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Mathematics meets physics

A contribution to their interaction in the 19$^{\text{th}}$ and the first half of the 20$^{\text{th}}$ century

Verlag
Harri
Deutsch

From Matrices to Hilbert Spaces: The Interplay of Physics and Mathematics in the Rise of Quantum Mechanics

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1 Introduction

In his *History of Functional Analysis*, the leading mathematician Jean Dieudonné points out how the history of this field ran counterwise to what a nowadays mathematician could imagine relying on the present way of introducing the topic. To make a long story short, Dieudonné emphasises how, in the development of functional analysis, the "linear algebra" type of understanding of the relevant issues came rather late, being historically preceded by the use of some tools today viewed as emblematic to the theory, but then not recognized as such. The theory of infinite systems of linear equations, of infinite determinants, of infinite bilinear forms and their normal forms, for their own sake or as a way to deal with integral equations, was first developed without reference to linear spaces and to typical problems associated with their endomorphisms. Also, the geometric interpretation of the problems that gave rise to functional analysis was absent from the early intuitions of its main founders. Only after Hilbert's results on the theory of integral equations and infinite forms were taken over and extended by his followers and students such as Hellinger, Schmidt, or Weyl, did the geometric point of view become explicit and recognized as an important insight to frame the theory[1].

When surveying the contributions of von Neumann who extended Hilbert's spectral theory to unbounded forms, Dieudonné mentions how these mathematical results were of highest importance to physicists having hard time to cope with the involved mathematics of quantum mechanics. Dieudonné's account offers ample ground for criticism as he conveys the impression that before the intervention of the mathematicians, physicists were much into the blue in what concerns the formal structure of their theory; he also fails to mention how the reflection on the foundations of quantum mechanics actually triggered von Neumann's results. These shortcomings, that one could possibly attribute to Dieudonné overly Bourbakist stand, are possibly minor if considered from the point of view of pure history of mathematics. However, beyond the question of sheer historical accuracy, Dieudonné's account thus misses the opportunity to pay due tribute to an important, if not

[1] Dieudonné 1981, pp. 2–3.

exemplary, episode from the rich history of fruitful connections between physics and mathematics. More importantly, by largely ignoring the physical context into which went invested some of the most important results of early functional analysis, Dieudonné fails to recognize that to a large extent, both communities were at the time facing the same lack, that of a geometrical, "linear algebra" intuition on their respective issues and problems. Indeed, my contribution endeavours to show how, in their respective way, physicists reached, in the crucial year 1926, a full understanding of the proper mathematical interpretation of the formalism of quantum mechanics, recognizing thus the prime importance of the linear structures and objects underlying their way to handle the formalism and put it to physical use. Their appraisal of this mathematical reality, known then as transformation theory, was the starting point of the developments that led Johann von Neumann to his abstract Hilbert space and his theory of self-adjoint unbounded operators and associated spectral theory.

2 Quantum theory: alternate formalisms and equivalences

The birth of quantum mechanics took place with a seminal paper of Werner Heisenberg in 1925[2]. The formal features of Heisenberg's approach were soon recognized to amount to (infinite) matrix manipulations by Max Born and Pascual Jordan[3] who subsequently elaborated, together with Heisenberg, the main features of matrix mechanics[4]. Dirac extended independently Heisenberg's original ideas as a calculus of abstract q-numbers in a series of papers from the same period[5]. Only a couple of months later, Erwin Schrödinger introduced in a series of four papers the differential equations of wave mechanics[6]. In the

[2] Heisenberg 1925. For a general history, see Jammer 1966, Mehra and Rechenberg 1982, 1987, Darrigol 1992.
[3] Born and Jordan 1925.
[4] Born, Jordan and Heisenberg 1926.
[5] Dirac 1925, 1926ab.
[6] Schrödinger 1926abcd.

same period, quantum theory even received a fourth formulation as an operator calculus due to Born and Wiener[7].

Thus, by mid 1926, quantum theory was associated with four different formalisms. The latter were differing by choices of basic ingredients and/or of logical order of presentation, and most of all, by different types of mathematical objects that were involved. Let us review their main characteristics.

2.1 Heisenberg's matrix mechanics

Born, Jordan and Heisenberg's formalism of matrix mechanics is deeply rooted in the classical theory of multiply periodic systems quantized with the help of the Bohr-Sommerfeld conditions[8]. It takes over some of the latter's formal features, replacing its characteristic Fourier expansions for physical magnitudes by arrays of numbers constructed from the corresponding Fourier amplitudes and frequencies. Thus, matrix mechanics associates to each of the physical quantities of a system a set of numbers $a(nm)\exp(2\pi i\nu(nm)t)$ understood as defining a (time-dependent) matrix $\mathbf{a}$[9]. For each degree of freedom indexed with integer k, and described by the coordinate q_k and associated momentum p_k, one imposes the fundamental relation between the corresponding canonical matrices:

$$\mathbf{p}_k\mathbf{q}_k - \mathbf{q}_k\mathbf{p}_k = -\mathrm{i}\hbar\mathbf{1}. \tag{1}$$

[7] Born and Wiener 1926.

[8] For an insightful account of the classical foundations and analogies that drove the early attempts at quantum theory before the advent of quantum mechanics, see Darrigol 1992.

[9] The integer indices n, m label the (discrete) set of stationary states of the system. The frequencies $\nu(nm)$ correspond to the transitions between state n and m according to Bohr's frequency conditions (see below). The origin of such expressions goes back to the use of multiple Fourier expansions inherited from the methods of celestial mechanics applied to the (planetary) models of the "old quantum theory". The successive harmonic terms of those series were providing, following Bohr's correspondence principle, information on the corresponding transitions between the stationary states of the quantum system. For the details of this correspondence, see Jammer 1966, p. 102 – 118, and Hund 1967; see also Darrigol 1992.

These relations enable to calculate products of quantum theoretical quantities[10]. Given a Hamiltonian matrix $\mathbf{H}$, the relations (1) ensure the validity of the canonical equations[11]

$$\dot{\mathbf{p}}_k = -\frac{\partial \mathbf{H}}{\partial \mathbf{q}_k}, \quad \dot{\mathbf{q}}_k = \frac{\partial \mathbf{H}}{\partial \mathbf{p}_k},$$

which account for the dynamics of the system. Bohr frequency conditions

$$h\nu(nm) = H_n - H_m \tag{2}$$

are recovered when the Hamiltionian matrix is diagonal, with H_n its n-th diagonal element (this corresponds to the energy of the n-th stationary state), and h Planck's constant. In matrix mechanics,the dynamical problem amounts thus to finding a set of matrices obeying (1) such that the corresponding Hamiltonian expressed in terms of the latter is diagonal. The main tool for diagonalization are the (canonical) transformations

$$\mathbf{H} \to \mathbf{S}^{-1}\mathbf{H}\mathbf{S}. \tag{3}$$

Born, Heisenberg and Jordan developed in their paper the stationary and time dependent perturbation theories, obtaining perturbative expansions for the diagonalization matrix $\mathbf{S}$. In this case the latter has an expansion of the form $\mathbf{S} = \mathbf{1} + \mathcal{O}(\epsilon)$ where ϵ is a small parameter, so that the computation of $\mathbf{S}^{-1}$ can be formally handled. The difficulty of computing $\mathbf{S}^{-1}$ in the general case will motivate soon research for alternate forms of the transformation (3). We shall shortly examine some examples of such.

It is of prime importance to emphasize here that in the matrix approach, matrices are understood simply as arrays of coefficients providing all the information that is directly observable, namely the amplitudes of the processes, which was the declared motivation of Heisenberg's first

[10] Canonical matrices for different degrees of freedom commute, i. e. $\mathbf{p}_k\mathbf{q}_l - \mathbf{q}_l\mathbf{p}_k = \mathbf{0}$, for $k \neq l$.

[11] $\mathbf{H}$, a function of the symbols $\mathbf{p}$ and $\mathbf{q}$, has its form suggested by the classical case. However, as in the quantum case the symbols $\mathbf{p}$ and $\mathbf{q}$ are matrices obeying the canonical commutation relations (1), the quantum Hamiltonian may eventually differ in its functional form from his classical counterpart due to the quantum non-commutativity of the symbols $\mathbf{p}$ and $\mathbf{q}$ which makes ambiguous their products.

paper. These matrices are however deprived of any operatorial meaning, i. e. they are not conceived as representatives of linear mappings within some linear space, left alone as acting on some physically meaningful objects.

