



The Equivalence Myth of Quantum Mechanics—Part I

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If only I knew more mathematics!
Erwin Schrödinger *

The author endeavours to show two things: first, that Schrödinger's (and Eckart's) demonstration in March (September) 1926 of the equivalence of *matrix mechanics*, as created by Heisenberg, Born, Jordan and Dirac in 1925, and *wave mechanics*, as created by Schrödinger in 1926, is not foolproof; and second, that it could not have been foolproof, because at the time matrix mechanics and wave mechanics were neither mathematically nor empirically equivalent. That they were is the Equivalence Myth. In order to make the theories equivalent and to prove this, one has to leave the historical scene of 1926 and wait until 1932, when von Neumann finished his magisterial edifice. During the period 1926–32 the original families of mathematical structures of matrix mechanics and of wave mechanics were stretched, parts were chopped off and novel structures were added. To Procrustean places we go, where we can demonstrate the mathematical, empirical and ontological equivalence of 'the final versions of' matrix mechanics and wave mechanics.

The present paper claims to be a comprehensive analysis of one of the pivotal papers in the history of quantum mechanics: Schrödinger's equivalence paper. Since the analysis is performed from the perspective of Suppes' *structural view* ('semantic view') of physical theories, the present paper can be regarded not only as a morsel of the internal history of quantum mechanics, but also as a morsel of applied philosophy of science. The paper is self-contained and presupposes only basic knowledge of quantum mechanics. Due to its length, the paper is published in two parts. Section 1 of the paper contains, besides an introduction, also the paper's five claims and a preview of the arguments supporting these claims; so Section 1 serves too as a brief summary of the paper for those readers who are not interested in the detailed arguments.

* Schrödinger in a letter to Wilhelm Wien, 27 December 1925; quoted in Moore (1989, p. 196).

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1. Introduction and Summary

In 1924 atomic physics was a lamentable hodgepodge of experimental regularities, cabalistic sum-rules, computational recipes, bold conjectures and above all unsolved problems (d'Abro, 1939; Heilbron, 1977; Jammer, 1966, Chap. 5). And then suddenly there were *two* atomic theories. First there was *matrix mechanics*, developed in 1925 by Werner Heisenberg, Max Born and Pascual Jordan (Göttingen) in a series of three papers in *Zeitschrift für Physik* (Heisenberg, 1925; Born and Jordan, 1925; Born *et al.*, 1926) and P. A. M. Dirac (Cambridge) in two papers in the *Proceedings of the Royal Society* (Dirac, 1925a; Dirac, 1925b).¹ Second there was *wave mechanics*, created by Erwin Schrödinger (Zürich) in a series of five papers in *Annalen der Physik* [Schrödinger (1926a; 1926b; 1926c; 1926d; 1926e)].²

By 1926 their mathematical equivalence already had been allegedly proven by Schrödinger and independently by Carl Eckart (Cambridge, U.S.A.), and by Wolfgang Pauli (Munich) in a letter to Jordan discovered by B. L. van der Waerden in 1972 (Schrödinger, 1926c; Eckart, 1926; Van der Waerden, 1973). About 15 years ago Linda Wessels emphasized that the nearly simultaneous emergence of two theories and *their* alleged almost unanimous acceptance by the physical elite barely 2 years later (at the Solvay Conference of October 1927 in Brussels) constitute a rare sequence of events in the history of physics and as such provides unique material for studying issues concerning the appraisal, comparison, pursuit, acceptance and interpretation of physical theories (Wessels, 1980, p. 59). Accordingly Wessels asserted that a careful study of the matrix-wave controversy was long overdue. Like the papers of Van der Waerden (1973), Wessels (1977; 1980; 1981), MacKinnon (1980) and Beller (1983; 1985; 1990; 1992; 1996) and part of De Regt's (1993) doctoral dissertation, the present paper can be seen as part of *Wessels' programme*.

The Equivalence Myth is that *matrix mechanics and wave mechanics were mathematically and empirically equivalent at the time when the equivalence proofs appeared and that Schrödinger (and Eckart) demonstrated their equivalence*.³ Since the story that first there were two entirely different theories that were subsequently proven equivalent by Schrödinger (and Eckart) is generically taken for granted, whereas in fact it is false, the term 'myth' seems appropriate. A survey of the physics library illustrates the ubiquity of the Equivalence Myth: it

¹ Collected, introduced and German papers translated into English, in Van der Waerden (1967).

² Translations in Schrödinger (1927).

³ Literature dealing explicitly with Schrödinger's and Eckart's equivalence proofs that the author was able to find: Hanson's confusing (1961), also published as Chapter VIII of Hanson (1963) and MacKinnon (1980, pp. 11–23), which are highly non-mathematical and therefore do not even come close to the heart of the matter; the historical works of Jammer (1966, pp. 270–275) and Mehra and Rechenberg (1987, pp. 636–684), who report the historical events, provide a wealth of internal background information (especially the latter), but omit critical analyses (*idem dito*); Van der Waerden (1973), where a gap in Schrödinger's proof is exposed; Emch (1983, pp. 288–289, 336–338), who views the proof as a precursor of von Neumann's unitary-uniqueness theorem; and Ludwig (1968, pp. 32–44), who supplies some mathematical scaffolding for Schrödinger's proof.

is to be found in text-books on quantum mechanics [Pauling and Wilson (1935, p. 417), Kramers (1937, p. 61), Royanski (1938, p. 341), Mott and Sneddon (1948, p. 356), Bohm (1951, §16.24), MacConnel (1958, p. 51), Powell and Crasemann (1961, p. 282), Messiah (1962, p. 47), Dicke and Wittke (1963, p. 176), Borowitz (1967, p. 244), Greiner (1989, p. 147), Bransden and Joachain (1989, p. 51), Peres (1993, p. 20)], in works of the founding fathers [Schrödinger (1926e; 1927, p. 58), Heisenberg (1929, p. 493), Born (1935, p. 128), Jordan (1936, p. 154)], in a variety of historical writings [d'Abro (1939, p. 810), Gamov (1966, p. 105), Jammer (1966, p. 271), Hund (1967, p. 139), Cline (1969, p. 159), de Broglie (1969, pp. 192–195), MacKinnon (1980, pp. 3, 11, 46), Wessels (1980, pp. 60, 69) and (1981, p. 192), Beller (1983, p. 470), (1992, p. 283) and (1996, p. 548), Forman (1984, p. 335), Mehra and Rechenberg (1987, pp. 636, 684), Wick (1995, p. 26)], in philosophical–foundational analyses [Reichenbach (1944, p. iv), Bub (1974, p. 2), Hughes (1989, pp. 45–46), Torretti (1990, p. 151), Van Fraassen (1991, p. 450), De Regt (1993, pp. 138, 145, 146, 156), Omnès (1994, p. 15)], in mathematical–foundational treatises [von Neumann (1932, p. 5), Ludwig (1968, p. 32), Prugovecki (1981, p. 296), Emch (1983, p. 288)], in pure mathematics monographs (Chae, 1995, p. 221), in scientific biographies [Moore (1989, p. 212), Kragh (1990, p. 31), Cassidy (1992, pp. 214–215)] and in autobiographies (Casimir, 1983, p. 53). Careful statements about the issue are rare.⁴

In order to understand Schrödinger's equivalence proof, we provide a synoptic description of matrix mechanics (Section 3) and wave mechanics (Section 4) as they were at the time when this proof appeared (March 1926). Then we give a comprehensive review of Schrödinger's equivalence proof, not Eckart's or Pauli's, for Schrödinger's is the most elaborate one and had the greatest historical impact (Section 5).

Ever since two sacred texts on quantum mechanics appeared, Dirac's *The Principles of Quantum Mechanics* (1930) and von Neumann's *Mathematische Grundlagen der Quantenmechanik* (1932), the state–observable characterisation of quantum mechanics has reigned—withstanding the remarkable differences between the two sacred texts. According to the state–observable characterisation the theory of quantum mechanics exhaustively describes physical systems in terms of measurable physical magnitudes, baptised *observables* by Dirac, and of *states* (Dirac, 1930, pp. 19, 25); from the state the probability measure regarding any observable of interest can in principle be calculated.⁵ Projecting the state–observable characterisation back into Schrödinger's equivalence proof prevents us from fully understanding what is really going on in the proof, for the only historically valid question reads: how Schrödinger intended his equivalence proof to be understood, not what we make of it from today's characterisation of quantum mechanics which simply did not exist at the time.

In Suppes' *structural view* of physical theories, according to which the

⁴ Tomonaga (1966, p. 162), Gibbins (1987, p. 24); Hanson (1961; 1963) denies the equivalence, but unfortunately for all the wrong reasons (*vide infra*).

⁵ See further any textbook of quantum mechanics.

essence of a physical theory lies in the mathematical structures it employs to describe physical systems, the equivalence proof, including part of Schrödinger's intentions, can legitimately be construed as an attempt to demonstrate the isomorphism between the mathematical structures of matrix mechanics and wave mechanics [Cf. Ludwig (1968, p. 32) and Wick (1995, p. 26)]. Matrix mechanics and wave mechanics such as they were around March 1926 are thus tailored in structural terms in Part II, Section 1.

