A brief history of the mathematical equivalence between the two quantum mechanics

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Abstract

The aim of this paper is to give a brief account of the development of the mathematical equivalence of quantum mechanics. In order to deal with atomic systems, Heisenberg developed matrix mechanics in 1925. Some time later, in the winter of 1926, Schrödinger established his wave mechanics. In the spring of 1926, quantum physicists had two theoretical models that allowed them to predict the same behaviour of the 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.

Keywords: Matrix mechanics, wave mechanics, mathematical equivalence.

Resumen

El objetivo de este artículo es ofrecer una breve reseña del desarrollo de la equivalencia matemática de las mecánicas cuánticas. Para tratar con los sistemas atómicos, Heisenberg desarrolló la mecánica matricial en 1925. Algún tiempo después, en el invierno de 1926, Schrödinger estableció su mecánica ondulatoria. En la primavera de 1926, los físicos cuánticos disponían de dos modelos teóricos que les permitían predecir el mismo comportamiento de los sistemas cuánticos, pero ambos eran muy diferentes. Schrödinger pensó que la equivalencia empírica podría ser explicada mediante una prueba de equivalencia matemática.

Palabras clave: Mecánica matricial, mecánica ondulatoria, equivalencia matemática.

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I. INTRODUCTION

Quantum physics grew out from attempts to understand the strange behaviour of atomic systems, which were capable of assuming discrete energy changes only. The heroic origin of quantum theory dates from December 14th, 1900. The *dramatis personae* of the prehistory of quantum theory (1900-1924) includes the names of Max Planck, Albert Einstein or Niels Bohr. However, old quantum physics was a bridge over troubled waters: 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)– into a meaningful statement in quantum physics. These rules revealed a dismaying state of affairs in 1924. In words of Bohr, Kramers & Slater [1]:

> "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."

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.

II. MATRIX MECHANICS

In 1925 Werner Heisenberg developed matrix mechanics (MM) in his paper *Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen* [2], although he did not even know what a matrix was, as 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

$$\ddot{x} = f(x), \tag{1}$$

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 matrices completely determined by the intensity and frequency of the emitted or absorbed atomic radiation. These matrices satisfied the so-called 'exact quantum condition'

$$PQ - QP = \frac{h}{2\pi i} I . \tag{2}$$

This equation was the only one of the formulae in quantum mechanics proposed by Heisenberg, Born & Jordan which contained Planck's constant h. Finally, a variational principle, derived from correspondence considerations, yielded certain motion equations for a general Hamiltonian H, which was a close analogue of the classical canonical equations

$$\dot{Q} = \frac{\partial H}{\partial P}\ ;\ \dot{P} = -\frac{\partial H}{\partial Q} . \tag{3}$$

Consequently, the basic matrix-mechanical problem was merely that of integrating these motion equations, *i. e.* the algebraic problem of diagonalizing the Hamiltonian matrix, whose eigenvalues were the quantum energy levels.

III. WAVE MECHANICS

In the winter of 1926 Erwin Schrödinger established his *Wellenmechanik* [3, 4]. The fundamental idea of wave mechanics (WM) was that the quantum phenomena had to be described adequately by specifying a definite wave function ψ . The wave equation that replaced the classical equation of motion was Schrödinger's equation:

$$\tilde{H}\psi = E\psi , \tag{4}$$

where $\tilde{H}$ is the operator obtained by substitution of q and p in the classical Hamiltonian by the operators

$$\tilde{Q} = x \tag{5}$$

and

$$\tilde{P} = -i\hbar \frac{\partial}{\partial x} . \tag{6}$$

The basic wave-mechanical problem was now that of solving this partial differential equation. The eigenvalues E_n were, according to Schrödinger, the quantum energy levels.

However one month before Schrödinger published his famous equation (4), the Hungarian physicist Cornel Lanczos wrote an integral equation as the first non-matricial version of quantum mechanics [5]. But if we transform the integral equation into a differential one, there results the Schrödinger equation (4) for stationary states [6].

Thus in the spring of 1926 quantum physicists disposed of two theoretical models in order to deal with such observable phenomena like the electromagnetic emission and absorption atomic spectra (quantum spectra). In other words, they had two different hypothetical reconstructions of quantum phenomena for the prediction of the same behaviour of the quantum system under investigation. Both of them were mathematically different but empirically equivalent. How could this fact be accounted for?

