Why were two theories (Matrix Mechanics and Wave Mechanics) deemed logically distinct, and yet equivalent, in Quantum Mechanics?

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Differences between MM and WM in 1926:

- **Formal:**
  - MM an algebraic approach employing the technique of manipulating matrices.
  - WM - differential equations (a basic partial differential wave equation at its heart)
- **Empirical:**
  - MM - spectral lines, and later (to some extent) the experiments with electron scattering.
  - WM - light interference experiments; the account of the energy values in experiments with hydrogen atoms

- **Ontological:**
  - Heisenberg stressed the discrete properties of the observed phenomena (e.g., spectral lines of different intensities)
  - Schrödinger perceived the field-like continuity of some key micro-physical phenomena as the main advantage of WM

- An argument for their supposed mathematical equivalence was first conceptualized and published by Schrödinger in 1926 - “On the Relation between the Quantum Mechanics of Heisenberg, Born, and Jordan, and That of Schrödinger”
- It was perceived as a major breakthrough – it predicated the future development of quantum mechanics

- F.A. Muller (1997a, 1997b) has deemed this equivalence a myth
  - Only later developments in the early 1930s, especially the work of mathematician John von Neumann (1932), provided sound proof of the mathematical equivalence

- The Copenhagen Interpretation of QM debunked as a myth a) forced on others by Bohr (Beller, 1999), or b) non-existent at the time (Howard, 2004) **– no good reasons for its existence**
  - CI commonly seen as largely predicated on the (alleged) equivalence

An Alternative View:

- Schrödinger's proof concerned a domain-specific ontological equivalence, of otherwise (empirically, logically and, perhaps, mathematically) distinct, theories – the domain being Bohr's atom
- Furthermore, even the full-fledged mathematico-logical equivalence of the theories did not seem out of the reach of the existing theories and methods, <u>although Schrödinger never intended to fully explore such a possibility in his proof paper</u>

- Only Bohr’s complementarity and Copenhagen Interpretation captured a more substantial convergence of, the subsequently revised (in light of the experimental results), theories.

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Muller's argument:

– Schrödinger attempted to prove the mathematical equivalence of MM and WM by demonstrating their *isomorphism* (the *explananas* of Schrödinger's overall argument), in order to explain their allegedly established empirical equivalence (*explanandum*)

Muller’s argument:

The myth of the empirical equivalence:

1. It was overlooked that the electron charge densities were smeared, and that this “made it conceivable to perform an *experimentum crucis* by charge density measurements” (Muller 1997a, 38)
2. Two cases insufficient as evidence of the purported empirical equivalence:
   - coinciding energy values for the hydrogen atom and “the few toy systems” (Muller 1997a, 49)
   - the quantisation of orbital angular momentum

Muller’s argument:
The myth of mathematical (logical) equivalence

“the 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 MM and WM” (Muller 1997a, 38).

Muller's argument:

Why the mathematical equivalence failed:

1. the absence of a state-space in MM prevented the direct mutual translation of sentences of WM and MM.
2. the language of MM could not refer to space, charge-matter densities, or eigenvibrations,[1] "because MM did not satisfy (in the rigorous model-theoretic sense) any sentence containing terms or predicates referring to these notions" (Muller 1997a, 39).

3. The failure of what Muller labels “Schrödinger-equivalence” – an attempted (Muller believes) proof of a “softer” equivalence – a failure which was due to the so-called “problem of moments” of the function not being treated in a satisfying way (as it was in Von Neumann’s proof)

The Empirical Evidence in Early QM

- **Schrödinger never committed himself to a strong view of empirical equivalence**, and it is actually very unlikely that anybody else believed in the full-blown empirical equivalence at the time
- The consequences of Schrödinger's theory, which contradicted Bohr's early view of radiation, were **probed experimentally by a series of crucial experiments** (Compton and Simon, 1925; Bothe and Geiger, 1926; Ramsauer)

- Nor could the experiments concerning the related issue of quantisation of the orbital angular momentum have contributed to the presumed (by Muller) agreement on the empirical equivalence.
- neither Schrödinger nor anybody else was certain whether or to what extent either of the two formalisms fully accounted for the observed properties of micro-physical processes, *nor whether either was indispensable*

Was Schrödinger’s proof, a proof of mathematico-logical equivalence?

- “[i]n what follows the very intimate *inner connection* between Heisenberg’s QM and my wave mechanics will be disclosed. From the formal mathematical standpoint, one might well speak of the *identity* of the two theories.” (Schrödinger, 1926a, 46).
- One or two distinct goals of the proof?

- <u>His explicit statements about the nature of the equivalence differ substantially</u>:
  - “both representations are – from the purely mathematical point of view – totally equivalent.” (letter to Wien, March 1926, Mehra and Rechenberg, 1982, 640)
  - In his second Communication he states that MM and WM “will supplement each other”
  - The obscure discussion of the mathematical/physical equivalence in the proof paper
  - Is Schrödinger’s mathematical point of view identical to that of Muller? Although not very usage of the phrase “mathematical equivalence” suggests this, let’s assume that it is. Was this the main goal of the proof?