We shall explain and argue for five claims. The first three—major—claims (I, II, IIIA) are historical in nature and are meant to challenge the Equivalence Myth; the other three—minor—claims (IIIB, IV, V) are foundational-mathematical in nature, of which the latter two (IV, V) were essentially established long ago but are added for the sake of elucidation and comprehension, and of which the first one (IIIB) is novel and is established by a little mathematical proof.

Claim I: at the time when Schrödinger's equivalence proof (March 1926) and Eckart's (September 1926) appeared, matrix mechanics and wave mechanics were neither mathematically equivalent (IA) nor empirically equivalent (IB). That matrix mechanics and wave mechanics were *ontologically* distinct, in the sense of making conflicting assertions concerning atomic reality, was obvious from the very beginning and recognised by all the players. But in arguing against the *mathematical* and *empirical* equivalence the author means to question at least all the testimonies of the Equivalence Myth referred to above. One reason for the failure of the mathematical equivalence is the fact that whereas matrix mechanics could in principle describe the evolution of physical systems over time (by means of the Born–Jordan equation), but limited itself unnecessarily to periodic phenomena, wave mechanics could not—Schrödinger's time-dependent wave-equation dates from 3 months later than his equivalence proof. Other reasons for the failure of mathematical equivalence are: the absence in matrix mechanics of a state space but its presence in wave mechanics (the space of wave-functions); the fact that Euclidean space and a set of charge–matter densities, both prominently present in wave mechanics, had no matrix-mechanical counterparts; and the fact that matrix mechanics produced the first theory of a quantised electromagnetic field by means of matrix-valued fields, whereas Schrödinger emphasised there was no need to tinker with the classical Maxwell equations in wave mechanics. The empirical non-equivalence between matrix mechanics and wave mechanics springs from the smeared charge densities, which made it conceivable to perform an *experimentum crucis* by charge measurements on electrons.

Claim II: the ontological difference between matrix mechanics and wave mechanics was entrenched in the mathematical structures characterising these two theories; therefore the superiority of wave mechanics with regard to *Anschaulichkeit*⁶ was not redundant verbal fluff, but was firmly rooted in the mathematical structure of wave mechanics and was not, and could not be, rooted in that of matrix mechanics. (Claim II is not a consequence of Claim I only,

⁶ Untranslatable; it is a proper mixture of 'visualizability', 'intuitiveness', 'pictoriability', 'comprehensibility', 'intelligibility' and 'understandability'.

because it also depends on which parts of the theory were stipulated to have ontological significance.) Euclidean space, the charge–matter densities and the eigenvibrations are elements of the wave-mechanical structure; all terms and predicates of the wave-mechanical language referring to these elements can only be dismissed after some ruthless chopping of the mathematical structure of wave mechanics. The matrix-mechanical language could not possibly refer to space, to charge–matter densities or to eigenvibrations, because the matrix-mechanical structure did not *satisfy* (in the rigorous model-theoretical sense) any sentence containing terms or predicates referring to these notions. Claims I and II are the subject matter of Part II, Section 2.

Claim IIIA: on the basis of a different, non-standard definition of ‘mathematical equivalence’, which we shall call *Schrödinger-equivalence* because it captures an intention of Schrödinger’s that the standard definition does not capture, the equivalence-proof fails too. The reigning state-observable characterisation will hinder our understanding of the gist of Schrödinger’s intentions, in a similar way as projecting back matrices in Heisenberg’s first paper hinders the understanding of that very paper (MacKinnon, 1977, p. 163). The failure of Schrödinger’s attempt to demonstrate Schrödinger-equivalence between matrix mechanics and wave mechanics is due to the fact that on closer inspection his appeal to ‘the moment problem’ in mathematics appears to be in vain.

Claim IIIB: Schrödinger-equivalence does nonetheless hold, which can be proved in a more contemporary setting by an appeal to von Neumann’s unitary-uniqueness theorem from 1931. Claims IIIA and IIIB are the topic of Part II, Section 3.

To attain equivalence, matrix mechanics was committed to the discovery of conditions governing the canonical matrices such that they generate an algebra, and such that corresponding wave-operators exist.

Claim IV: the shift in mathematical perspective *from* looking upon an infinite matrix as a mathematical entity in its own right, as the founding fathers originally did, *to* looking upon an infinite matrix as a partial specification of a linear operator acting on the Hilbert-space of complex sequences, as required by the reigning state-observable characterisation of quantum mechanics, resolves the problem. Claim IV, obvious from our present understanding of quantum mechanics, will nonetheless be exemplified briefly in Part II, Section 4, for the sake of completeness.

In Part II, Section 5 we formulate an Equivalence Theorem (Claim V): the ‘final versions’ of matrix mechanics and wave mechanics, which exhibit the familiar state-observable characterisation and are therefore quite distinct from their historical progenitors, can be proven to be mathematically and empirically equivalent. We shall not prove this Equivalence Theorem because all the ingredients of such a proof are available elsewhere. Finally, we indicate the precise connection between the final versions of matrix mechanics and wave mechanics on the one hand and *orthodox quantum particle mechanics* on the other hand; we take the last mentioned to be von Neumann’s edifice (1927a; 1927b; 1931; 1932).

This paper ends with a speculative remark on the distinction formal-

ism/interpretation in quantum mechanics, which Heisenberg surreptitiously introduced to justify his use of the wave-mechanical equations (Part II, Section 6).

2. Mathematical Preamble

Our nomenclature and notation coincide with those used in Prugovecki's book, which can be viewed as a self-contained, expanded and modernised version of von Neumann's book (Prugovecki, 1981; von Neumann, 1932). For the purposes of the present paper we need the following additional definitions and notational deviations.

For the sake of expediency, we treat 'morphism' and 'structure-preserving map' as synonyms. Two members \mathfrak{U} and \mathfrak{V} of two families of set-theoretical structures are *isomorphic* (notation: $\mathfrak{U} \simeq \mathfrak{V}$) iff there exists a bijective morphism between them; whenever both structures \mathfrak{U} and \mathfrak{V} are ordered n -tuples of set-theoretical structures, \mathfrak{U} is isomorphic to \mathfrak{V} iff there exist n bijective morphisms between their n respective slots (= elements). Two sets are *equinumerous* iff they have the same cardinality. Notation of natural numbers is as follows: $\mathbb{N}_0 := \{0, 1, 2, 3, \dots\}$; $\mathbb{N} := \{1, 2, 3, \dots\}$; and $\mathbb{N}_n := \{1, 2, 3, \dots, n\}$, where $n \in \mathbb{N}$.

A *Hilbert-vector* (Cooke, 1950, p. 224) is an element of some Hilbert-space \mathcal{H} . The inner product of Hilbert-vectors ψ and ϕ is denoted as $\langle \psi | \phi \rangle$, and an ordered pair as $\langle \psi, \phi \rangle$. $D(\hat{A}) \subseteq \mathcal{H}$ and $R(\hat{A}) \subseteq \mathcal{H}$ denote the domain and range of operator \hat{A} , respectively (operators wear hats); recall that domains are defined as (not necessarily topologically closed!) vector spaces. The operator \hat{A} is *complete* iff it has a complete set of eigenvectors in \mathcal{H} . Hilbert-vectors of \mathcal{H} are *Weyl-equivalent* iff they differ by a complex overall factor of modulus 1 ('a phase factor'); $\mathbb{P}\mathcal{H}$ is the ensuing projective Hilbert-space of rays (Weyl, 1931, p. 75).

A *Schmidt-sequence* s is a denumerable sequence of complex numbers s_n such that the sum of the $|s_n|^2$ converges; $l^2(\mathbb{N})$ is the Hilbert-space of all Schmidt-sequences.⁷ Denote by e^n the sequence all of whose elements equal 0 except the n th element, which equals 1: $e_m^n = \delta_{nm}$, where δ_{nm} is the Kronecker-delta; the set $\{e^n\}$ of these Schmidt-sequences is an orthonormal basis for $l^2(\mathbb{N})$, called the *natural basis*. A *sequence-operator* \hat{a} is an operator acting on a Schmidt-sequence.

By a *matrix* we mean a complex matrix with denumerably many rows and columns, unless stated otherwise. A matrix B is *bounded* iff Bs is a Schmidt-sequence whenever s is a Schmidt-sequence.⁸ A matrix Q is a *Schrödinger-Eckart matrix* iff Qs is a Schmidt-sequence for every s in some vector space that is dense in $l^2(\mathbb{N})$. A matrix is a *Wintner-matrix*⁹ iff its rows and columns are Schmidt-sequences. The product of two Wintner-matrices always exists. The

⁷ The structure $l^2(\mathbb{N})$ to which these sequences give rise was first explored by Erhardt Schmidt in 1928; cf. Wintner (1929, p. 278).

⁸ The historically important *Hilbert-matrices* coincide with the bounded matrices, as a result of Theorem 9.4 III in Cooke (1950, p. 246); Crone (1971) solved the long-standing problem of characterising a bounded matrix in terms of its matrix elements only.