2.2 Dirac's q-numbers

Inspired by Heisenberg's results, Dirac derived the formalism of quantum theory insisting on the essential non commutativity of the symbols associated to quantum quantities, which he consequently called q-numbers in opposition to ordinary commuting scalars. Classically, given a system described in the Hamiltonian scheme by the (generalized) coordinates q_k and the associated momenta p_k, the time evolution of any physical quantity, say $A = A(p_k, q_k)$, is given by its Poisson bracket with the Hamiltonian $H = H(p_k, q_k)$

$$\dot{A} = \{A, H\} \equiv \sum_k \frac{\partial A}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial H}{\partial q_k}\frac{\partial A}{\partial p_k}$$

In particular, for the coordinates and momenta themselves, one has

$$\dot{p}_k = \{p_k, H\} = -\frac{\partial H}{\partial q_k}; \quad \dot{q}_k = \{q_k, H\} = \frac{\partial H}{\partial p_k}.$$

Analysing the formalism that Heisenberg introduced in his 1925 foundational paper, Dirac recognized that the quantum case involved in general non-commuting q-number analogues of the q_k's and p_k's, and the prescription that any classical Poisson bracket $\{A, B\}$ of any two quantities A and B goes into the corresponding quantum bracket $\frac{\mathrm{i}}{\hbar}[\mathbf{A}, \mathbf{B}] \equiv \frac{\mathrm{i}}{\hbar}(\mathbf{AB} - \mathbf{BA})$ of the q-analogues. Dirac's approach was in principle more general than that of Born, Jordan and Heiseberg since, concentrating on the non-commutative q-numbers algebra, he did not give necessarily these numbers an explicit realization in terms of matrices[12].

2.3 Schrödinger's wave mechanics

Schrödinger's approach is physically based on the view of classical mechanics as a limiting case (long-wave approximation) of wave mechanics

[12] Dirac 1925, 1926ab.

in analogy with the geometric optics with respect to wave theory of light[13]. Consequently, Schrödiger considered the energy levels E of the stationary states of the quantum system in a potential V as associated to a wave function ψ, in general a complex valued function defined over the configuration space of the system parametrized with the coordinates q_k. The wave function ψ is a solution of the eigenvalue equation[14]

$$\triangle\psi - \frac{8\pi^2}{h^2}(E - V)\psi = 0.$$

This equation is formally obtained from the energy relation

$$(H(p_k, q_k) - E)\,\psi = 0, \tag{4}$$

where in the Hamiltonian

$$H(p_k, q_k) = \frac{1}{2}\sum_k p_k^2 + V(q_k)$$

of the system, one has substituted for the momenta p_k the partial derivatives

$$p_k \to -i\frac{h}{2\pi}\frac{\partial}{\partial q_k}$$

The dynamics of the system is given by the time-dependent equation

$$\left(\triangle - \frac{8\pi^2}{h^2}V\right)\psi = i\frac{4\pi}{h}\frac{\partial}{\partial t}\psi$$

where E in (4) has been replaced this time by $i\frac{h}{2\pi}\frac{\partial}{\partial t}$.

[13] Schrödinger 1926abcd, in particular 1926b.

[14] The mass of the particle has been set to 1. Below, $\triangle$ is the (negative of the) Laplacian operator, given in (rectangular) coordinates by

$$\triangle = -\sum_k \frac{\partial^2}{\partial q_k^2}$$

2.4 The operator calculus of Born-Wiener

Let us also mention for the sake of completeness that, because matrix mechanics was impractical to formulate in the case of non periodic systems [15], Born and Wiener formulated an alternative formalism for quantum theory choosing as the fundamental formal devices linear operators[16]. I shall omit to comment on this approach as it did not play a major role in the developments that are pertaining to my topic. Let me just emphasize that Born and Wiener operators are not equivalent to those of the Hilbertian theory[17].

2.5 Problems of Equivalence

Dirac's q-numbers could be easily represented in terms of Born Jordan matrices thus showing immediately the equivalence of Dirac's formalism with the matrix one. In his early paper "Quantum Mechanics and a Preliminary Investigation of the Hydrogen Atom"[18], Dirac, studying the quantum analogue of action-angle variables, introduced the fundamental interchange relations

$$
\begin{aligned}
e^{i(\alpha q)} f(q_r, p_r) &= f(q_r, p_r - \alpha_r \hbar), \qquad (5)\\
f(q_r, p_r) e^{i(\alpha q)} &= e^{i(\alpha q)} f(q_r, p_r + \alpha_r \hbar),
\end{aligned}
$$

$$
\text{with} \quad (\alpha q) \equiv \sum_{r=1}^{f} \alpha_r q_r, \qquad (6)
$$

[15] As we have seen, the integer indices labelling the matrices directly refer to the stationary states of the theory which are the eigenstates of the Hamiltonian. Now, whenever the latter has a continuous spectrum, the matrices are clearly ill-defined: even if one is ready to consider a continuous range for the index labelling their lines and columns, one ends up with mathematical trouble, for instance singularities (Dirac's functions) on their diagonal.

[16] Born and Wiener 1926.

[17] Pauli, when trying to understand the equivalence between matrix and wave mechanics, introduced operators as well, but in a form different from that of Born and Wiener, see Mehra and Rechenberg 1987, chap. IV. The operator approach was used also by others in their attempts to prove the equivalence of matrix and wave mechanics; among others, C. Eckart (Eckart 1926ab). Actually, Cornelius Lanczos proposed as early as end of 1925 a systematic way of obtaining continuous equations equivalent to matrix ones using integral equations and the formalism of Green functions (Lanczos 1926), but did not provide any new application, see below.

[18] Dirac 1926a.

where the index r runs over the degrees of freedom, and f stands here for a function of the q_r and p_r. This enabled him to deal with the quantum analogues of the classical multiply periodic expansions of the form

$$x = \sum_{\alpha} x_{\alpha}(J_r) e^{i(\alpha w)}.$$

used in the "old quantum theory". Commuting the x_α across the $e^{i(\alpha w)}$, and using the canonical commutation relations, Dirac could obtain q-number formulas displaying the same structural features as the ones of matrix mechanics. This lead, in Dirac's terms, to the proof of the possibility of representing his q-numbers by Heisenberg's matrices of c-numbers, defining the corresponding "matrix scheme". Dirac studied later this correspondence in a more general setting acting directly with q-numbers on Schrödinger's eigenfunctions[19].

The situation was much more puzzling in what concerned the relation of matrix mechanics with Schrödinger's wave formalism. Quite early, it was understood that both formalisms yielded the same physical predictions. The first proof of the equivalence of wave mechanics with matrix mechanics was given by Schrödinger himself[20]. For each pair of (normalized) eigenfunctions of his equation, say ψ_n and ψ_m, and a physical quantity $A(p_k, q_k)$, Schrödinger showed that the expressions

$$A_{nm} = \int dq \psi_n A(q, \frac{\partial}{\partial q}) \psi_m.$$

defined the coefficients of the corresponding Heisenberg matrix[21]. Schrödinger's proof was sufficient as far as practical considerations were concerned. One could then freely choose between his approach and the rival matrix formalism depending on the problem at hand. Actually, the differential formalism of wave mechanics soon supplanted the matrix one. However, Schrödinger's proof, a kind of dictionary between both approaches was not providing any clue about the mathematical reasons

[19] Dirac 1926b.

[20] Schrödinger 1926e.

[21] Although Schrödinger realized that, to some extent, the square modulus $\psi\psi^* = |\psi|^2$ played the role of a weight function in the configuration space (this interpretation can be found in Schrödinger 1926d, pp. 109 – 139), the full probabilistic meaning of $|\psi|^2$ came only with Born's statistical interpretation.

that were making it possible. Let us consider a bit closer the situation. As mentioned, Born and Jordan matrices were not understood as associated to linear transformations in some (linear) space. Accordingly, in the matrix formalism, there are just no column matrices (vectors) on which these matrices could 'act'. With hindsight, these vectors would, if present, formally correspond to (quantum) states of the system, but in the matrix formalism, we are just in the "Heisenberg representation" where observables (matrices), but not states, evolve with time and the dynamical equations are about observables-matrices and not states-vectors. This makes it plain why matrix mechanics was not necessitating, as far as physical reasons go, any reference to a linear space underlying its formalism. Given that, at the time, in mathematics too, one could deal with diagonalization problems in the language of the normal form of bilinear forms, and that other 'linear' problems were treated in a non-coordinate free approach, we see that matrix mechanics and its use were not requiring any geometric form of intuition to be associated to its formal features.

Similar observations can be done with respect to wave mechanics, albeit for different formal reasons. Here, one considers a partial differential equation defining an eigenvalue problem. The eigenvalues are associated to stationary solutions of the time-dependent equation and refer to time-constant physical configurations of the system. Because the equation is linear, one can take linear combinations of its solutions to obtain new ones. However, the linear span of the solutions is devoid of any physical meaning beyond the physical meaning attributed to the solutions themselves. Thus, Schrödinger's solutions are not representing quantum states, they provide just the density of matter waves of the system. Since Schrödinger is attributing to the solutions an interpretation in terms of configurations of matter waves, he does not associate either to its differential expressions $A(p_k, q_k)$ an operatorial meaning in the linear span.