IV. THE MATHEMATICAL EQUIVALENCE BETWEEN MATRIX MECHANICS AND WAVE MECHANICS

Schrödinger thought that the empirical equivalence could be explained by means of a proof of mathematical equivalence. Were he able to prove the mathematical equivalence of MM and WM, then a weaker equivalence should also hold: both mechanics would necessarily be empirically equivalent. That was the aim of his paper *Über das Verhältnis der Heisenberg-Born-Jordanschen Quantenmechanik zu der meinen* of May, 1926 [7]. In his own words:

> "Considering the extraordinary differences between the starting-points and the concepts of Heisenberg's quantum mechanics and of the theory which has been designated 'undulatory' or 'physical' mechanics, and has lately been described here, it is very strange that these two new theories agree *with one another* with regard to the known facts, where they differ from the old quantum theory. [...] That is really very remarkable, because starting-points, presentations, methods, and in fact the whole mathematical apparatus, seem fundamentally different. [...] In what follows the very intimate *inner connection* between Heisenberg's quantum mechanics and my wave mechanics will be disclosed. From the formal mathematical standpoint, one might well speak of the *identity* of the two theories."

However Schrödinger was not able to establish the mathematical equivalence between WM and MM due to conceptual and technical difficulties [8, 9, 10, 11]. He did prove indeed that WM is contained in MM, but not the reciprocal, and this is a serious flaw. To be precise: given an arbitrary complete orthonormal system of proper wave functions $\{\varphi_k\}$, Schrödinger was able to show that each operator $\tilde{F}$ of WM could be related to a matrix *F* of MM in the following way:

$$\Theta_{\{\varphi_k\}} : \{ \textit{Operators of WM} \} \to \{ \textit{Matrices of MM} \},$$

$$\tilde{F} \mapsto F = \begin{pmatrix} F_{11} & F_{12} & \cdots & \cdots \\ F_{21} & \ddots & & \\ \vdots & & F_{mm} & \\ \vdots & & & \ddots \end{pmatrix} =$$

$$= (F_{mn}) = (\int_{-\infty}^{+\infty} \varphi_m^*(x)\tilde{F}(\varphi_n)(x)dx), \quad (7)$$

i. e., as Schrödinger [7] claims: "a matrix element is computed by *multiplying* the function of the orthogonal system denoted by the *row*-index [...] by the result arising from using our operator in the orthogonal function corresponding to the *column*-index, and then by *integrating* the whole over the domain". In particular, Schrödinger obtained:

$$\tilde{Q} \overset{\Theta}{\mapsto} (Q_{mn}) = (\int_{-\infty}^{+\infty} \varphi_m^*(x) x \varphi_n(x)dx) \quad (8)$$

and

$$\tilde{P} \overset{\Theta}{\mapsto} (P_{mn}) = (-i\hbar \int_{-\infty}^{+\infty} \varphi_m^*(x) \frac{\partial}{\partial x} \varphi_n(x)dx) \quad (9)$$

where the results *Q* and *P* satisfy Heisenberg's formal rules (the so called 'exact quantum condition'). The main issue here was whether or not the algebraic morphism Θ is an isomorphism.

Obviously morphism Θ between operators in WM and matrices in MM is not an isomorphism, since every undulatory operator is assigned a different matrix (thus Θ is injective), but not necessarily every matrix in MM comes from an operator (surjectivity condition). Θ is injective because "$\tilde{F}$ is fixed *uniquely* by the matrix (F_{mn})" [7]. But it is not surjective because for each operator $\tilde{F}$ of WM the matrix *F* of MM is a Wintner matrix (i. e. its rows and columns are of sumable square), and the original postulates in Heisenberg's MM do not require *a priori* the matrices to be Wintner ones [8, 10]. Schrödinger proved that no more than one operator of WM can be mapped onto a given matrix of MM (because of injectivity), but he did not prove that there always exists an operator of WM corresponding to any arbitrary matrix of MM (surjectivity), as von Neumann [12] noticed. Moreover, his morphisms Θ depended on the fixed system of proper wave functions $\{\varphi_k\}$, and these functions cannot be reconstructed from the numerically given matrices, since Schrödinger's mathematical problem of momenta cannot be solved in general [11].