⁹ Wintner (1929, p. 122) baptised them '*Q*-matrices', from the German 'Quadrat'.

relations between all these matrices are as follows (\mathcal{M}_{bnd} is the set of bounded matrices, etc.):¹⁰

$$\mathcal{M}_{\text{bnd}} \subset \mathcal{M}_{\text{Wintner}} \quad \text{and} \quad \mathcal{M}_{\text{bnd}} \subset \mathcal{M}_{\text{SE}}. \quad (1)$$

A subset G of matrices (operators) of a matrix (operator), *algebra* $\mathfrak{A}(G)$, by definition closed under addition and multiplication and containing the unit matrix (operator) consists of the *generators* iff G is the smallest subset of $\mathfrak{A}(G)$ such that every element of the matrix (operator) algebra can be written as a polynomial of the elements in G ; the set G is *irreducible* iff the only element that commutes with all the generators is (a scalar multiple of) the unit matrix (operator).

An element $\psi \in L^2(\mathbb{R}^n)$, the Hilbert-space of all complex functions on \mathbb{R}^n whose modulus is square-integrable, is called a *wave-function*; a basis for $L^2(\mathbb{R}^n)$ is called a *wave-basis*. A *wave-operator* \hat{A} is an operator acting on a wave-function; two wave-operators \hat{A} and \hat{B} are called *Lebesgue-equivalent* iff their action upon a wave-function ψ yields two wave-functions $\hat{A}\psi$ and $\hat{B}\psi$ that are Lebesgue-equivalent (i.e. all their definite Lebesgue-integrals coincide).

3. Matrix Mechanics

The historical emergence of matrix mechanics has been described exhaustively.¹¹ We present matrix mechanics as an axiomatised theory, much as in the *Dreimännerarbeit* of Born *et al.* (1926).¹² The postulates apply to an atomic system of Nd degrees of freedom ($d \in \mathbb{N}_3$), consisting of $N \in \mathbb{N}$ material particles.

3.1. Postulate M1

Each Cartesian component of the classical magnitudes *momentum* and *position* corresponds in matrix mechanics to a time-dependent, Hermitian matrix $P_k(t)$ and $Q_k(t)$, respectively, called *canonical matrices* ($k \in \mathbb{N}_{Nd}; n, m \in \mathbb{N}$):¹³

$$P_k(m, n; t) := P_k(m, n)e^{i\omega(m, n)t} \quad \text{and} \quad Q_k(m, n; t) := Q_k(m, n)e^{i\omega(m, n)t}, \quad (2)$$

¹⁰The first 'C' is the content of a Corollary in Cooke (1950, p. 259); the second 'C' is trivial.

¹¹See Van der Waerden (1967, pp. 28–35), Jammer (1966, pp. 208–227) and Beller (1983); see Mehra and Rechenberg (1973, pp. 62–138) for the most elaborate exposition of all the founding papers of matrix mechanics; Tomonaga (1962, pp. 204–259) and Ludwig (1968, pp. 17–25) provide rational reconstructions; elucidating from a mathematical point of view is Emch (1983, pp. 252–276), who focusses on Born and Jordan (1925), and elucidating from a historical point of view is MacKinnon (1977), who analyses Heisenberg (1925); easy and written from a working physicist's point of view is d'Abro (1939, pp. 810–863).

¹²We ignore the operator reformulation of a part of matrix mechanics by Born and Wiener (1926), because it is now regarded as a dead end and because Schrödinger ignored it too.

¹³To avoid doubly indexed matrices, we assume that in the case of, say $N = 2$ and $d = 3$, $k = 1$ refers to the x -component matrix pertaining to the first particle, ..., $k = 6$ refers to the z -component matrix of the second particle; etc.

where the frequency $\nu(m, n) := \omega(m, n)/2\pi$ of the emitted or absorbed electromagnetic radiation of the atomic system in the transition $m \rightleftharpoons n$ obeys the following two conditions: (M1a) $\nu(m, n) + \nu(n, l) + \nu(l, m) = 0$, where $m, n, l \in \mathbb{N}$ are assumed to refer to the labels of the atomic spectral lines; and (M1b) if $n \neq m$, then $\nu(n, m) \neq 0$. The canonical matrices, the set of which is denoted by C_{mx} ,¹⁴ obey the following *canonical commutation relations*:

$$[P_k(t), Q_j(t)] = -i\hbar\delta_{jk}1 \quad \text{and} \quad [P_k(t), P_j(t)] = [Q_j(t), Q_k(t)] = 0, \quad (3)$$

where δ_{jk} is the Kronecker-delta and 1 and 0 the unit and zero matrices, respectively.¹⁵ Pairs $\langle P_k(t), Q_k(t) \rangle$ are called *canonical (ly conjugated) pairs*. *QEP*¹⁶

Condition (M1a) regarding the frequencies, which was known at the time as the phenomenological Rydberg–Ritz combination rule, was postulated by Heisenberg in 1925 solely to achieve consistency with H. A. Kramer’s phenomenological dispersion formula (Van der Waerden, 1967, pp. 29–33). Condition (M1b) merely asserts that transitions result in the emission or absorption of electromagnetic radiation (non-zero frequency). Born and Jordan saw that the relations (3), which presuppose the existence of the products $Q_j(t)P_k(t)$ and $P_k(t)Q_j(t)$, force the canonical matrices to be infinite (Van der Waerden, 1967, p. 291).

3.2. Postulate M2

All physical magnitudes correspond to time-dependent, Hermitian, matrix-valued polynomial functions of the canonical matrices. *QEP*

In their ‘Fundamental Principle III’ Born *et al.* restricted the class $\mathcal{F}(C_{mx})$ of matrix-valued functions of the canonical matrices to polynomials; so $\mathcal{F}(C_{mx}) = \mathfrak{A}(C_{mx})$, where the latter is the *canonical matrix algebra*, generated by C_{mx} . But further on in the *Dreimännerarbeit*, they asserted that certain relations hold for ‘every function $F(P_k(t), Q_j(t))$ which can be formally expressed as a power series’ (Van der Waerden, 1967, pp. 325, 281, 327). To presuppose the existence of arbitrary polynomial expressions of *unbounded infinite* matrices in $\mathfrak{A}(C_{mx})$ is mathematically as baffling as it is bold; it will be one of the troublesome issues taken up in the present paper.

3.3. Postulate M3

The physical magnitude *energy* corresponds to a Hermitian, diagonalizable matrix-valued function $H = H(P_k(t), Q_j(t)) \in \mathcal{F}(C_{mx})$, called the *Hamiltonian*

¹⁴ Throughout this paper the subscripts ‘mx’ and ‘wv’ indicate that the subscripted mathematical entity belongs to matrix mechanics or wave mechanics, respectively.

¹⁵ Eq. (38) of Born and Jordan (1925), eq. (12) of Dirac (1925a) in Van der Waerden (1967, pp. 36–38, 292, 42, 315) and Jammer (1966, pp. 220, 238).

¹⁶ *Quod erat ponendum*; signals end of Postulate’s formulation—supposed to be a joke!

matrix. The only possible energy values are the diagonal elements E_n of the diagonalised H , which we collect in the set $\sigma_{\text{mx}}(H)$. *QEP*

Notice that in contrast to Postulate M3 the diagonal elements of $P_k(t)$ and $Q_j(t)$ are not postulated to have any physical significance. There is a cogent reason for the absence of such a postulate: neither member of a canonical pair can be diagonal.¹⁷ For non-degenerate atomic systems ($\nu(m, n) \neq 0$ for some n, m) Born *et al.* derived that H is diagonalizable; for degenerate atomic systems their derivation crashed.¹⁸

3.4. Postulate M4

The frequency $\nu(m, n)$ of the emitted or absorbed electromagnetic radiation of an atom in transition $m \rightleftharpoons n$ is given by Bohr's 1913 frequency condition:

$$h\nu(m, n) = E_m - E_n, \quad (4)$$

where E_m, E_n are elements of $\sigma_{\text{mx}}(H)$ (*vide* Postulate M3). *QEP*

For non-degenerate atomic systems Bohr's frequency condition could be derived from the other postulates;¹⁹ once again, for degenerate atomic systems this derivation crashed [Born *et al.* (1926) in Van der Waerden (1967, pp. 343–345)].

3.5. Postulate M5

A postulated matrix version of Hamilton's Principle of Least Action was shown to lead to the matrix versions of the classical Hamilton equations.²⁰

$$\dot{Q}_k(t) = \frac{\partial H}{\partial P_k(t)} \quad \text{and} \quad \dot{P}_k(t) = -\frac{\partial H}{\partial Q_k(t)}, \quad (5)$$

where the definitions of the partial matrix-mechanical derivatives closely resemble the familiar definition of ordinary differential calculus.²¹ *QEP*

3.6. Postulate M6

The intensity $I_k(m, n)$ of the electromagnetic radiation emitted or absorbed by an atom in a transition $n \rightleftharpoons m$ with frequency $\nu_k(m, n)$ polarised in direction k is proportional to the square of the absolute value of the corresponding matrix-element of $Q_k(t)$:

$$I_k(m, n) \propto |Q_k(m, n; t)|^2, \quad (6)$$

¹⁷ This is established by an easy *reductio ad absurdum* argument using the fact that the trace of products and sums of finite matrices equals the products and sums of their traces, respectively.