As we see, the way both formalisms were used and interpreted was not requiring any recognition of the importance of the linear structure underlying both. Given that the latter is the key to grasp the nature of the mathematical relationship between matrix and wave mechanics, the proper mathematical understanding of this relation had to remain obscure for some time. The appraisal of the intrinsic relevance of the linear structure underlying matrix and wave mechanics actually emerged out of the necessity to work out the dynamic equations in different coordinate schemes i. e. to understand how to perform, at the level of the quantum treatment, the analogue of a classical (canonical) transformation of variables used to describe the system. As we will see, learning how to do it provided a strong hint to understand the relationship between both eigenvalue problems of matrix and wave mechanics. It is within these developments that the linear stucture underlying both formalisms started to be granted some attention, until it received a central place in the formulation of quantum mechanics as the space of quantum states. Thus, the problem of quantum canonical transformations led to the "transformation theory" of London, Dirac and Jordan, which in turn triggered von Neumann's theory of quantum mechanics as an operator calculus in abstract Hilbert space in which one-dimensional spaces (rays) describe pure states.

3 The question of transformations of coordinates

Whatever the formalism of quantum mechanics put to use, matrix or wave, in the practical applications there arose immediately the need to understand how to take advantage of the various coordinate schemes that physicists were widely using in classical mechanics. This implied to work out, at the quantum level, the transformations analogous to the canonical transformations of the classical formalism. In particular, one wished to recover in matrix or wave mechanics the computational convenience and physical heuristics of the action-angle techniques, and more generally of cyclic coordinates, the more so as these techniques were underlying the computational scheme of the "old quantum theory" of multiply periodic systems[22]. To much surprise, it was discovered that the taking over of the canonical techniques in the realm of quantum formalism was not quite easy. Actually, instead bringing more insight, the early uses of transformations of variables prompted new questions and lead sometimes to paradoxical statements. But this was eventually to good effect: in need to clarify what were exactly the quantum counterparts of classical transformations, quantum physicists were

[22] See Darrigol 1992.

forced to face problems where the linear structure of the formalism was most manifest. Not only were the problems of the transformation of coordinates eventually solved, the insight gained on this occasion was instrumental in the obtention of the transformation theory and the Hilbert space formalism.

3.1 Canonical transformations

The concept of canonical transformation received its full understanding in the works of Carl G. J. Jacobi in the middle of the 19th century[23]. Jacobi, following Hamilton's reformulation of analytical mechanics[24], simplified the theory and made it a powerful tool for solving mechanical problems. For generalized coordinates q_k and corresponding momenta p_k, obeying the canonical equations

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad \dot{q}_k = \frac{\partial H}{\partial p_k},$$

a canonical transformation q_k, $p_k \to Q_i$, P_i defines a set of new variables Q_i and P_i, functions of the former q_k and p_k, which are required to be canonical as well, i. e. there exists a new Hamiltonian function, K, such that:

$$\dot{P}_i = -\frac{\partial K}{\partial Q_i}, \quad \dot{Q}_i = \frac{\partial K}{\partial P_i}.$$

Jacobi identified the most general canonical transformation q_k, $p_k \to Q_i$, P_i, as obtained by considering a generating function, say $V = V(q_k\,, P_i, t)$ with the relations

$$\begin{aligned} Q_i &= \frac{\partial V}{\partial P_i}, \\ p_k &= \frac{\partial V}{\partial q_k}, \\ K &= H + \frac{\partial V}{\partial t}. \end{aligned} \tag{7}$$

[23] Jacobi 1866.
[24] Hamilton 1834.

The first two relations, together with their inversions, yield the transformation formulas, whereas the last one defines the new Hamiltonian K.

The theory of canonical transformations is an important tool in the Hamilton-Jacobi theory of solving the dynamics of the system. A powerful way to solve the Hamilton-Jacobi equation for the function S characterizing the geometry of the possible trajectories of the system:

$$0 = H(q_k, \frac{\partial S}{\partial q_k}) + \frac{\partial S}{\partial t}, \tag{8}$$

is indeed to try to express it in a set of canonical variables where it is separable[25]. One can then introduce yet another transformation of variables where the dynamics of the system are particularly simple to picture in periodic terms, where the new momenta (called then 'action variables') are constant in time, and their canonical conjugates are evolving linearly in time (called then 'angles'). The Hamilton-Jacobi theory became popular in the second half of the 19th century mainly among astronomers busy with celestial mechanics. The latter developed sophisticated perturbation methods which enabled to solve (8) by successive approximations. Owing to the similarity between the dynamical problems of celestial mechanics, and Bohr's atomic theory, these same techniques were next applied to the field of quantum theory and constituted the formal core of the "old quantum theory" of multiply periodic systems.

With the advent of quantum mechanics, the concept of a canonical transformation went transposed to the quantum case. In their paper from November 1925, Born, Jordan and Heisenberg defined a canonical transformation, as a transformation $\mathbf{p}, \mathbf{q} \to \mathbf{P}, \mathbf{Q}$ preserving the fundamental commutation relations[26]:

$$\mathbf{pq} - \mathbf{qp} = -i\hbar\mathbf{1} \Leftrightarrow \mathbf{PQ} - \mathbf{QP} = -i\hbar\mathbf{1}.$$

[25] For an introductory review of the Hamilton-Jacobi theory, see for example Goldstein 1980, or the beautiful book of Lanczos 1986. For a more rigorous and deeper approach to the mathematical implications of the Hamilton-Jacobi theory, see instead Rund 1966.

[26] For the sake of simplicity, the authors considered initially the case of a single degree of freedom, see Born, Heisenberg and Jordan 1926.

The authors recognized that the conjugation by an arbitrary matrix $\mathbf{S}$:

$$\begin{aligned}\mathbf{q} &\to \mathbf{S}^{-1}\mathbf{q}\mathbf{S} \equiv \mathbf{Q} \\ \mathbf{p} &\to \mathbf{S}^{-1}\mathbf{p}\mathbf{S} \equiv \mathbf{P}\end{aligned} \tag{9}$$

is a canonical transformation. They postulated further that *any* canonical transformation is of that form. The proof of that statement came four month later in a paper by Jordan[27]. Reducing the problem to the case of one degree of freedom (one could combine transformations multiplying the corresponding matrices), Jordan showed that for any canonical transformation one could obtain the form (9) considering $\mathbf{S}$ as a solution of the differential equation

$$\mathbf{R}\mathbf{S} + \frac{\partial \mathbf{S}}{\partial \mathbf{q}} = 0 \tag{10}$$

where $\mathbf{R}$ is defined by $\mathbf{P} - \mathbf{p} = -i\hbar\mathbf{R}$. When $\mathbf{R}$ does not depend on $\mathbf{q}$, Jordan could provide an explicit solution to (10) in the form of a 'normal ordered' exponential

$$\mathbf{S} = Exp(-\mathbf{R}, \mathbf{q}) \equiv \sum_{n=0}^{\infty} \frac{(-\mathbf{R})^n \mathbf{q}^n}{n!}.$$

The same exponential can be used to construct the quantum analogue of a classical canonical transformation with generating function

$$V(q, P) = \sum_k v_k(q) P_k. \tag{11}$$

This was an important practical result as this is the general form of a point-transformation where by definition the new generalized coordinates are only functions of the old ones. Indeed, one has:

$$\begin{aligned}Q_k &= \frac{\partial V}{\partial P_k} = v_k(q); \\ p_k &= \frac{\partial V}{\partial q_k} = \sum_l \frac{\partial v_l}{\partial q_k}(q) P_l\end{aligned}$$

Jordan thus proved that all the point-transformations used in classical mechanics could be transposed to the quantum case.

[27] Jordan 1926a, submitted April 27.

Jordan contributed two months later a second paper[28] where he extended this result showing that given a generating function generalizing (11):

$$V(P,q) = \sum_n f_n(P) g_n(q),$$

the transformation defined by the formulas (7) was quantum canonical. He proved this result showing explicitly the following relation between the generating function $\mathbf{V}(\mathbf{q},\mathbf{P})$ (understood as a matrix) and the corresponding matrix $\mathbf{S}$

$$\ln \mathbf{S} = \sum_{n=1}^{f} \mathbf{q}_n \mathbf{P}_n - \mathbf{V}(\mathbf{q},\mathbf{P}).$$

Indeed, one can then prove that

$$\mathbf{p}_k = \mathbf{S}\mathbf{P}_k^{-1}\mathbf{S}^{-1} = \frac{\partial \mathbf{V}}{\partial \mathbf{q}_k},$$
$$\mathbf{q}_k = \mathbf{S}\mathbf{P}_k\mathbf{S}^{-1} = \frac{\partial \mathbf{V}}{\partial \mathbf{P}_k}.$$

Jordan's results were crucial for the very consistency of the quantization procedure. Indeed, as we will see now, the difficulties met in the quantization of systems involving cyclic coordinates led to the fundamental problem of investigating the equivalence between quantum problems stemming from canonically equivalent versions of a same classical problem. Thus, the problem adressed was to provide a quantum equivalent of the theory of classical canonical transformations, with the requirement that classically equivalent problems, once quantized, are equivalent too and hence describe the same physical situation.