Applying Dirac's basic concepts formulated later on in quantum mechanics, I can claim that Schrödinger tried to prove the equivalence between *observables*, *i. e.* between the operators of WM and the matrices of MM. However he could not even attempt to construct the equivalence between *states*, *i. e.* the wave functions in WM, because MM did not have any *space of states*. Indeed the notion 'stationary state' did not occur in MM, as Muller [11] claims:

> "The absence of states in matrix mechanics was not a mathematical oversight of the founding fathers. On the contrary, Heisenberg counted the abolition of such unobservable relics from the old quantum theory, wherein (stationary) states were identified with electron orbits, as a personal victory."

In order to show the importance of this handicap, it suffices to note, according to Beller [13], that whereas WM was able of conceptualising a single stationary state by means of a standing wave, whose frequency was identified with a spectral term, MM lacked of this capability, as von Neumann [12] noticed.

Carl Eckart's simultaneous proof of mathematical equivalence [14] contained all the essential mistakes of Schrödinger's paper. Eckart's approach is a special case of Schrödinger's method. Thus the result is the same: the action of the wave operators on an arbitrary function cannot be calculated from the knowledge of the numerical matrices.

In the autumn of 1926 Paul Dirac formulated the theory of general linear transformations, which corresponded to the canonical transformations of classical mechanics, and are nowadays known as the unitary transformations in Hilbert space. Dirac was the first who pointed out the difference between *states* and *observables* of a physical system, a distinction which was present in WM (wave functions/wave operators) but not in MM, where only matrices were considered. How could then states be accounted for in MM? The states were, according to Dirac, the eigenvectors of the matrix *H* of MM, *i. e.* the elements of the transformation matrix of *H*, which were just the proper functions of Schrödinger's wave equation.

But the difficulties of formulating a mathematically tractable version of Dirac's quantum mechanics were quite formidable, due, among other reasons, to the pathological Dirac's improper δ-function. Dirac's *Principles of Quantum Mechanics*, 1930 [15], was criticized by von Neumann because of its lack of mathematical rigour. Therefore Jammer [16] claimed that "Full clarification on this matter has been reached only by John von Neumann when he showed in 1929 that, ultimately due to the famous Riesz-Fischer theorem in functional analysis, the Heisenberg and Schrödinger formalism are operator calculi on isomorphic (isometric) realizations of the same Hilbert space and hence equivalent formulations of one and the same conceptual substratum". Von Neumann's *Mathematical Foundations of Quantum Mechanics*, 1932 [12], was the definitive mathematical framework for the new quantum physics.

Von Neumann solved the quarrel of the mathematical equivalence as he showed that Heisenberg's MM –focused on discrete matrices and sums– and Schrödinger's WM –focused on continuous functions and integrations– are algebraic isomorphic operator calculi (the structure of the *observables*) on topological isomorphic and isometric realizations of the same Hilbert space (the structure of the *states*), and this thanks to the famous functional analysis theorem of Riesz & Fischer. Von Neumann identified the space of wave functions with

$$L^2(R) = \{ f : R \rightarrow C \mid f \text{ Lebesgue measurable and } \|f\|_2 = \left(\int_{-\infty}^{+\infty} f^*(x) f(x) dx\right)^{1/2} < \infty \} \quad (10)$$

and the space of states in MM, postulated by Dirac, with the space of sequences

$$\ell^2 = \{ (z_n) : \|(z_n)\|_2 = \left(\sum_{n=1}^{\infty} z_n^* z_n\right)^{1/2} < \infty \}, \quad (11)$$

from which every matrix in MM can be generated (this was a later development which was not originally present in Heisenberg's theory). And for this two spaces the Riesz-Fischer theorem claims that, given a complete orthonormal system $\{\varphi_k\}$,

$$\Phi_{\{\varphi_k\}} : L^2(R) \rightarrow \ell^2,\ \psi \mapsto (\langle \psi, \varphi_k \rangle)_{k=1}^{+\infty} \quad (12)$$

is an isometric isomorphism, *i. e.* "L^2 and ℓ^2 are isomorphic [...] it is possible to set up a one-to-one correspondence between L^2 and ℓ^2 [...] and conversely in such manner that this correspondence is linear and isometric" [12].

IV. CONCLUSION

Summing up, the existence of these two apparently very different formulations of quantum theory is not accidental and they are indeed alternative isomorphic expressions of the same underlying mathematical structure. Thus, *due to this isomorphism, MM and WM must always yield the same empirical predictions*.

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