¹⁸ Van der Waerden (1967, pp. 328–329, 343–345). The restriction to diagonalizable Hamiltonian matrices implies a restriction to point-spectra.

¹⁹ Heisenberg (1925) in Van der Waerden (1967, p. 273), Born and Jordan (1925) in Van der Waerden (1967, pp. 38, 294); cf. Part II, Section 2.2.

²⁰ Born and Jordan (1925) in Van der Waerden (1967, p. 290), eq. (35).

²¹ Van der Waerden (1967, p. 282), Mehra and Reichenberg (1982, pp. 69, 97–98); we do not need these definitions in this paper.

where t is arbitrary²² and where $Q_k(t)$ is expressed in the diagonal representation of H. *QEP*

Born and Jordan realised that a quantum theory of matter (atoms, electrons) had to be supplemented by a quantum theory of (electromagnetic) radiation. They set out to formulate the Maxwell equations in matrix language. In classical electrodynamics the electromagnetic field is characterised by two vector-valued functions $\mathbf{E}(\mathbf{r}, t), \mathbf{B}(\mathbf{r}, t) \in \mathbb{R}^3$ on space–time, whose points are here arbitrarily labelled by Cartesian coordinates $\mathbf{r} \in \mathbb{R}^3$ and $t \in \mathbb{R}$:²³

$$\mathbf{E}(\mathbf{r}, t) := E_x(\mathbf{r}, t)\mathbf{e}_x + E_y(\mathbf{r}, t)\mathbf{e}_y + E_z(\mathbf{r}, t)\mathbf{e}_z, \quad (7)$$

$$\mathbf{B}(\mathbf{r}, t) := B_x(\mathbf{r}, t)\mathbf{e}_x + B_y(\mathbf{r}, t)\mathbf{e}_y + B_z(\mathbf{r}, t)\mathbf{e}_z, \quad (8)$$

which solve the Maxwell equations.

3.7. Postulate M7

Each component of the electromagnetic field corresponds to a space–time-dependent, Hermitian matrix. Define the *vector–matrix* for the electric and the magnetic field as follows:

$$\vec{\mathbf{E}}(\mathbf{r}, t) := E_x(\mathbf{r}, t)\mathbf{e}_x + E_y(\mathbf{r}, t)\mathbf{e}_y + E_z(\mathbf{r}, t)\mathbf{e}_z, \quad (9)$$

$$\vec{\mathbf{B}}(\mathbf{r}, t) := B_x(\mathbf{r}, t)\mathbf{e}_x + B_y(\mathbf{r}, t)\mathbf{e}_y + B_z(\mathbf{r}, t)\mathbf{e}_z. \quad (10)$$

These vector–matrix-valued fields are postulated to obey the free *matrix Maxwell equations*, which are obtained by replacing the vectors \mathbf{E} and \mathbf{B} in the familiar Maxwell equations with their vector–matrix analogues. *QEP*

We next bring some consequences of these postulates into the limelight, for future reference.

(m1) The problems posed by the (an)harmonic oscillator and the rigid rotator were solved in matrix mechanics. By means of an ingenious and laborious calculation, Pauli obtained the frequencies of the Balmer series of the hydrogen spectrum, and their shift when hydrogen is exposed to a homogeneous electric field (Stark effect, discovered in 1913) and to crossed electric and magnetic fields; Dirac obtained a few results independently.²⁴ At this stage matrix mechanics could hardly be said to have superseded the old Bohr–Sommerfeld model as far as the empirical content was concerned. According to Van der Waerden and Jammer, Pauli’s achievement nevertheless managed to convince most physicists that matrix mechanics was the way to create order out of chaos [see Van der Waerden (1967, p. 58) and Jammer (1966, pp. 241–242)]. But according to Beller,

²² The time t can be taken arbitrarily because the norm of each matrix element $Q_k(m, n; t)$ is time-independent.

²³ Born and Jordan (1925, Section 4) and Born *et al.* (1926, Section 4.3); Van der Waerden did not include these sections in (1967, iv, pp. 277); see also Mehra and Rechenberg (1982, pp. 87–90, 129–156).

²⁴ Pauli (1926), Dirac (1925b), Mehra and Rechenberg (1982, pp. 174–185), Van der Waerden (1967, pp. 57–59, 387–415). In 1972 Vleck (1973, pp. 30–31) discovered that Dirac had cheated.

victorious squeaks came exclusively from the hills around Göttingen; everywhere else the physicists were all sitting on the fence, watching how these awkward infinite matrices were invading atomic physics (Beller, 1983).

(m2) The conservation of orbital angular momentum was established. The introduction of orbital angular momentum matrices, elements of $\mathcal{F}(C_{mx})$, obeying a novel commutation relation led to the result that in atomic transitions orbital angular momentum changes only in integer units of Planck's constant (Van der Waerden, 1967, pp. 364–369). This was in fact a well-established selection rule of experimental spectroscopy. Here matrix mechanics provided a theoretical explanation for a phenomenological regularity.

(m3) On the assumption that the Hamiltonian matrix H can be decomposed in a sum of two matrices depending only on $P_k(t)$ and $Q_j(t)$, respectively, Born and Jordan derived that any physical magnitude corresponding to a matrix-valued polynomial function $F(P_k(t), Q_j(t))$ satisfies the following equation of motion (Born and Jordan, 1925; Van der Waerden, 1967, p. 293, eq. (43)):

$$i\hbar \dot{F}(P_k(t), Q_j(t)) = [F(P_k(t), Q_j(t)), H]. \quad (11)$$

This *Born–Jordan equation* is always incorrectly called ‘the Heisenberg equation’.

(m4) A *canonical transformation* $P \mapsto P'$, $Q \mapsto Q'$ is a transformation that leaves the canonical commutation relations (3) invariant. Born and Jordan showed that similarity transformations are canonical transformations:

$$P' = SPS^{\text{inv}} \quad \text{and} \quad Q' = SQS^{\text{inv}}, \quad (12)$$

where S must be a unitary matrix ($S^\dagger = S^{\text{inv}}$) iff the Hermiticity is to be conserved; we then speak of *unitary transformations*.²⁵ The importance of canonical transformations lies in the fact that if the diagonalizable $H(P_k(t), Q_j(t))$ is not a diagonal matrix, then there must be a unitary matrix U such that

$$H'(P'_k(t), Q'_j(t)) := UH(UP_k(t)U^{\text{inv}}, UQ_j(t)U^{\text{inv}})U^{\text{inv}} \quad (13)$$

is a diagonal matrix.

(m5) Jordan derived from Postulate M7 a number of interesting results, one of which we mention. The intensity of Hertzian dipole radiation polarised in the direction of k , associated with the transition $n \rightleftharpoons m$, appeared to be equal to

$$I_k(m, n) = \frac{4e^2}{3c^2} \omega^4(m, n) |Q_k(m, n; t)|^2, \quad (14)$$

which provided a magnificent justification for expression (6) of Postulate M6. [See Van der Waerden (1967, p. 38) and Mehra and Rechenberg (1982, p. 90, eq. (190)). Matrix mechanics anno 1926 included the first serious attempt, entirely due to Jordan, to formulate a quantum field theory (Van der Waerden, 1967, p. 38).]

²⁵ Born and Jordan (1925), Van der Waerden (1967, pp. 330, 351); compare Weyl (1931, pp. 96–98).

4. Wave Mechanics

De Broglie's hypothesis concerning matter waves, Hamilton's principle of least action, wave optics, Einstein–Bose gas theory and the demand for an *anschauliche* theory of what is happening in atomic reality, all stimulated the neurons of Schrödinger's brain when it was in the process of creating wave mechanics.²⁶ The postulates below are to be found almost *verbatim* in Schrödinger's first three papers [Schrödinger (1926a; 1926b; 1926c) in Schrödinger (1927, pp. 1–40, 45–61)]; they apply to one material particle (the electron) in three-dimensional Euclidean space.

4.1. Postulate W1

Each Cartesian component of the classical magnitudes *momentum* and *position* corresponds in wave mechanics to a wave-operator acting on a suitable complex function ψ , defined on \mathbb{R}^3 . These so-called *canonical wave-operators* are defined as the differential operator (up to a factor $-i\hbar$) and the multiplication operator, as follows:

$$\hat{P}_k \psi(\mathbf{q}) := -i\hbar \frac{\partial \psi(\mathbf{q})}{\partial q_k} \quad \text{and} \quad \hat{Q}_j \psi(\mathbf{q}) := q_j \psi(\mathbf{q}), \quad (15)$$

where $j, k \in \mathbb{N}_3$ and $\mathbf{q} := \langle q_1, q_2, q_3 \rangle \in \mathbb{R}^3$. C_{wv} denotes the set of the six canonical wave-operators. *QEP*

The only motivation for the introduction of these wave-operators was the fact that they obey canonical commutation relations analogous to (3):

$$[\hat{P}_k, \hat{Q}_j] = -i\hbar \delta_{jk} \hat{1} \quad \text{and} \quad [\hat{P}_k, \hat{P}_j] = [\hat{Q}_j, \hat{Q}_k] = \hat{0}. \quad (16)$$

Initially these canonical wave-operators played no part whatsoever in wave mechanics: Schrödinger only invented these wave-operators when pursuing his equivalence proof (cf. Section 5). This initial *absence* is perfectly intelligible, for we currently think of these operators as having something to do with the *measured* momentum and position in space of a *particle*, but wave mechanics was not (intended by Schrödinger as) a particle theory since it was a *wave* theory; and waves 'occupy' non-denumerably many positions in space simultaneously, whether measured or not.