3.2 The quantization of action-angle pairs: an unexpected difficulty

Action-angle techniques achieved considerable popularity among atomic physicists following their efforts to generalize Bohr's quantization of the circular orbits of the hydrogen atom. The solution of this problem led

[28] Jordan 1926b, submitted July 6.

to a set of well-defined prescriptions (the Bohr-Sommerfeld conditions) allowing the quantization of multiply periodic systems where one could introduce action-angle variables, a class of systems already known to 19th century astronomers and mathematicians involved into problems of celestial mechanics. Thanks to the analyses of Karl Schwarzschild, Paul Epstein, and Niels Bohr[29], some of the results of these astronomers and mathematicians, from Delaunay to Poincaré, became known to the quantum community. The systems considered were of the separable type, i. e. cases where the Hamilton-Jacobi equation could be separated and the motion understood as a superposition of one-dimensional periodical components characterized by an angle variable, growing uniformly in time, and a conserved action integral. These multiply periodic systems fitted well the physical models of Bohr's atomic theory where, save for the quantization prescriptions, atoms were expected to be considered in analogy to planetary systems with the help of the arsenal of perturbation methods. As it turned out, this analogy led eventually to a dead-end: genuine quantum effects such as spin and quantum statistics, showing up respectively in the anomalous Zeeman effect and Helium spectra, effects resisting the 'semi-classical' methods of the "old quantum theory", were instrumental in the advent of quantum mechanics. Actually, it was already clear that the quantum theory of multiply periodic systems could not be the last word: because of its requirement of an underlying periodicity, it was inoperative in situations as simple as free motion, not to speak of scattering, or of transitions between stationary states.

Given the canonical form of the equations of matrix mechanics, inviting to take advantage as much as possible of the analogy with the classical theory, it was natural to try to import into its formal developments the arsenal of techniques developed by 19th century astronomers and their 20th century quantum heirs[30]. However, quantization using the action-angle variables turned out unexpectedly difficult to handle in the matrix context: a straightforward application of the rules of quantization to a couple of action-angle variables appeared impossible.

[29] Schwarzschild 1916, Epstein 1916ab, Bohr 1918.

[30] For instance the papers of Born and Brody 1921, Epstein 1922, Born and Pauli 1922.

Indeed, the commutation relations (1) can not be imposed because of the time-constancy of the action variable[31].

The problem appears already in simplest case of the rotator. Using the angular variable φ and the associated momentum p_φ, the classical Hamiltonian of the rotator is[32]:

$$H = \frac{1}{2A} p_\varphi,$$

with A, in analogy to the mass, is the moment of inertia of the rotator. The angular coordinate is cyclic which ensures the time-conservation p_φ. In matrix mechanics, the latter become matrices, and the conservation of p_φ requires it to commute with the Hamiltonian so that it is diagonal, which is incompatible with the canonical relations (1) as a simple inspection shows. To circumvent the difficulty of quantization using the cyclic variable φ, several authors proposed to express the rotator in a different set of canonical variables where quantization could be carried out. In a paper submitted just before the first one of Jordan, Igor Tamm proposed a (point) transformation[33] going to the libration coordinate q and its associated momentum p_q using as generating function $V = p_q \sin\varphi$, so that

$$p_\varphi = \frac{\partial V}{\partial \varphi} = p_q \cos\varphi, \quad \text{and} \quad q = \frac{\partial V}{\partial p_q} = \sin\varphi, \tag{12}$$

and the corresponding classical Hamiltonian:

$$H = \frac{1}{2A}\left\{p_q^2 - p_q^2 q^2\right\}.$$

After a proper symmetrization of this Hamiltonian, Tamm was then able to comput he spectrum of the stationary states. Relying on his transformation (12) he further proposed a general scheme to deal with problems involving cyclic coordinates. However, in a note added in the proofs (dated May 22), apparently unaware of Jordan's result, Tamm asked the following general question[34]:

31 An explicitation of this difficulty is to be found in a later paper of Jordan (Jordan 1927, p. 3), see also the section on Jordan's transformation theory below.

32 I have changed below Tamm's notations.

33 Tamm 1926, submitted April 23.

34 Tamm 1926, pp. 696 – 697.

«Das zur Behandlung des Rotators angewandte Verfahren führt zu der Frage, ob es berechtigt ist zur Lösung eines Problems, das durch Angabe einer «klassischen» Hamiltonschen Funktion definiert ist, eine «klassische» kanonische Transformation der Variablen auszuführen und erst dann die transformierte Hamiltonsche Funktion nach Umschreiben in Matrizenform in die Quantenmechanik zu übernehmen. Das heisst, liegen zwei klassische Hamiltonsche Funktionen $H(p,q)$ und $H'(P,Q)$ vor, die vermittelst einer klassischen kanonischen Transformation ineinander übergeführt werden können und schreibt man H und H' in Matrizenform um, so fragt es sich, ob die nach den Regeln der Quantenmechanik durchgeführte Lösung der beiden Hamiltonschen Probleme zu gleichen Energiewerten führt oder nicht.»

It is difficult to prove the equality of spectra of the matrices H and H' without Jordan's first result. The concept of a (quantum) canonical transformation as a change of variables preserving the canonical commutation relations does not entail in a straightforward way the invariance of the spectrum of the related Hamiltonians. Such a result is on the other hand easily obtained when one can use the form (9)[35].

Tamm further observed that given a classical transformation with the generating function $V(q,P)$ written as a sum of monomials of the form $q^i P^j$, when replacing systematically all the variables by matrices, the relations

$$\mathbf{p} = \frac{\partial \mathbf{V}}{\partial \mathbf{q}}; \quad \mathbf{Q} = \frac{\partial \mathbf{V}}{\partial \mathbf{P}} \tag{13}$$

define a transformation which is canonical. Although unable to prove in general that the energy spectrum was left invariant, except in some peculiar cases (he missed Jordan's result!), Tamm conjectured it was true and hence conjuctured further that the answer to his question was in general affirmative[36]:

«[...] die am Anfang des Nachtrages erwähnte Frage, wenn nicht allgemein, so doch in vielen Fällen [ist] zu bejahen, denn es

[35] One already finds an example in section three of Born, Heisenberg and Jordan paper where they discuss the uniqueness of the diagonalizing procedure, proving the well-definedness of the quantum dynamical problem.

[36] Ibid, p. 698.

> ist gleichgültig, ob die Transformation [13] vor oder nach der Umschreibung der klassischen Hamiltonschen Funktion in der Matrizenform ausgeführt wird.»

Tamm's question on the identity of spectra for classically equivalent Hamiltonians was not an isolated concern: a similar investigation can be found in a slightly posterior contribution of Otto Halpern from Vienna, with the title «Notiz über die Quantelung des Rotators und die Koordinatenwahl in der neuen Quantenmechanik»[37]. Halpern quantized the rotator using instead the Poincaré transformation

$$p_q = -\sqrt{2p_\varphi}\sin\varphi \quad \text{and} \quad q = \sqrt{2p_\varphi}\cos\varphi,$$

with the resulting Hamiltonian

$$H' = \frac{(p_q^2 + q^2)^2}{8A}$$

of which he then duely studied the spectrum. If Tamm's concern about the soundness of his procedure came only after he completed his paper as his note suggests, Halpern realised the same problem right from the start: indeed, he ended his paper with the following commentary[38]:

> «Es läge nun nahe, diesen recht einfachen Rechenvorgang, der jedes zyklische Problem auf die «Potenz» eines Oszillatorenproblems umformt, ganz allgemein zur Integration aller gequantelten Probleme heranzuziehen, die ja nach Einführung der Wirkungsvariablen durchweg zyklische Systeme geworden sind. Rechnet man dies für einige Fälle aus, so ergibt sich ein vollkommenes Versagen dieses Versuchs. Dies hat im folgenden seine Ursache. Betrachten wir zunächst die Hamiltonsche Funktion **H** in Matrizengestalt, die wir durch Transskription des klassischen Ausdrucks H in kartesischen Koordinaten gewonnen haben, und gehen wir von den Matrizen $\mathbf{x}$, $\mathbf{p}_x$ zu neuen Matrizen $\mathbf{q}, \mathbf{p}$ über, so daß auch bei dieser Transformation die Vertauschungsrelation
>
> $$\mathbf{p}_x\mathbf{x} - \mathbf{x}\mathbf{p}_x = \mathbf{p}\mathbf{q} - \mathbf{q}\mathbf{p} = -\,i\hbar\mathbf{1}$$
>
> gewahrt bleibt, so ergibt sich: $\mathbf{H}\,(\mathbf{x},\,\mathbf{p}_x) \to \mathbf{H}'\,(\mathbf{p},\,\mathbf{q})$. Dadurch werden die Werte der Energieniveaus nicht geändert, wie aus dem

[37] Halpern 1926, submitted June 5.

[38] Ibid, p. 10.

> Eindeutigkeitssatz von Born-Heisenberg-Jordan folgt. Dieser Matrizentransformation entspricht eine Berührungstransformation mit dem Ergebnis
>
> $$x, p_x \to q, p; H(x, p_x) \to H'(q, p).$$
>
> Wenn wir jetzt H' in Matrizengestalt aufschreiben, so geht sie nicht in die Form $\mathbf{H}'$ über, sondern etwa in $\mathbf{H}^*$. $\mathbf{H}^*$ aber würde andere Termwerte liefern als $\mathbf{H}'$. [...] Daraus folgt zwingend, daß es für die Anwendung der Matrizenrechnung notwendig ist, die Hamiltonsche Funktion des Systems in *kartesischen* Koordinaten in den Matrixkalkül herüberzunehmen. *Innerhalb* der Matrizenrechnung sind dann alle Koordinaten erlaubt, die unter Wahrung der Vertauschungsrelation auseinander hervorgehen.»

