \frac{\partial}{\partial n} \int p q' dt = \frac{1}{2\pi i} \frac{\partial}{\partial n} \oint p dq \\
 &= \frac{1}{2\pi i} \frac{\partial}{\partial n} J = \frac{1}{2\pi i} \frac{\partial}{\partial n} nh = \frac{1}{2\pi i} h = \frac{h}{2\pi i}.
 \end{aligned} \tag{11}$$

The non-diagonal elements of the matrix D are zero because

$$D' = (PQ - QP)' = (2\pi i v_{m,n} d_{m,n} \exp(2\pi i v_{m,n} t))_{m,n} = 0 \tag{12}$$

if and only if $d_{m,n} = 0$ (for $m \neq n$).

That matrix equation (10) was the only one of the formulae in quantum mechanics proposed by Heisenberg, Born and Jordan, in the known as ‘Dreimännerarbeit’ (1926), which contained Planck’s constant h , and it was a re-interpretation of the Bohr-Sommerfeld quantum conditions. In fact, this equation was engraved on Born’s tombstone as an epitaph.

Finally, a variational principle, derived from correspondence considerations, yielded certain motion equations for a general Hamiltonian $H = H(Q, P)$, which was a close analogue of the classical canonical equations:

$$\begin{cases} \dot{Q} = \frac{\partial H}{\partial P} \\ \dot{P} = -\frac{\partial H}{\partial Q} \end{cases} \tag{13}$$

The exact quantum condition (10) together with these equations of motion (13) were sufficient to define all matrices and hence the experimentally observable properties of the atom.

Consequently, the basic matrix-mechanical problem was merely that of integrating these motion equations (13), i.e. the algebraic problem of diagonalizing the Hamiltonian matrix H , whose eigenvalues were the quantum energy levels. Born, Jordan and Heisenberg applied the rules of matrix mechanics to a few highly idealized problems and the results were quite satisfactory. However, there was, at that time, no rational evidence that their matrix mechanics would prove correct under more realistic conditions. The first physically important application of Göttingen’s matrix theory was made several months later by Wolfgang Pauli, who calculated the stationary energy values of the hydrogen atom, and found complete agreement with Bohr’s formulae.

‘The three-men mechanics’ managed to avoid the problems posed by old quantum theory: on the one hand, it substituted the electron orbits by discrete states defined by

way of matrices; on the other hand, the satisfactory explanation of the hydrogen spectrum created the expectation that finally it would be possible to explain multielectronic atoms.

Summing up, *matrix mechanics* was presented in a fully developed form in the famous ‘three-men’s paper’ of Born, Heisenberg and Jordan (and also in Dirac’s first paper on quantum mechanics, received 7 November 1925, which contained an analogous theory of such non-commutating symbols P and Q , inspired by a lecture of Heisenberg in Cambridge). This theory was based upon four hypotheses:

MM₁. The behavior of a quantum mechanical system is determined by the (Hermitian) matrices $Q = (q_{mn} e^{2\pi i t v_{mn}})$ and $P = (p_{mn} e^{2\pi i t v_{mn}})$ (one matrix Q for every coordinate q , and one P for every momentum p) where the amplitudes and the frequencies satisfy:

$$q_{mn} = q_{nm}^* \quad (14)$$

$$p_{mn} = p_{nm}^* \quad (15)$$

$$v_{mn} = -v_{nm} \quad (16)$$

$$v_{mn} \neq 0 \quad \text{for } m \neq n \quad (17)$$

$$v_{rs} + v_{st} = v_{rt} \quad (18)$$

MM₂. The quantum mechanical matrices Q and P satisfy the exact quantum condition:

$$PQ - QP = \frac{h}{2\pi i} I \quad (19)$$

where I is the identity matrix.

MM₃. Equations of motion

$$\dot{Q} = \frac{\partial H}{\partial P}, \quad \dot{P} = -\frac{\partial H}{\partial Q}. \quad (20)$$

MM₄. If Q and P verify the last three axioms, then the Hamiltonian H is a diagonal matrix, having as diagonal elements the energy values, i.e. $\sigma(H) = \{E_n\}$. Otherwise it is necessary to find a *canonical transformation* (nowadays called *unitary transformation*), that is an orthogonal matrix S such that $S^{-1}HS$ is diagonal (in this case $S^{-1}QS$ and $S^{-1}PS$ verify **MM₁**-**MM₃**).

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