4.2. Postulate W2

All physical magnitudes correspond to wave-operator-valued functions of the canonical wave-operators. *QEP*

²⁶ Wessels (1977) traces Schrödinger's route to wave mechanics and Regt (1993, pp. 138–159) isolates the purely philosophical factors; Mehra and Rechenberg (1982, pp. 367–576) describe the rise of wave mechanics in their distinctive whirligig of details; Jammer (1966, pp. 242–277) provides a briefer account; Ludwig (1968, pp. 25–31) reconstructs wave mechanics rationally from classical-mechanical point-mechanics; Emch (1983, pp. 276–295) looks at wave mechanics through von Neumann's spectacles; and MacKinnon (1980) addresses the rise and fall of 'Schrödinger's interpretation of the wave-function'.

Schrödinger required these functions to be polynomials in \hat{P}_k , in order to replace $P_k(t)$ meaningfully by $-i\hbar\partial/\partial q_k$ in matrix expressions [Schrödinger (1926c; 1927, p. 27)]. We remain provisionally silent about the precise mathematical characterisation of the set $\mathcal{F}(C_{\text{wv}})$ of allowed wave-operator-valued functions, as did Schrödinger, but we let it include all polynomials.

4.3. Postulate W3

The physical magnitude *energy* of an electron corresponds to a complete²⁷ Hermitian wave-operator-valued function $\hat{H} = \hat{H}(\hat{P}_k, \hat{Q}_j) \in \mathcal{F}(C_{\text{wv}})$, called the *Hamiltonian wave-operator*, whose eigenvalue-equation reads:

$$\hat{H}\psi(\mathbf{q}) = E\psi(\mathbf{q}). \quad (17)$$

The only possible values for the energy are the eigenvalues E_n of \hat{H} , which we collect in the set $\sigma_{\text{wv}}(\hat{H})$; the solutions ϕ_n of the eigenvalue-equation (17) are the so-called *eigenvibrations* of the atomic system. *QEP*

We prefer to take the eigenvalue equation (17), called *the time-independent Schrödinger equation*, as a postulate, notwithstanding Schrödinger's two distinct derivations.²⁸ The eigenvibrations (ϕ_n) are the wave-functions upon which \hat{H} acts as multiplication by a constant (E_n). The Hermiticity of \hat{H} entails the orthogonality of $\{\phi_n\}$ as well as the fact that the energy values are real numbers. The Hamiltonian wave-operator $\hat{H} := \hat{H}_{\text{free}} + V(\mathbf{q})\hat{1}$ is assumed to consist of a free and a potential term, where the potential V is some well-behaved function on \mathbb{R}^3 .²⁹ Equation (17) then turns out to be a second-order, linear, parabolic, homogeneous partial differential equation, which poses, when boundary and initial conditions are added, a determinate problem for all $E_n \in \sigma_{\text{wv}}(\hat{H})$.

4.4. Postulate W4

The frequency $\nu(m, n)$ of the emitted or absorbed electromagnetic radiation of an atom in the transition $m \rightleftharpoons n$ is given by Bohr's frequency condition (4):

$$E_m - E_n = h\nu(m, n), \quad (18)$$

where $E_m, E_n \in \sigma_{\text{wv}}(\hat{H})$ are the energy values of the eigenvibrations m and n , respectively. *QEP*

²⁷ See Section 2.

²⁸ Schrödinger (1926a; 1926b; 1927, pp. 1–2, 13–27); see Wessels (1977, pp. 330–335), MacKinnon (1980, pp. 4–6).

²⁹ Whether the potential term is an element of $\mathcal{F}(C_{\text{wv}})$ is at this juncture undecidable because it is not necessarily a polynomial. But 'well-behaved' is taken to imply the existence of a Taylor expansion for $V(\mathbf{q})$, every approximation of which can be rewritten as a polynomial in \hat{Q} , which would make the approximation an element of $\mathcal{F}(C_{\text{wv}})$; to write an *infinite* power series in \hat{Q} , one first needs to specify a topology. For an elementary rigorous treatment of the mentioned Hamiltonian wave-operator, see Prugovecki (1981, pp. 354–369).

4.5. Postulate W5

Electrons are smeared charge-matter densities in space, the electric charge density being

$$\rho(\mathbf{q}) := e\psi^*(\mathbf{q})\psi(\mathbf{q}) = e|\psi(\mathbf{q})|^2, \quad (19)$$

where e is the electron charge. *QEP*

The wave-function ψ must of course be normalised to obtain the total electron charge 'after integration of ρ over \mathbb{R}^3 :

$$\int_{-\infty}^{+\infty} \rho(\mathbf{q}) \, d\mathbf{q} = e. \quad (20)$$

So wave-functions reside in $L^2(\mathbb{R}^3)$. Replacing the electron's charge e with its mass m_e yields a similar formula for the matter density (Tomonaga, 1966, pp. 17–23), although Schrödinger did not explicitly write it down. [In March 1926 Schrödinger did not yet have the particular definition (19) for the charge density; it saw the light of day in his fifth founding paper of wave mechanics 3 months later [Schrödinger (1926e; 1927, p. 120)]. But Schrödinger did have another definition. Since what is important for the present discussion is the fact that Schrödinger had a charge density $\rho : \mathbb{R}^3 \rightarrow \mathbb{R}$, not which particular definition for this mapping he had, we have taken the definition that would survive as the most promising one. For the purposes of the present paper, *this* historical incongruency is harmless.]

This ends our description of the five postulates of wave mechanics as it was in March 1926. A sixth postulate (W6) concerning the intensity of electromagnetic radiation will be added in the next section. We report the main consequences of these postulates.

(w1) Schrödinger solved the problems posed by the harmonic oscillator, the rigid rotator with fixed and with free axes, and the non-rigid rotator; furthermore, he calculated the frequencies of the Balmer series of the hydrogen spectrum, by solving the eigenvalue equation (17) of the Hamiltonian for one electron in the Coulomb field of an atomic nucleus ('Kepler problem') [Schrödinger (1926a; 1926b; 1927, pp. 2–8, 30–40)]. Schrödinger also derived the continuous part of the spectrum: $[0, \infty)$; the fact that the corresponding eigenvibrations (plane waves) make serious trouble for the total charge formula (20) was ignored.

(w2) The quantisation of angular momentum, and the implied integer selection-rule, constituted a success that matched consequence (m2) of matrix mechanics.

Schrödinger's eigenvalue equation (17) was soon used by all physicists, the founding fathers of matrix mechanics included. Solving a linear partial differential equation, something physicists had been accustomed to for centuries, was so much easier than to diagonalise an unbounded infinite matrix. Eventually, it was not wave mechanics as expounded above which was accepted but a quite distinct version (*vide* Part II, Section 5).

5. The Equivalence Proof

Schrödinger opened his equivalence paper as follows (1926c; 1927, pp. 45–46, his italics):

Considering the extraordinary differences between the starting-points and the concepts of Heisenberg's quantum mechanics [= matrix mechanics] and of the theory which has been designated 'undulatory' or 'physical' mechanics [= wave mechanics] [...] 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. Above all, however, the departure from classical mechanics in the two theories seems to occur in diametrically opposed directions. In Heisenberg's work the classical continuous variables are replaced by systems of *discrete* numerical quantities (matrices), which depend on a pair of integral indices, and are defined by *algebraic* equations. The authors themselves describe the theory as a "true theory of a discontinuum". On the other hand, wave mechanics shows just the reverse tendency; it is a step from classical point-mechanics towards a *continuum-theory*. In place of a process described in terms of a finite number of dependent variables occurring in a finite number of differential equations, we have a continuous *field-like* process in configuration space, which is governed by a *single partial differential* equation, derived from a Principle of [Least] Action.

So the *explanandum* is 'the agreement with regard to the known facts' of matrix mechanics and wave mechanics (coinciding energy values for the hydrogen atom and for a few toy systems, and quantisation of orbital angular momentum), and the ensuing equivalence proof is offered as the *explanans*. In this section we present the explication of this *explanans*. After (a) an introductory remark, we (b) treat the purported isomorphism of the canonical matrix- and wave-operator algebras, (c) expand wave mechanics by a sixth postulate concerning the intensity of electromagnetic radiation, and (d) immerse ourselves in wave mechanics to understand the part of the proof wherein the wave-functions are constructed from the matrices.

(a) Schrödinger effectively proposed a generalisation of his postulates for the application to atomic systems consisting of $N \in \mathbb{N}$ 'particles' in $d \in \mathbb{N}_3$ dimensions, just as in matrix mechanics; we shall not spell out this generalisation to an arbitrary number of degrees of freedom (from \mathbb{R}^3 to configuration space \mathbb{R}^{Nd}), which proceeds straightforwardly. For the sake of simplicity, we shall confine ourselves to the simplest case ($N = 1$ and $d = 1$), unless indicated otherwise; generalisations of the equivalence proof again proceed straightforwardly. Henceforth we also walk the familiar route of writing the row- and column-indices of the matrices as subscripts: $Q_{mn}(t) := Q_1(m, n; t)$, etc.