Reaching a negative conclusion contrary to Tamm's, Halpern makes a statement certainly puzzling to the modern reader used to coordinate-independent statements: this shows just how much there still was to be achieved before a proper understanding of the situation was enventually obtained.

3.3 Quantum analogues of the action-angle techniques

Various approaches to the problem of the quantization using cyclic coordinates were further provided by London, Dirac, and others. I mentioned already Dirac's approach when discussing his equivalence proof of the q-number calculus with matrix mechanics. His fundamental relations (5) were used again by Fritz London three months later[39]. The latter proposed to circumvent the difficulty to quantize an action-angle pair p and q considering as a substitute for (1) the derived relation

$$\mathbf{pE}(\mathbf{q}) - \mathbf{E}(\mathbf{q})\mathbf{p} = -i\hbar\frac{\partial \mathbf{E}}{\partial \mathbf{q}} = -i\hbar\mathbf{E}(\mathbf{q}), \tag{14}$$

where $\mathbf{E}(\mathbf{q})$ was defined formally as the exponential $\mathbf{E}(\mathbf{q}) = \sum \mathbf{q}^s/s!$. Contrary to (1), (14) makes sense for a time-constant, hence diagonal matrix $\mathbf{p}$. London could then discuss the eigenvalues of the action matrix $\mathbf{J}$ and the resulting relationship between the 'transition' and the 'classical' (*Umlauf*) frequencies. London considered next the problem

[39] London 1926a, submitted May 22.

of the form of quantum canonical transformations. Observing that the Born-Jordan-Heisenberg form (9) of the canonical transformations was unpractical to use because of the necessity of computing the inverse $\mathbf{S}^{-1}$(this is in general tractable only for infinitesimal cases), London proposed an alternative. He proved that given an arbitrary (matrix) function $\mathbf{S}(\mathbf{q}, \mathbf{P})$, the transformation defined by

$$\mathbf{Q} = \frac{\partial \mathbf{S}}{\partial \mathbf{P}}; \quad \mathbf{p} = \frac{\partial \mathbf{S}}{\partial \mathbf{q}},$$

was canonical, i. e. he generalized Jordan's result which he apparently was not yet aware of. He immediately applied his result to the oscillator and rotator problems, going to action-angle variables and using as well his newly obtained relation (14).

4 Towards a proper understanding of the mathematical structure: London's early transformation theory

London's work on quantum canonical transformations lead him to penetrate deeper than anybody else before the mathematical structure of the new quantum theory. In a paper submitted October 16 which established him firmly as one of the pioneers of transformation theory[40], London reached a clear understanding of the importance of the linear and functional structures involved in the kind of problems considered in quantum theory.

London opened his paper observing that in the recent wave mechanics of Schrödinger the full power of the canonical formalism was not yet taken advantage of[41]:

> «Die Beschreibung des Schwingungsvorganges, in welchen Schrödinger das quantenmechanische Geschehen aufgelöst hat, bedient sich ausschließlich des «q-Raumes» als Mannigfaltigkeit der mathematischen Formalismen. Es ist bekannt, welche außerordentliche Symmetrie die klassische Mechanik annimmt, wenn man statt der Koordinaten und ihrer zeitlichen Ableitungen die Koordinaten

[40] London 1926b.
[41] Ibid, p. 193.

> und Impulse als «kanonische» Variable einführt, und sich dadurch die Möglichkeit erschließt, die Lösung des mechanischen Problems auf die Aufsuchung einer Transformation auf uniformisierende Variable zurückzuführen.
>
> Die Übertragung dieses Ideenkreises auf die Wellenmechanik ist von prinzipieller Bedeutung; sie soll in ihren Grundzügen im folgenden skizziert werden. Dabei wird uns die Parallele zu der bereits vorliegenden Transformationstheorie[42] der Matrizenmechanik von Vorteil sein.»

London observed that in the Schrödinger equation

$$\mathbf{H}(q, \frac{\partial}{\partial q})\Psi(q) = E\Psi(q), \tag{15}$$

the changes of variables used until then corresponded solely to point transformations, namely $Q = F(q)$. He proposed consequently to consider the most general formal differential relations

$$\begin{aligned} \mathbf{Q} &= \mathbf{F}(q, \frac{\partial}{\partial q}), \\ \frac{\partial}{\partial \mathbf{Q}} &= \mathbf{G}(q, \frac{\partial}{\partial q}), \end{aligned}$$

where the second one is constrained by the necessity to preserve the canonical relation

$$\frac{\partial}{\partial \mathbf{Q}}\mathbf{Q} - \mathbf{Q}\frac{\partial}{\partial \mathbf{Q}} = 1.$$

F and **G** can be obtained, drawing on London's, and Jordan's earlier results, from a single 'generating' expression $\mathbf{S} = \mathbf{S}(q, -i\hbar\frac{\partial}{\partial \mathbf{Q}})$ using the Jacobi representation

$$\begin{aligned} \mathbf{p} &= -i\hbar\frac{\partial}{\partial q} = \frac{\partial \mathbf{S}}{\partial q}, \\ \mathbf{Q} &= \frac{\partial \mathbf{S}}{\partial \mathbf{P}}. \end{aligned} \tag{16}$$

[42] Notice the use of this word which suggests that the problem by then has become a topic by itself. London refers here to the canonical transformation papers of Jordan as well as to his own commented above.

On the other hand, one can construct an operator **T** implementing this transformation (16) as a conjugation (9). The proof of the equivalence of (15) with the transformed eigenvalue problem,

$$\begin{aligned} &\mathbf{H}^*(\mathbf{Q}, \frac{\partial}{\partial \mathbf{Q}})\Psi^*(Q) = E\Psi^*(Q), \quad \text{where} \\ &\qquad \mathbf{H}^*(\mathbf{Q}, \frac{\partial}{\partial \mathbf{Q}}) \equiv \mathbf{T}^{-1}\mathbf{H}(\mathbf{Q}, \frac{\partial}{\partial \mathbf{Q}})\mathbf{T}, \end{aligned}$$

becomes trivial provided one recognizes that the solutions of the transformed problem are related to the previous ones by the action of T:

$$\mathbf{T}(\mathbf{Q}, \frac{\partial}{\partial \mathbf{Q}})\Psi^*(Q) = \Psi(Q). \tag{17}$$

The most striking part of the paper is London's realization of the proper mathematical meaning of a canonical transformation. London rightly insists on the operatorial meaning of the Q and P symbols, bringing to the forefront the 'linear algebra' structure of the problem[43]. The rather forceful style of the following quote from his paper clearly witnesses London's awareness of the importance of his insight[44]:

> «Wir werden [...] zwangläufig zu einer Deutung des ganzen Transformationszusammenhanges geführt, welche bereits in der Matrizenmechanik mehrfach geahnt worden ist, aber in ihr noch nicht vollständig zum konkreten Ausdruck gelangen konnte.
>
> Wir sind ausgegangen von Transformationen von Operationen [16]. Das bedeutet folgendes: Ich habe in einem Gebiet eine Abbildung H, welche jeden Gegenstand x in einen anderen Gegenstand y des Gebietes überführt. Außerdem habe ich eine andere Abbildung **T**, welche das ganze Gebiet mitsamt seiner Abbildung H in ein neues Gebiet abbildet. x gehe dabei in x^*, y in y^* über. Die «abgebildete Abbildung» $\mathbf{H}^*$ führt dann x^* in y^* über.

[43] London rightly noted that this algebraic reality had been hinted at previously by Born, Jordan and Heisenberg (in connection with the theory of Hermitian forms), and Born and Wiener (operators acting on formal series).

[44] Ibid, pp. 197 – 198.

$$\begin{array}{ccc} y & \overset{\mathbf{T}}{\Longrightarrow} & y^* \\ \uparrow \mathbf{H} & & \uparrow \mathbf{H}^* \\ x & \overset{\mathbf{T}}{\Longrightarrow} & x^* \end{array}$$

Benutzt man statt $x^* \to y^*$den Umweg $x^* \to x \to y \to y^*$, so ergibt sich die bekannte Darstellung für die Transformation einer Transformation:

$$\mathbf{H}^* = \mathbf{T}^{-1}\mathbf{H}\mathbf{T}.$$

Dieser Zusammenhang hatte von Anfang an in der Matrizenmechanik die Frage nahegelegt: Wenn die kanonischen Transformationen $\mathbf{T}^{-1}\mathbf{Q}\mathbf{T}$ die Form von Transformationen von Transformationen haben, an welchen Dingen x greift dann $\mathbf{T}$ unmittelbar an? Die Antwort auf diese Frage gibt Gleichung [17]: Die Dinge x sind Schrödingers neue Zustandsgröße Ψ, deren Schwingungsvorgänge durch eine Reihe von Eigenfunktionen Ψ_k beschrieben werden. Der Operator $\mathbf{T}$ führt gemäß [17] diese Reihe gliedweise über in ein anderes System Ψ_k^* von Eigenfunktionen.»