The motivation for the proof:

- the equation $\Delta\psi + 8\pi^2 m_o/h^2\, [E - E_{pot}\, (x, y, z)]\, \psi = 0$ will have a solution for E_n
- **Schrödinger's solution of the hydrogen atom eigenvalue equation of his first and second communication of 1926 resulted in Bohr's energy levels**
- Given that WM and Bohr's model agreed with respect to the eigenvalues and stationary energy states, the question was whether WM and MM agreed with respect to eigenvalues and, thus, to stationary states as well

- Schrödinger’s expression of the “intimate connection” between MM and WM, rather than his reference to the “mathematical equivalence” of the two, indicates the central goal of the proof
- The analysis of both **the structure and the content of the proof** indicates this

The proof:

- ***Part 1*** of the proof establishes the preliminary connection between MM and WM
- "I will first show how to each function of the position and momentum-co-ordinates there may be related a matrix in such a manner, that these matrices, in every case, satisfy the formal calculating rules of Born and Heisenberg (among which I also reckon the so-called 'quantum condition' or 'interchange rule')" (1926a, 46).

- Since Born-Heisenberg's matrix relation **pq** - **qp** = $(h/2\pi i)\mathbf{1}$ corresponds to the WM relation $[(h/2\pi)(\partial/\partial q)]\, q\psi - q\,[(h/2\pi i)(\partial/\partial q)]\,\psi = (h/2\pi i)\psi$, a differential operator $F[(h/2\pi i)(\partial/\partial q), q]$ can be associated with the function of momentum and position $F = F(p, q)$.
- If the phase velocity functions, $uk = uk\,(q)$, in the configuration space of the position q form a complete orthonormal set, then an equation

$Fjk = \int u^*j\, [F, uk]\, dq$, can be derived that determines the elements of the matrix Fjk.

- Thus, as this argument goes, in this very particular sense, any equation of WM can be consistently translated into an equation of MM.

- ***Part 2*** provides the *unidirectional argument for the domain-specific equivalence* by constructing suitable matrices from eigenfunctions

- Relying on the insights of Part 1, Schrödinger replaces the *ui* of the *uk* = *uk* (*q*) with the eigenfunctions of his wave equation. Thus, he obtains an operator function: [*H*, *ψ*] = *Eψ*. The operator's eigenvalues *Ek* satisfy the equation [*H*, *ψk*] = *Ek ψk*. As it turns out, solving this equation is equivalent to diagonalizing the matrix *H*.
  - In other words, the *H* turned out to be diagonal with respect to the specified basis (diagonalization of a matrix is a particular orthogonal transformation of the so-called quadratic form, i.e., its rotation).

- In the final and decisive step of Part 2, Schrödinger demonstrates that the matrices constructed in accordance with the elements of matrix *Fjk* given by the above-stated equation, with the help of some auxiliary theorems, satisfy the Born-Jordan-Heisenberg laws of motion.
  - More precisely, **the Heisenberg-Born-Jordan laws of motion** (Born, Heisenberg and Jordan, 1926) **initially derived purely from MM point of view, are satisfied by (as Schrödinger characterizes the decisive step in the Introduction) "assigning the auxiliary role to a definite orthogonal system, namely to the system of *proper functions* [Schrödinger's italics] of that partial differential equation which forms the basis of my wave mechanics"** (1926a, 46).

- **Yet if we believe that providing a logical proof of the isomorphism between MM and WM was the central goal of the proof, Part 3 of the text must be at least as essential as Part 2**, as it tries (and ultimately fails) to establish the reciprocal equivalence required by such a goal
- But: unlike the pressing issue dealt with in Part 2, **the issue addressed in Part 3 is an ‘academic’(in a pejorative sense of the word) one** of logical isomorphism requiring the proof of reciprocal equivalence

Schrödinger's intentions:

- Schrödinger states that "the equivalence actually exists, and it also exists conversely." But he never fully demonstrates this, nor does he make an outstanding effort to do so. Instead, he provides a vague idea of how one might proceed in proving this sort of logical equivalence
- More precisely, as Muller (1997a, 56) correctly pointed out, **Schrödinger does not prove the bijectivity of the Schrödinger-Eckart mapping (which assigns one matrix to each wave-operator), necessary for isomorphism**

- The isomorphism of MM and WM would have made sense as the *explanans* and as the key, and perhaps, the only goal of the proof, only if a full-blown empirical equivalence was established.
- The modest demonstration was more desirable, especially because establishing Bohr's model as an acceptable "big picture" did not require the logical equivalence (i.e., bi-directional derivation to prove isomorphism)

- Schrödinger apparently gets his priorities straight. He explicitly states that he will offer only "a short preliminary sketch" (1926a, 47) of the full-fledged reciprocal equivalence, i.e., the connection between MM and WM, taken in the opposite direction from that demonstrated in Part 2
- Schrödinger tentatively says, "The following *supplement* [Schrödinger's italics] to the proof of equivalence given above is interesting" (Schrödinger 1926a, 58), before going on to discuss the possibility of the construction of WM from MM and its implications for the epistemological status of WM.