(b) Consider the putative canonical wave-operator algebra $\mathfrak{A}(C_{\text{wv}})$ generated by C_{wv} , and the putative canonical matrix algebra $\mathfrak{A}(C_{\text{mx}}^0)$ generated by C_{mx}^0 , where the latter contains only $P := P(0)$ and $Q := Q(0)$; all their elements are polynomials over \mathbb{C} of their two generators. We use the word 'putative',

because the question whether the canonical wave-operators and the *unbounded infinite* canonical matrices do generate *algebras* is non-trivial; in March 1926 the tacit affirmative answer was at best a mathematical conjecture and at worst speculation. Let us reflect for a moment on whether matrix mechanics and wave mechanics *need* fully fledged algebras in the first place.

The quantisation programme of the old quantum theory was to find quantum-mechanical counterparts of (all) magnitudes in classical physics. Dirac's famous quantisation rule of replacing the Poisson brackets in classical expressions with $i\hbar$ times the commutator, and concomitantly replacing classical dynamical variables ('*c*-numbers') with operators ('*q*-numbers'), revived the quantisation programme in quantum mechanics (Dirac, 1925b; Van der Waerden, 1967, pp. 58, 420–421).

If the canonical wave-operators and the canonical matrices generate algebras, then one has rolled out a red carpet for the quantisation programme: all polynomial expressions, which include Taylor-approximations to n th order (n arbitrary) of appropriate functions, are mathematically allowed. Without algebras, the quantisation programme may produce diverging expressions, which are both mathematically and physically unacceptable. The non-existence of the canonical *algebras* would however not necessarily be a *physical* drawback: as long as a sufficient number of polynomials of the canonical elements exist *that correspond to all the relevant physical magnitudes* (kinetic and potential energy, angular momentum), the physicist is in business. Hence to get off the ground, the quantisation programme needs at least the guarantee that *some* polynomials exist, like the monomials QP and PQ of Postulate M2, like P^2 , which occurred in all Hamiltonian matrices considered, and like Q^2 (Q^3), which occurred in the (an)harmonic oscillator. But it is precisely this modest requirement that puts the matrix-mechanic in the predicament of having to check all his needed matrix expressions by hand, for the postulates of matrix mechanics do not provide the necessary guarantees. The fact that *some* polynomials of physical relevance did indeed appear to exist [consequence (m1), Section 3] was the springboard for a leap to the existence of *all* polynomials—a move not uncharacteristic of the theoretical physicist. We provisionally follow the founding fathers in assuming the existence of the fully fledged canonical algebras $\mathfrak{A}(C_{wv})$ and $\mathfrak{A}(C_{mx}^0)$.

Another issue we provisionally pay little attention to is the notion of *self-adjointness*, which would become a pearl in von Neumann's crown. Taking the adjoint is an example of what is currently known in mathematical physics as a **-map*;³⁰ consequently the canonical algebras $\mathfrak{A}(C_{wv})$ and $\mathfrak{A}(C_{mx}^0)$ are called **-algebras*; henceforth we leave this implicit.

Enter Schrödinger.

Suppose the canonical matrices $P, Q \in C_{mx}^0$ correspond to the canonical wave-operators $\hat{P}, \hat{Q} \in C_{wv}$, respectively. Then to every polynomial of \hat{P} and \hat{Q} there should correspond the same polynomial of P and Q , and *vice versa*. For example,

³⁰ A map $A \mapsto A^*$ is a **-map* iff $(A^*)^* = A$, $(AB)^* = B^*A^*$, $(A + B)^* = B^* + A^*$ and $(cA)^* = \bar{c}A^*$.

$$\hat{F}(\hat{P}, \hat{Q}) := \hbar \hat{Q}^2 \hat{P} - 2\pi i \hat{Q} \hat{P} \hat{Q} \hat{P} + 8\hat{Q}^3 \hat{P}^2 \hat{Q}^2 \quad (21)$$

corresponds to

$$F(P, Q) := \hbar Q^2 P - 2\pi i Q P Q P + 8Q^3 P^2 Q^2. \quad (22)$$

Due to the non-commutativity of the putative algebras, the order of the factors in each term is essential. Consider furthermore the set $\mathcal{F}(C_{wv})$ of wave-operator-valued functions of the canonical wave-operators and the set $\mathcal{F}(C_{mx}^0)$ of matrix-valued functions of the canonical matrices. The existence of these sets of functions, which are taken to include all polynomials, is an even bolder mathematical conjecture. A one-to-one correspondence between the sets $\mathcal{F}(C_{mx}^0)$ and $\mathcal{F}(C_{wv})$ would presumably be a straightforward extension of the correspondence displayed in (21) and (22).

The pivotal question which has to be answered before the correspondence displayed in (21) and (22) can take off is: *which* matrices P and Q correspond to the differential operator \hat{P} and the multiplication operator \hat{Q} (of Postulate W1), respectively? The following considerations provide an answer to this question.

Suppose that \hat{A}, \hat{B} are arbitrary Hermitian wave-operators and that $\{\phi_n\} \subset D(\hat{A}) \cap D(\hat{B})$ is an orthonormal basis for $L^2(\mathbb{R})$. Define the wave-operators $\hat{\Sigma} := \hat{A} + \hat{B}$ and $\hat{\Pi} := \hat{A}\hat{B}$. Next Schrödinger defines the following complex numbers, for each pair $\langle j, k \rangle$ of natural numbers:³¹

$$A_{jk} := \int_{-\infty}^{+\infty} \phi_j^*(q) \hat{A} \phi_k(q) dq, \quad (23)$$

and *mutatis mutandis* for B_{jk}, Σ_{jk} and Π_{jk} . Formula (23), also discovered by Eckart and Pauli [Eckart (1926, pp. 720, 723), Pauli in Van der Waerden (1973, p. 281)], is the illuminating connection between ‘the discrete matrices’ and ‘the continuous waves’; its provenance lies in Hilbert’s theory of quadratic forms and integral equations, wherein infinite matrices appeared for the very first time. Kornel Lanczos (Frankfurt am Main) had used a similar formula in a paper (December 1925) which addressed the connection between matrix mechanics and Hilbert’s theory of integral equations; Schrödinger knew this paper because he referred to it [see Lanczos (1926, p. 813), Schrödinger (1927, p. 60); cf. Van der Waerden (1973)]. Notice that $\Pi_{jk} \in \mathbb{C}$ iff $\hat{B}\phi_k \in D(\hat{A})$.³² Thence we obtain four infinite *matrices*: A, B, Σ and Π , for which Schrödinger showed that:

$$\Sigma = A + B \quad \text{and} \quad \Pi = AB. \quad (24)$$

Equations (23) define what we shall call a *Schrödinger–Eckart mapping*, which assigns matrices to wave-operators:

$$f_\phi : \mathfrak{A}(C_{wv}) \rightarrow \mathfrak{A}(C_{mx}^0), \quad \hat{A} \mapsto f_\phi(\hat{A}) = A, \quad (25)$$

where the subscript ϕ indicates that the wave-basis $\{\phi_n\}$ is chosen. Together with the fact that $f_\phi(\hat{1}) = 1, f_\phi(\hat{0}) = 0$ and the fact that the Schrödinger–Eckart mapping f_ϕ (25) preserves the relation ‘is the adjoint of’:

³¹ We omit Schrödinger’s redundant ‘density functions’ from all integrals.

³² Notice that in general the domains of $\hat{\Sigma}$ and $\hat{\Pi}$ do not coincide.

$$f_\phi(\hat{A}^\dagger) = f_\phi(\hat{A})^\dagger = A^\dagger, \quad (26)$$

equations (24) demonstrate that f_ϕ preserves the structure of the wave-operator algebra and the matrix algebra, i.e. it is a *morphism*.³³

$$\begin{aligned} f_\phi(\hat{A} + \hat{B}) &= f_\phi(\hat{A}) + f_\phi(\hat{B}) = A + B \\ f_\phi(\hat{A}\hat{B}) &= f_\phi(\hat{A})f_\phi(\hat{B}) = AB. \end{aligned} \quad (27)$$

The Schrödinger–Eckart mapping f_ϕ assigns one matrix to each wave-operator—or actually to each class of Lebesgue-equivalent wave-operators (cf. Section 2). How about the converse? In a footnote (!) Schrödinger wrote (Schrödinger, 1927, p. 52, his italics):

In passing it may be noted that the converse of this theorem is also true, at least in the sense that certainly *not more than one* linear differential operator [wave-operator] can belong to a given *matrix*.