London expanded further the eigenfunctions Ψ_k on the system formed by the Ψ_i^*,

$$\Psi_k(Q) = \sum_i T_{ik}\Psi_i^*(Q), \tag{18}$$

and proved that the matrices built out of the Schrödinger matrix elements T_{ik},

$$T_{ik} = \int \bar{\Psi}_i^* \mathbf{T} \Psi_k^* dQ$$

were unitary

$$\mathbf{T}^\dagger \mathbf{T} = \mathbf{1}. \tag{19}$$

He interpreted then the corresponding linear transformations as "rotations" (*Drehungen*) in the linear space that, remarkably enough, he insightfully related to Hilbert's name[45]:

[45] Ibid, p. 199. London refered here to the linear space that Hilbert used, extending Fredholm's pioneering results (Fredholm 1900, 1903), in his studies of the spectral

> «[19] charakterisiert die Abbildung [18] als eine «*Drehung*» (im Hermiteschen Sinne) des von den orthogonalen Eigenfunktionen ausgespannten «Koordinatenachsensystems» im *Hilbertschen* Funktionenraum von unendlich vielen Dimensionen. Die kanonischen Transformationen der Matrizen sind dann die von dieser Drehung *induzierten* Transformationen beliebiger linearer Transformationen des Simultansystems der Ψ_k.»

London devoted the rest of his paper applying his formal understanding of what canonical transformation are to obtain in a unified way solutions of problems involving action-angle coordinates. Since, in the latter, the Hamiltonian $\mathbf{H}$ is by definition only a function of the $\mathbf{J}_k = i\hbar \frac{\partial}{\partial w_k}$, the wave equation is easily solved yielding as eigenfunctions the exponentials. This is, finally identified, the quantum counterpart of the simplicity which the use of action-angle variables brings to classical mechanics. Then, applying the transformation, (17), one can compute explicitly the solutions corresponding to the old variables scheme. As London puts it, the action-angle variables correspond to the use of the exponentials for the complete system, and other choices map this system to other complete sets.

Apparently after completing his work, London realized that a whole mathematical trend was related to his own results. In a footnote, he mentioned the works of Pincherle and Cazzaniga on "distributive functional operations"[46]. In Pincherle's language, the "distributive" property corresponds to what we call today linearity, and the papers London refers to develop elements of a theory of formal operations on functional spaces. Another reference is to Paul Lévy's *Leçons d'analyse fonctionnelle*, which deals with functional spaces insisting much on the "geometrical" (linear space) aspect of the situation. London's comments were the second time, after Born's, Jordan's and Heisenberg's remarks on the relevance for the matrix formalism of the theory of the diagonalization of infinite forms, that physicists were explicitly pointing to the importance for quantum physics of a new mathematical

problem of bounded forms (Hilbert 1906, and Hilbert 1912 for a collection of all his papers devoted to the topic), that today we name l^2. See Dieudonné 1981, chapt. V, and Steen 1973 for detailed accounts. See also below the section on the contribution of John von Neumann.

[46] Pincherle 1897, 1905; Cazzaniga 1899.

field of functional analysis. The final episode, where to occur with the mathematical elaboration of transformation theory by von Neumann.

Before we continue next with an examination of transformation theory, it is fair to recall the unfortunate fate of Lanczos' continuous field-like formulation of matrix mechanics which preceded, this is important to mention, Schrödinger's wave mechanics[47]. Would his work been better understood and accepted at the time, the recognition of the linear structure of quantum mechanics would have been accelerated and its relation to the mathematics of functional analysis taken earlier advantage of. Indeed, as early as November 1925, Lanczos succeeded in translating the discontinuous matrix equations into integral equations using the theory of Green functions. One of the weaknesses of his approach, but, with distance, one of his most glorious anticipations, was Lanczos' use of a kernel associated to an orthogonal system of functions. Lanczos fully realized the lack (at the time!) of a physical motivation for his construction, but emphasized that the situation would radically change in case the orthogonal system were to receive a physical meaning. Then, the equation defining the kernel would make the whole difference and the continuous 'field-like' (*feldmäßige*) formulation would supersede the matrix one[48]:

> «Daraus ergibt sich für die prinzipielle Bewertung der beiden Auffassungen folgendes Bild. Sind alle physikalischen Tatsachen von der Beschaffenheit, daß sie uns prinzipiell immer nur die Koeffizienten der Matrizen liefern können, so gebührt der matrizenmäßigen Darstellung der Vorzug (wenigstens vom positivistischen Standpunkt aus !), weil sie kein prinzipiell unerreichbares Element in die Beschreibung der Tatsachen hineinbringt. Die Sachlage ändert sich aber, wenn dem Kern eine physikalische Bedeutung zukommt. In diesem Falle muß die feldmäßige Darstellung als die adäquatere gelten, weil die matrizenmäßige Formulierung insofern weniger liefert, als sie nur die Eigenwerte des Kernes geben kann, das System der Eigenfunktionen aber unbestimmt läßt.»

Lanczos' proposal did not receive the attention it retrospectively deserved, even not when the first proofs of the equivalence between matrix

[47] Lanczos 1926.
[48] Ibid, pp. 820 – 821.

and wave formalism hit the stage. This is actually quite surprising given the first rank mathematical abilities of those who at the time played down Lanczos' contribution, namely Schrödinger and Pauli themselves[49]. This will be remained as one of the missed opportunities in this story. Be it as it may, Lanczos deserves retrospectively his part of recognition as one of those whose intuition of the mathematics involved was developing (retrospectively) in the right direction.

5 The wave function acquires physical meaning

There are many sides to the crucial contribution of wave mechanics to the shaping and final understanding of quantum mechanics. Here, I want to emphasize the very importance of the wave function, more precisely its formal role within the formalism, before (at least conceptually) the issue of its physical interpretation was raised. Because in wave mechanics we are, retrospectively, in the "Schrödinger picture", the wave function, as an explicit formal ingredient of the Schrödinger formalism, offers a potential 'handle' on which the object soon to be recognized as operators, can simply 'act'. This is plain with the differential operators of Schrödinger, but we just saw that London recognized a deeper picture where there was advantage to fancy "distributive operations" on a space spanned by the wave functions. Let us remember that Heisenberg's matrices were not understood as standing for mathematical objects endowed with an operatorial meaning. They were conceived as a convenient way to write down transition amplitudes, making manifest the manipulation (matrix) rules governing matrix mechanics. Again, we meet here the discrepancy of past and old conceptions. Today we think of matrices, and of the associated operations (multiplication, trace, determinant) as derived concepts, making those of linear spaces and linear mapping as the fundamental ones. The former are mere 'numerical' consequences of the latter as soon as a basis has been chosen. Such a

[49] Pauli and Schrödinger criticized Lanczos' contribution invoking the curious argument that in Lanczos' theory, instead of the eigenvalues, there appeared their inverses. Indeed, such was the case because of the mathematical tradition in writing down the Fredholm problem. However, this was of a purely notational importance, and besides, Lanczos himself stated in his paper on p. 816 the correct relation with the energy eigenvalues.

point of view was certainly foreign to the founding fathers of quantum mechanics. Moreover, and more importantly, they lacked any physical motivation to ask for the substrate on which one could think the action of the matrices. This is where the issue of the physical meaning of the wave function enters the stage.

As brilliant as was London's mathematical understanding of the situation, he missed the full story. Although he correctly identified the transformation equations between the amplitudes, he did not realize their physical meaning. One should however not consider this as London's lack of insight. At the time of London's paper, Born's statistical interpretation of the squared modulus of the wave function was hardly known. We thus come to the next crucial event, which made finally possible Dirac's and Jordan's full accounts, physically and mathematically, of the transformation theory.

The context of Born's proposal is well known and I shall not recall here the details. Let us however notice that Born's interpretation emerged, almost as a mere byproduct, out of a longstanding interest of Born to reformulate the theory in order to be able to handle typically non periodic situations where the spectra were continuous. The operator theory that he developed together with Wiener (the one that I alluded to above) was explicitely within this program. It is remarkable that Born's persistance in dealing with the problem eventually make him hit on this crucial ingredient of the theory. The statistical interpretation was merely mentioned in the preliminary notice[50], but in his subsequent paper[51], Born made his proposal explicit. In case of a superposition of Schrödinger eigenfunctions:

$$\psi = \sum_n c_n \psi_n, \tag{20}$$

Born interpreted the square moduli $|c_n|^2$ as the probability for the system to be in the state n. Going to to the continuous case, and using the Fourier expansion

$$\psi(x) = \frac{1}{2\pi} \int c(k) e^{ikx} \, \mathrm{d}k,$$

[50] Born 1926a, submitted June 25.
[51] Born 1926b, submitted July 21.

he again interpreted $|c(k)|^2$ as a relative frequency for the interval $(2\pi)^{-1}dk$ centered at k. One will however not find directly in Born's paper the emblematic statement that $|\psi(x)|^2$ yields a density of probability. Within Born's logic at that time, this would have required to consider an improper expansion of the type

$$\psi(x) = \int \psi(x)\delta(x-y)\,\mathrm{d}y,$$

which he did not. This is certainly related to the fact that Born did not grant (20) the meaning of a representative of a state. It was for him rather something of a statistical mixture[52].