- How did others perceive the proof and equivalence?
  - Bohr’s 1928 letter to Schrödinger: Bohr is still concerned with an (implicit) assumption of MM regarding stationary states as a limitation on the applicability of WM

    In the interpretation of experiments by means of the concept of stationary states, we are indeed always dealing with such properties of an atomic system as dependent on phase relations over a large number of consecutive periods. *The definition and applicability of the eigensolutions of the wave equation are of course based on this very circumstance*.

- Other proofs
  - Pauli thought he has found “a quite simple and general way [to] construct matrices satisfying the equations of the Göttingen mechanics”
  - The influence of Wigner-Klein-Jordan’s proof
  - Dirac’s proof
  - Eckart’s proof

- Later commentators understood Schrödinger’s proof in the same spirit as Von Neumann (and Muller is right in claiming this) because of the changing tide in quantum physics.
- The second stage of the quantum revolution had already begun, and physicists concentrated their efforts on the formal aspects of research, grounded on firmly established experimental results.

- Appendix

- WM and MM

"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. I refer, in particular, to the peculiar "half-integralness" which arises in connection with the oscillator and the rotator." (1926a, 45)

- Early agreement of MM and WM (II Comm.):

Already in (1926c) while discussing the rotator case, S. notes the agreement between MM and WM, with respect to the quantum energy levels: "Considering next the proper values, we get … $E_n = (2n + 1)/2\ h\nu_o$; $n = 0, 1, 2, 3, \ldots$ Thus as quantum levels appear so-called "half-integral" multiples of the "quantum of energy" peculiar to the oscillator, *i.e.* the *odd* multiples of $h\nu_o/2$. The intervals between the levels, which alone are important for the radiation, are the same in the former theory. It is remarkable that our quantum levels are *exactly* those of Heisenberg's theory." (p. 31)

- <u>Bohr's energy-states and eigenvalues:</u>
  - <u>In (1926b, 8)</u> Schrödinger starts from the wave mechanical assumptions and derives the expression $-E_\iota = m(e^2)^2 / 2K^2\iota$ where "the well known Bohr energy-levels, corresponding to the Balmer lines, are obtained, if the constant ***K***, introduced in for reasons of dimensions, we give the value $K = h / (2\pi)$, from which comes $-E_\iota = 2\pi^2 m (e^2)^2 / h^2\iota^2$."
  - <u>In (1926c, 27-28),</u> at the end of the discussion of the case of the rotator, Schrödinger generalizes the expression of an earlier derived wave function (div grad $\psi - (1/u^2)\,\ddot{\psi}$) in the following way: "For it is possible to generalize by replacing div grad ψ by $f(qk)$ div $\{[1 / f(qk)]$ grad $\psi\}$, where f may be an arbitrary function of the q's, which must depend in some plausible way on E, $V(qk)$, and the coefficients of the line elements."
  - Later on, he comments on the agreement between energy values in Bohr's theory and eigenvalues (discussed on p. 26), emphasizing the advantage of his approach: "… the quantum levels are *at once* defined as the *proper values* of equation (18) [wave equation], which *carries in itself its natural boundary conditions*." (p. 29) The entire argument for the advantage of the wave-mechanical approach in the second Communication was predicated on this agreement.

- *The so-called "problem of moments"*, referred to in Part 3, has to do with the preliminary discussion of the full-fledged logical proof and an attempt to argue for epistemological advantage of WM. Thus, Schrödinger promises "[t]he functions can be constructed from the numerically given matrices." (p. 58) If so, "the functions do not form, as it were, an *arbitrary* and *special* "fleshly clothing " for the bare matrix skeleton, provided to pander to the need of the intuitiveness." In order to show this, he invokes the totality of the "moments" of a function...

The moment problem

- The moment of a function
  - In physics: the magnitude of force applied to a rotational system at a distance from the axis of rotation
  - In mathematics: the *n*-th moment of a (real-valued) function $f(x)$ of a real variable concerning a value c is

$$\mu'_n = \int_{-\infty}^{\infty} (x-c)^n f(x)dx$$

  - The problem of moments – finding characterizations of sequences μ'_n $(n = 1, 2, 3,\ldots)$ which are sequences of moments of f (i.e., inverting the mapping that takes the measure μ *to the sequences of moments*)

- Schrödinger’s moment problem is a version of the Hamburger moment problem in which the supportt of μ is allowed to be the whole real line

- The totality of the integrals ($\int P(x)u_i(x)u_k(x)dx$) forms the totality of the moments (when i and k are fixed) of the function $u_i(x)u_k(x)$- *the functions* $u_i(x)$ *are to be found* in the equation relating the matrices with WM relations
- The totality of the moments determines a function uniquely (under very general assumptions that S. does not specify, nor can he)