The matrix-elements A_{jk} on the j th column can be seen as the expansion coefficients of the image of the basis-element ϕ_j under \hat{A} (Eckart, 1926, pp. 720–723):

$$\hat{A}\phi_j = \sum_{k=1}^{\infty} A_{kj}\phi_k, \quad (28)$$

so the action of a wave operator \hat{A} , such that $f_\phi(\hat{A}) = A$, on an arbitrary wave-function ψ having expansion coefficients c_j is given by:

$$\hat{A}\psi = \sum_{j=1}^{\infty} c_j \sum_{k=1}^{\infty} A_{kj}\phi_k. \quad (29)$$

Equation (29) purports to define the inverse of the Schrödinger–Eckart mapping f_ϕ (25):

$$f_\phi^{\text{inv}} : \mathfrak{A}(C_{\text{mx}}^0) \rightarrow \mathfrak{A}(C_{\text{wv}}), \quad A \mapsto f_\phi^{\text{inv}}(A) = \hat{A}. \quad (30)$$

Notice however that the requirement $\hat{A}\phi_j \in L^2(\mathbb{R})$ (below Postulate W5) implies by expansion (28) that the columns of A have to be Schmidt-sequences:

$$\infty > \int_{-\infty}^{+\infty} |\hat{A}\phi_j(q)|^2 dq = \sum_{k=1}^{\infty} |A_{kj}|^2. \quad (31)$$

Whenever \hat{A} is Hermitian (like \hat{P} , \hat{Q} and \hat{H}), the matrix $A = f_\phi(\hat{A})$ is Hermitian too; whence it follows that A must be a Wintner matrix. Notice also that the requirement $\hat{A}\psi \in L^2(\mathbb{R})$ implies by expansion (29):³⁴

$$\infty > \int_{-\infty}^{+\infty} |\hat{A}\psi(q)|^2 dq = \sum_{k=1}^{\infty} \left| \sum_{j=1}^{\infty} c_j A_{kj} \right|^2. \quad (32)$$

³³ See Section 2. A morphism which preserves the relation ‘is the $*$ -image of’ (see footnote 30) is an example of what is called a $*$ -*morphism*; we leave this again implicit in the text.

³⁴ The assumption that A is a Wintner matrix, which we just above stumbled upon, does not help us here because it does not entail equation (32) (elementary exercise).

Since the postulates of matrix mechanics do not require the matrices to be Wintner matrices, or to satisfy any other (stronger) criteria, they may or may not have a corresponding wave-operator. As Schrödinger implies in the last quotation, it is indeed the case that the existence of *more than one* wave-operator corresponding to a given matrix would destroy the putative equivalence of matrix mechanics and wave mechanics; the mapping f_ϕ (25) prevents this destruction (up to Lebesgue-equivalence, *supra*). But one may equally wonder whether *less than one* wave-operator corresponding to a given matrix is not equally destructive for equivalence: f_ϕ^{inv} (30) must be defined on $\mathfrak{A}(C_{\text{mx}}^0)$ such that the range of f_ϕ^{inv} coincides with $\mathfrak{A}(C_{\text{wv}})$ to qualify as the inverse of f_ϕ . Physically speaking, if some matrix of matrix mechanics, say a Hamiltonian matrix for the sake of argument, does not have a corresponding Hamiltonian wave-operator, then matrix mechanics can handle situations where wave mechanics fails. That would destroy the purported equivalence. Remarkably, in the same footnote from which we quoted above, one stumbles upon Schrödinger's confession to this effect:

[...] we have not proved that a linear operator [wave-operator], corresponding to an arbitrary matrix, *always exists*.

The conclusion is that any inference at this stage that f_ϕ (25) is bijective, which is apparently considered necessary by Schrödinger for the equivalence of matrix mechanics and wave mechanics, would be a *non sequitur*. We shall resolve this issue in Part II, Section 4.

We continue our exposition. The mapping f_ϕ (25) answers the pivotal question posed above; the canonical matrices $P := f_\phi(\hat{P})$ and $Q := f_\phi(\hat{Q})$ are:

$$P_{mn} = -i\hbar \int_{-\infty}^{+\infty} \phi_m^*(q) \partial_q \phi_n(q) dq, \quad (33)$$

$$Q_{mn} = \int_{-\infty}^{+\infty} \phi_m^*(q) q \phi_n(q) dq. \quad (34)$$

As a consequence of the structure-preserving nature of the Schrödinger–Eckart mapping f_ϕ , the resulting matrices P and Q obey the canonical commutation relations (3), something which Schrödinger explicitly showed. Recall our observation below Postulate W1 in Section 4: Schrödinger introduced the canonical wave-operators \hat{P} and \hat{Q} in wave mechanics solely in order to have something from which to construct the canonical matrices.

The Hamiltonian matrix-elements are:

$$H_{mn} := \int_{-\infty}^{+\infty} \phi_m^*(q) \hat{H} \phi_n(q) dq. \quad (35)$$

This Hamiltonian matrix $H := f_\phi(\hat{H})$ is diagonal iff

$$\hat{H} \phi_n = E_n \phi_n, \quad (36)$$

because only then we do have that $H_{mn} = \delta_{mn} E_n$. Suppose, for the sake of expediency, that the arbitrarily chosen wave-basis $\{\phi_n\}$ solves equation (36),

that is, it contains the *eigenvibrations* of the atomic system under consideration. Diagonalising the H of matrix mechanics is the same as solving the time-independent Schrödinger equation (17) of wave mechanics; \hat{H} is complete iff H is diagonalizable. The energy basis $\{\phi_n\}$ is a physically preferred basis, because of all wave bases, only the eigenvibrations characterise the atomic system under consideration; and only in this basis do we obtain H in diagonal form, containing all the energy values on its diagonal. All other Hamiltonian matrices, obtained by performing unitary transformations, are empirically insignificant in matrix mechanics (they are in general not diagonal).

By assuming the time-dependence of $P(t)$ and $Q(t)$ as given by definitions (2), Schrödinger rewrote the matrix-mechanical Hamilton equations (5) as follows:

$$h\nu(m, n)Q_{mn} = [H, Q]_{mn} \quad \text{and} \quad h\nu(m, n)P_{mn} = [H, P]_{mn}. \quad (37)$$

He argued that the matrices $P = f_\phi(\hat{P})$, $Q = f_\phi(\hat{Q})$ and $H = f_\phi(\hat{H})$, constructed by means of equations (33), (34) and (35), respectively, where ϕ now refers to the energy basis $\{\phi_n\}$, obey equation (37). Hence, again, the energy basis is a physically preferred basis because it generates the solutions of the matrix-mechanical equations of motion, as Schrödinger emphasised (Schrödinger, 1927, p. 54); other bases allegedly do not. Schrödinger furthermore showed that partial differentiation, properly defined, of a wave-operator-valued polynomial $\hat{F}(\hat{P}_k, \hat{Q}_j) \in \mathfrak{A}(C_{wv})$ yields equations identical to ones arrived at by Born, Heisenberg and Jordan if wave-operators are substituted for matrices [Van der Waerden (1967, p. 327, eq. (6)), ; Schrödinger (1926b; 1927, p. 51, eqs (14) and (15))].

(c) In his second founding paper Schrödinger had confessed that wave mechanics could not calculate the intensity of the spectral lines, something which matrix mechanics in principle was able to do [Schrödinger (1926b; 1927, p. 30)]. Empirical equivalence lost. But from his own proof Schrödinger learned how to express spectral-line intensities in wave mechanics, by looking at the matrix-mechanical formula (6). Empirical equivalence regained—hopefully.

5.1. Postulate W6

The intensity $I_k(m, n)$ of electromagnetic radiation with frequency $\nu_k(m, n)$ polarised in direction k and emitted or absorbed in the transition $n \rightleftharpoons m$ is proportional to:

$$I_k(m, n) \propto \left| \int_{-\infty}^{+\infty} \phi_m^*(\mathbf{q}) \hat{Q}_k \phi_n(\mathbf{q}) d^3 q \right|^2, \quad (38)$$

where we have taken $d = 3$. *QEP*

So besides extending wave mechanics by adding the canonical wave operators (Postulate W1) whilst in the process of proving equivalence,³⁵ Schrödinger was here extending wave mechanics once more by another brand new postulate (Van der Waerden, 1973, p. 277). Schrödinger was not just attempting to prove the

³⁵ Section 4, below Postulate W1.

equivalence of matrix mechanics and extant wave mechanics, but he was also *expanding* extant wave mechanics on the spot *to make* it equivalent to matrix mechanics. As the inventor of wave mechanics, Schrödinger naturally had every right to expand *his* theory.

Recall that $|Q_k(m, n)|^2$ in matrix mechanics is proportional to $I_k(m, n)$ in the diagonal representation of H (Postulate M6). Hence we arrive once more at the conclusion that the energy basis is a physically preferred basis; in all other bases the proportionality (38) fails to hold.

(d) We enter the final part of the proof, which seems never to have been understood properly.³⁶ Then Schrödinger asserted that (Schrödinger, 1927, p. 58, *his italics*):

The equivalence *actually* exists, and it also exists *conversely*. Not only can the matrices be constructed from the eigenfunctions as shown above, but also, conversely, the functions can be constructed from the numerically given matrices.

We should be puzzled. So far Schrödinger has investigated the correspondence between wave-operators and matrices by means of mapping f_ϕ (25) and that investigation seemed to be more-or-less finished when he had purportedly arrived at the conclusion that f_ϕ is an isomorphism. Then, implicitly respecting the reigning state-observable characterisation of quantum mechanics, one would next expect to see the *states* treated, for the *observables* have been dealt with. There is only one problem with this line of reasoning: the concept of the quantum-mechanical state had still to be born (it can be projected back into wave mechanics with some wriggling, but most certainly not into matrix mechanics; cf. Part II, Section 2). To understand Schrödinger's words properly, we need to break away from the state-observable hegemony and immerse ourselves in wave mechanics. Here we go.