Because of this, an important step had still to be made, namely characterize directly $|\psi(x)|^2$as a density of probability, and then generalize this intepretation to other quantities obtained from the wave function. This had to be Wolfgang Pauli's contribution. In his paper on transformation theory that we shall comment shortly, Jordan acknowledges indeed Pauli's generalization of Born's insight refering to a note in a paper by Pauli still in print at that time[53]. What Pauli had in mind is exposed more explicitely in his letter to Heisenberg[54]. There, Pauli first extends Born's interpretation to the squared modulus of the wave function *in momentum space* and then considers even more general possibilities. Let me quote him extensively[55]:

> «Die historische Entwicklung hat es mit sich gebracht, daß die Verknüpfung der Matrixelemente mit der Beobachtung zugänglichen Daten auf dem Umweg über die emittierte Strahlung vorgenommen wird. Ich bin aber jetzt mit der ganzen Inbrunst meines Herzens davon überzeugt, daß *die Matrixelemente mit prinzipiell beobachtbaren kinematischen (vielleicht statistischen) Daten der betreffenden Teilchen in den stationären Zuständen verknüpft sein müssen* [...] Nun ist es so: alle *Diagonal*elemente der Matrizen (wenigstens von Funktionen der p allein oder der q allein) kann man überhaupt schon jetzt kinematisch deuten. Denn man kann ja zunächst nach der Wahrscheinlichkeit fragen, daß in einem

52 This is clear in his paper "Das Adiabatenprinzip in der Quantenmechanik" (Born 1926c, pp. 168 – 169).

53 «Über Gasentartung und Paramagnetismus», Pauli 1927, p. 83.

54 Pauli to Heisenberg, letter dated October 19, in Hermann, von Meyenn and Weisskopf 1979.

55 Pauli to Heisenberg, ibid, p. 347.

bestimmten stationären Zustand des Systems die Koor[di]naten q_k seiner Teilchen $(k = 1, .., f)$ zwischen q_k und $q_k + \mathrm{d}q_k$ liegen. Die Antwort hierauf ist

$$\left|\psi(q_1 \dots q_f)\right|^2 \mathrm{d}q_1 \dots \mathrm{d}q_f,$$

wenn ψ die Schrödingersche Eigenfunktion ist [...] Es ist dann klar, daß die Diagonalelemente der Matrix jeder q-Funktion

$$F_{nn} = \int F(q_k) \left|\psi(q_1 \dots q_f)\right|^2 \mathrm{d}q_1 \dots \mathrm{d}q_f,$$

sein müssen, da sie physikalisch "Mittelwert von F im n-ten Zustand" bedeuten. Hier kann man einen mathematischen Witz machen: Es gibt auch eine entsprechende Wahrscheinlichkeitsdichte im *p-Raum*: Hierzu setze man an (eindimensional formuliert, der Einfachheit halber)

$$p_{ik} = \int p\varphi_i(p)\tilde{\varphi}_k(p)\,\mathrm{d}p;$$
$$\frac{\mathrm{i}}{\hbar}q_{ik} = -\int \varphi_i \frac{\partial\tilde{\varphi}_k}{\partial p}\,\mathrm{d}p = +\int \frac{\partial\varphi_i}{\partial p}\tilde{\varphi}_k\,\mathrm{d}p.$$

(~ bedeutet konjugiert komplexe Größe; es unterscheidet sich im allgemeinen $\tilde{\varphi}_k$ und φ_k nicht nur durch einen konstanten Faktor. Orthogonalität besagt

$$\int \varphi_i\tilde{\varphi}_k\,\mathrm{d}p = \begin{Bmatrix} 0, & i \neq k \\ 1, & i = k \end{Bmatrix}$$

Multiplikationsregel und Relation $pq - qp = -\mathrm{i}\hbar 1$ sind erfüllt.)

Sie sehen, daß ich gegenüber der gewöhnlichen Vorschrift die Bildungsgesetze für die Matrizenelemente p_{ik} und q_{ik} aus den Eigenfunktionen vertauscht habe. Aus der Matrixrelation des Energiesatzes $p^2/2m + V(q) = E$ gewinnt man

$$\left[\frac{p^2}{2m} + V(-\mathrm{i}\hbar\frac{\partial}{\partial q})\right]\varphi = E\varphi$$

V als Operator gedacht, etwa Potenzreihe in $\frac{\partial}{\partial q}$. Beim harmonischen Oszillator, wo die Hamilton-Funktion symmetrisch in p und q ist, ist auch φ das Hermitesche Polynom [...] Jedenfalls gibt es also auch eine Wahrscheinlichkeit dafür, daß im n -ten Quantenzustand p_k zwischen p_k und $p_k + \mathrm{d}p_k$ liegt, und die ist gegeben durch

$$\left|\varphi_n(p_1 \dots p_f)\right|^2 \mathrm{d}p_1 \dots \mathrm{d}p_f$$

also

$$F(p)_{nn} = \int F(p)\,|\varphi_n(p)|^2\,\mathrm{d}p_1 \ldots \mathrm{d}p_f»$$

According to Pauli, if the system is in a state corresponding to the n-th Schrödinger (normalized) eigenfunction, $\varphi(q)$, the probability for the coordinate q to have a value in the interval q and $q + dq$ is given by $|\varphi(q)|^2\,dq$. Now, rephrasing Pauli's thought, and using a notation closer to what Jordan will use soon (see next section), given two (Hermitian) quantities p and E, one can consider as well the function $\varphi(p, E)$ such that $|\varphi(p, E)|^2\,dp$ be the (relative) probability for p to have a value in the interval between p and $p + dp$, assuming that the value of E was y.

Pauli's thinking was crucial in so far that it drew attention to a possibility of a *systematic* way of obtaining physical information out of quantum computations (one will find precisely this motivation in Dirac's paper on transformation theory, see next section). This eventually ended up the effective bias towards the basis of energy eigenstates making physicists recognize the generality of the eigenvalue problem as associated to *any* physical question. Born's interpretation associates to the n-th Schrödinger wave function, i. e. to the wave function representing a state of energy $E = E_n$, the density of probability of position q defined by the square norm $|\varphi_n(q)|^2$. More generally, one can similarly consider a basis of (function) eigenstates of (any) quantity β, so, instead of definite energy wave functions, one considers definite β wave functions. This had two important consequences on the formal understanding of the situation. First, it emphasized the role of the wave functions which prior to this were considered (unless one granted them physical meaning following the physical picture of an undulatory matter "à la Schrödinger") as mere 'handles' to formulate the eigenvalue problem (but see the discussion at the beginnig of this section). Then, it prompted the necessity to concentrate on the relations between the various amplitudes related to different physical questions. This opened the way to an appreciation of the linear structure underlying the problem from (another) point of view, this time dictated by physical interpretation.

6 The physicists' final appraisal: Jordan's and Dirac's transformation theories

With the acknowledgment of the central role played by wave functions and the understanding of the canonical transformations as implementing unitary transformations in the functional space of the wave functions, the situation was ripe for a final statement refounding the theory on new formal principles and unifying previous apparently disparate approaches. Jordan and Dirac reached more or less simultaneously the same results, but it will come as no surprise for anybody knowing a little of their personalities and contexts, to learn how different their styles and reasonings were.

In what concerns chronology, Dirac's paper came first[56]. It is characteristic of Dirac's scientific style, deceptively simple, yet full of pregnant consequences and insights. Dirac's declared motivation, as already mentioned, was not to study the general scheme of changes of variables, but rather to provide a *systematic* way of obtaining physical information out of quantum computations. Acknowledging the various *ad hoc* prescriptions assigning physical meaning to the c-numbers issued from quantum computations, Dirac proposed the following problem as exhausting the means of quantum theory to provide physical information. Consider a "constant of integration" $\mathbf{g}$ (Dirac's expression for a representative of a physical magnitude), depending on a set of canonically conjugated q-numbers $\boldsymbol{\xi}_r$ and $\boldsymbol{\eta}_r$ parametrizing the system. Because the $\boldsymbol{\xi}_r$ and $\boldsymbol{\eta}_r$ do not commute, one cannot assign in a unique way a numerical value to $\mathbf{g}$ when assigning one to $\boldsymbol{\xi}_r$ and $\boldsymbol{\eta}_r$. Therefore, and taking into account previous prescriptions, the only information one can retrieve, given numerical assignements, say, to the $\boldsymbol{\xi}_r$, is the density of distribution of the $\mathbf{g}$-values on the $\boldsymbol{\eta}_r$-space. Thus, although one cannot follow the transitions in the $\mathbf{g}$-values, it is still possible to specify the fraction of the $\boldsymbol{\eta}_r$-space corresponding to a given value.