In wave mechanics the mathematical representatives of the physical magnitudes are the wave-operators and in matrix mechanics they are the infinite matrices. In both theories the mathematical representatives of the canonical physical magnitudes are postulated to generate similar structures, *videlicet* the canonical algebras $\mathfrak{A}(C_{wv})$ and $\mathfrak{A}(C_{mx})$. But the *canonical wave-operators* and the *canonical matrices* play quite different roles in their respective theories. In matrix mechanics the canonical matrices P_k and Q_j *vary from one physical problem to another*; they help to characterise the atomic system under consideration: the squared norms of the elements of Q in the diagonal representation of H are the intensities, other solutions Q' of the matrix-mechanical canonical commutation relations have no empirical significance. In contrast, in wave mechanics the canonical wave-operators *do not vary from one physical problem to another*; the canonical physical magnitudes position and momentum, whose wave-mechanical significance we indicated to be obscure,³⁷ are mathematically

³⁶ In all the literature on Schrödinger's proof mentioned in the Introduction it is simply ignored or taken for granted. Unjustifiably so, as we shall see. Van der Waerden (1973) is possibly the only exception, if interpreted with extreme charity, but in any case he did not pursue the matter.

³⁷ Section 4, below Postulate W1.

represented by the same *fixed* wave-operators for all atomic systems, namely the multiplication operator \hat{Q}_j and the differential operator (up to a constant) \hat{P}_k . In wave mechanics it is the collection of eigenvibrations $\{\phi_n\}$ that *varies from one physical problem to another*. What matrix mechanics and wave mechanics have in common is the fact that their Hamiltonians H and \hat{H} vary from one physical problem to another, and consequently so do their demonstrably identical sets of energy values $\sigma_{mx}(H)$ and $\sigma_{wv}(\hat{H})$. Now, a different Hamiltonian wave-operator \hat{H}' *does not have an effect on* the fixed canonical wave-operators \hat{P}_k and \hat{Q}_j , but does have an effect on the collection $\{\phi'_n\}$ of eigenvibrations and the set of eigenvalues $\sigma_{wv}(\hat{H}')$, both of which characterise the atomic system under consideration, because they solve the time-independent Schrödinger equation (17). A different Hamiltonian matrix H however *does have an effect on* the canonical matrices P_k and Q_j in the diagonal representation of H ; moreover, these matrices solve the matrix-mechanical Hamilton equations (5), in which H occurs.

Thence, an N -particle atomic system having Nd degrees of freedom is individuated in matrix mechanics by H , $\sigma_{mx}(H)$, C_{mx} , and in wave mechanics by \hat{H} , $\sigma_{wv}(\hat{H})$, $\{\phi_n\}$.

We next import this understanding into the equivalence proof. Returning to the last quotation, Schrödinger has tacitly changed his mathematical perspective on what has been 'shown above'. The phrase 'the matrices can be constructed from the eigenfunctions' alludes to a mapping, M say, that assigns matrices to eigenvibrations:

$$M : \Phi_{wv} \rightarrow \{\mathfrak{A}(C_{mx}^0)\}, \quad \{\phi_j\} \mapsto M(\{\phi_j\}) = \mathfrak{A}(C_{mx}^0), \quad (39)$$

given the fixed wave operators in $\mathfrak{A}(C_{wv})$, where Φ_{wv} is the set of all wave bases, and $\{\mathfrak{A}(C_{mx}^0)\}$ is the collection of all canonical matrix algebras each of which is generated by a distinct canonical pair $\langle P, Q \rangle$. Let us first spell out the connection between this new mathematical perspective and the old one.

Specifically, the connection between: (i) mapping M (39), which Schrödinger claimed to have considered 'above' but in actual fact did not appear to have been considered 'above'; and (ii) the Schrödinger–Eckart mapping f_ϕ (25), which Schrödinger did appear to have considered 'above', is: *given the canonical wave-operator algebra* $\mathfrak{A}(C_{wv})$, the set of all matrices determined by the (energy) basis $\{\phi_n\}$ coincides with the canonical matrix algebra iff for each matrix A there is a wave-operator \hat{A} related to A by the Schrödinger–Eckart mapping f_ϕ (25). Symbolically,

$$M(\{\phi_j\}) = \mathfrak{A}(C_{mx}^0) \quad \text{iff} \quad \forall A \in \mathfrak{A}(C_{mx}^0), \exists \hat{A} \in \mathfrak{A}(C_{wv}) : f_\phi(\hat{A}) = A. \quad (40)$$

(If f_ϕ is an isomorphism, it suffices to let the quantifiers run over the generator sets.) We now arrive at a rigorous rendition of Schrödinger's words as an assertion of *the invertibility of the mapping* M (39). In other words, there exists a mapping which assigns wave bases to matrices:

$$M' : \{\mathfrak{A}(C_{mx}^0)\} \rightarrow \Phi_{wv}, \quad \mathfrak{A}(C_{mx}^0) \mapsto M'(\mathfrak{A}(C_{mx}^0)) = \{u_j\}, \quad (41)$$

such that

$$M' \circ M = I_{wv} \quad \text{and} \quad M \circ M' = I_{mx}, \quad (42)$$

where I_{wv} is the identity on Φ_{wv} and I_{mx} is the identity on $\{\mathfrak{A}(C_{mx}^0)\}$, because equations (42) identify M' as the inverse of M .

To verify equations (42), we need to know whether such a mapping M' (41) exists. We now follow Schrödinger almost *verbatim* (Schrödinger, 1927, p. 58). Suppose a matrix Q is given. Then by matrix multiplication all matrices Q^n can be calculated. [Notice that the existence of the fully fledged matrix algebra $\mathfrak{A}(C_{mx}^0)$ is needed to license the last mentioned assertion!] Schrödinger looked for a collection of eigenvibrations $\{u_j\}$, assuming them to be mutually orthogonal, real-valued, positive, twice differentiable and vanishing (asymptotically) for large q , such that $f_u(\hat{Q}^n) = Q^n$ for all n . Hence we obtain the following denumerable system of Riemann-integral equations:

$$(Q^n)_{jk} = \int_{-\infty}^{+\infty} q^n u_j(q) u_k(q) dq. \quad (43)$$

Then Schrödinger declared (Schrödinger, 1927, p. 58):

The totality (43) of these integrals, when j and k are fixed, forms what is called the totality of the *moments* of the function $u_j u_k$. And it is known that, under very general assumptions, a function is determined by the totality of its moments. So all the products $u_j u_k$ are uniquely fixed, and thus also the squares u_j^2 and therefore also u_j itself.

Thus by declaring that the subalgebra $\mathfrak{A}(Q)$ of $\mathfrak{A}(C_{mx}^0)$, generated by Q only, determines the basis $\{u_j\}$, Schrödinger was proposing the following definition of M' :

$$M'(\mathfrak{A}(Q)) = \{u_j\} \quad \text{iff} \quad \{u_j\} \text{ solves equation (43) uniquely.} \quad (44)$$

If the system of Riemann-integral equations (43) does not have a unique solution, then M' is not even a mapping and by implication the mapping M (39) is not bijective. Equivalence doomed. We can however see that *if* 'Schrödinger's moment problem' (43) is uniquely solvable, *then* equation (42) is satisfied, by virtue of the connection (40), and the conclusion that the mapping M is bijective follows immediately. Equivalence saved—hopefully.

In Part II, Section 3 we shall address the purported bijectivity of the mapping M (39), and delve into the connection between 'Schrödinger's moment problem' (43) and what was known in mathematics at the time as 'the power moment problem'. Interestingly, Schrödinger hardly says a word about that connection, nor does he mention what the 'very general assumptions' are, which the functions u_j are tacitly assumed to fulfil.

This completes our review of Schrödinger's proof of his assertion that matrix mechanics and wave mechanics 'are completely equivalent from the mathematical point of view' [Schrödinger (1926c; 1927, p. 57)].

Let us summarise our analysis. We noted in (c) that the threat of the empirical non-equivalence of matrix mechanics and wave mechanics caused by the fact that wave mechanics did not contain a clue of how to calculate radiation intensities

was averted by Schrödinger by adducing a novel wave-mechanical postulate. The problem of whether the putative canonical algebras really are algebras being set aside, we ascertained in (b) that their mathematical equivalence (isomorphism) was not yet demonstrated because the bijectivity of the Schrödinger–Eckart mapping was not proved. We noted Schrödinger's confession to this effect, despite his confident conclusion of the 'complete mathematical equivalence'. Finally, in (d) we immersed ourselves in wave mechanics to understand the need to solve Schrödinger's moment problem, and we felt fobbed off with fair promises. So already we can conclude that the putative proof is not entirely foolproof. We shall subsequently find out what is right and what is wrong with the proof as it stands, disclose which features of extant matrix mechanics and wave mechanics are ignored in the proof, and point out how to attain equivalence in the von Neumann manner.

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