In order to work out his proposal, Dirac needed general transformation formulas for passing from a given 'matrix scheme' to another one labelled with the values of a (maximal) commuting set of quantities, like the $\boldsymbol{\xi}_r$ above. This amounts to picking up the basis of $\boldsymbol{\xi}_r$ simultaneous

[56] Dirac 1926c, submitted December 2.

eigenfunctions. Dirac expressed his transformation formulas using the continuous formalism of integral operators, duely mentioning at that point Lanczos' 'field-like' representation[57]. This highly suggestive formalism is possible only at the price of introducing the singular δ-functions and its derivatives, which John von Neumann will refrain from using later (see next section).

I shall not go here more into details about Dirac's paper as the material is nowadays fairly standard. I turn instead to Jordan's contribution whose style since then faded into relative oblivion.

Jordan's paper «Ueber eine neue Begründung der Quantenmechanik»[58] is resolutly of a foundational style. It aims at a unification of previous approaches[59], and uses an axiomatic style together with a rather formal wording. Let us remember that at the time Jordan was at the University of Göttingen, in Max Born's *Institut für theoretische Physik*[60], where he obtained his Ph.D. in 1924 and became privat dozent in 1926. Born had close relations with Hilbert. We know that Jordan, on the other hand, was helping Richard Courant, Hilbert's close friend, in preparing the latter's book, *Methoden der Mathematischen Physik*[61]. Not much is known however about Jordan's possible direct contacts with Hilbert but one can only guess that given Hilbert's fame and Jordan's

[57] It is indeed quite edifying to see Dirac pay this tribute to Lanczos.

[58] Jordan 1926cd. Jordan's paper was received in December 1926, and published in the 1926 volume in 1927. Some results of Jordan's paper were presented at a session of the *Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse*, on the 14 January 1927. The text of this communication (Jordan 1926c) appeared in the *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen* from the year 1926. Jordan's *Zeitschrift für Physik* paper (Jordan 1926d) offers more details but some of the lines from the *Nachrichten* are worth quoting as well.

[59] The issue of deriving a unifying approach to the various quantum formalisms is discussed in Jammer 1966, pp. 293 – 322.

[60] For historical details about the Göttingen Physics Institute and the University, see Mehra and Rechenberg, vol. 1, chapter III.

[61] It is while working on the latter that Jordan got acquainted with the matrix methods. Jordan became Courant's assistent (*Hilfsassistent*) in 1922 to help the latter in his lectures on partial differential equations; he then went to Born. See Reid 1976, pp. 93, 113, also Jammer 1966, p. 207.

own inclinations towards abstraction, Hilbert must have exerted some influence on him[62].

Jordan put forward in his introduction the general problem of the meaning of a change of variables in quantum theory, making explicit the link with his previous works on canonical transformations[63]:

> «Nach Schrödinger ist einer Hamiltonschen Funktion $H(p,q)$ eine Schwingungsgleichung
>
> $$\left\{ H(-\mathrm{i}\hbar\frac{\partial}{\partial y}, y) - W \right\} \varphi(y) = 0$$
>
> zuzuordnen [...] Ich habe mir die folgende Frage vorgelegt: Statt der p, q mögen durch eine kanonische Transformation neue Veränderliche P, Q eingeführt werden, wobei $H(p,q) = \bar{H}(P,Q)$ werden möge. Dann wollen wir mit $\bar{H}$ die neue Wellengleichung
>
> $$\left\{ \bar{H}(-\mathrm{i}\hbar\frac{\partial}{\partial x}, x) - W \right\} \psi(x) = 0$$
>
> bilden. Wir erhalten so zu jeder kanonischen Transformation ein besonderes $\psi(x)$. Wie verhalten sich diese $\psi(x)$ zu der ursprünglichen Funktion $\varphi(y)$? Die Beantwortung dieser Frage wird sich aus den späteren Betrachtungen ergeben.
>
> Ihre Untersuchung führte zur Feststellung sehr allgemeiner formaler Zusammenhänge in den quantenmechanischen Gesetzen, welche die in den bisherigen Formulierungen niedergelegten formalen Tatsachen als spezielle Fälle in sich enthalten. Dabei ergab sich auch eine engere Verbindung zwischen den verschiedenen bislang entwickelten Darstellungen der Theorie. Bekanntlich ist die Quantenmechanik in vier verschiedenen, selbständigen Formen entwickelt worden; außer der ursprünglichen Matrizentheorie liegen vor die Theorie von Born und Wiener, die Wellenmechanik und die Theorie der q-Zahlen. Die Beziehungen der letzteren drei Formulierungen zur Matrizentheorie sind bekannt; jede Formulierung führt zu den gleichen Endformeln wie die Matrizentheorie, soweit diese selber reicht. Dabei standen jedoch die drei späteren Formulierungen *untereinander* ohne eigentliche

[62] It seems that Jordan followed all of Hilbert's lectures on physical topics (Mehra and Rechenberg 1982, vol. 3, p. 49) and his taste for philosophical questions should have offered a favorable ground for axiomatics.

[63] Jordan 1926d, pp. 809 – 10.

> innere Verbindung da; es fehlte sogar der allgemeine Beweis, daß sie auch dort, wo sie über die Matrizentheorie hinausgehen, zu äquivalenten Ergebnissen führen.»

Jordan made central in his treatment the notion of the probability amplitude associated to a pair of mechanical quantities: doing so, he was amplifying Wolfgang Pauli's generalization of Born's statistical interpretation of the wave-function as a probability distribution[64]. After characterizing his amplitudes with the help of some postulates[65], Jordan recognized further as a decisive feature of the quantum probability amplitudes their combination law that he dubbed 'interference of probabilities'. Considering the amplitude $\psi(x,y)$ for the pair of quantities Q and q, and φ as above, he showed that $\Phi(x,y)$, the amplitude for a value x of Q, given the value y of β, was related to the former amplitudes by[66]

$$\Phi(x,y) = \int \psi(x,z)\varphi(z,y)\,\mathrm{d}z.$$

Jordan renounced on the other hand to state the canonical commutation rules as part of the fundamental requirements of the theory[67]. He preferred to introduce instead the concept of a canonical pair of quantities in the following definition: If the amplitude $\rho(x,y)$ for a value x of p given a value y of q is

$$\rho(x,y) = \exp(-\mathrm{i}\frac{xy}{\hbar})$$

[64] See the previous section.

[65] Ibid, pp. 813–814.

[66] Following the discussion of Pauli's generalization of Born's interpretation of the square modulus of ψ, the formula below expresses just a change of basis from a basis of q-eigenstates to the basis of Q-eigenstates. In Dirac's bra-ket notation this would run as

$$< x \mid z >= \int \mathrm{d}y < x \mid y >< y \mid z >$$

where $\mid y >$ denotes (the y) element of the q basis, $\mid x >$ denotes (the x) element of the Q basis, and $\mid z >$ is (the z) element of a third basis related to the quantity β. One can view then this formula as a relationship between Q- and q-coordinates of a state function of definite value of β.

[67] See his *Zeitschrift* paper 1926d, p. 812. The canonical commutation rules shall be recovered indirectly using the concept of canonically conjugated quantities, see Jordan's postulate D.

then p is said *canonically conjugated* to q. His next postulate stated then (postulate D, p. 814) that for each q one has an associated conjugated moment p. This has as a consequence that the function $\rho(x,y)$ obeys the following differential equations:

$$\left(x - \mathrm{i}\hbar\frac{\partial}{\partial y}\right)\rho(x,y) = 0$$
$$\left(\mathrm{i}\hbar\frac{\partial}{\partial x} - y\right)\rho(x,y) = 0$$

Now, assume that for a mechanical quantity Q the amplitude for $Q = x$ given $q = y$ is $\varphi(x,y)$ and the amplitude for $Q = x$ given $p = y$ is $\Phi(x,y)$. Then, according to the definition of $\rho(x,y)$ above,

$$\varphi(x,y) = \int \Phi(x,z)\rho(z,y)dz$$

which Jordan wrote, introducing the linear operator $T = \int \mathrm{d}z\Phi(x,z)$, as

$$\varphi(x,y) = T \cdot \rho(z,y).$$

It follows that $\varphi(x,y)$ obeys the differential equation

$$\left(-TxT^{-1} - \mathrm{i}\hbar\frac{\partial}{\partial y}\right)\varphi(x,y) = 0 \qquad (21)$$
$$\left(-\mathrm{i}\hbar T\frac{\partial}{\partial x}T^{-1} - y\right)\varphi(x,y) = 0.$$

Keeping fixed a given quantity Q, Jordan associated thus to each other quantity q an operator $-\mathrm{i}\hbar T\frac{\partial}{\partial x}T^{-1}$. He defined then the addition and multiplication of the mechanical quantities using the addition and multiplication of the associated operators. He showed further that when choosing $Q = q$ its associated operator turned out to be x and that of the conjugate momentum P corresponded to $-\mathrm{i}\hbar\frac{\partial}{\partial x}$. Because the operators one might construct out of x and $-\mathrm{i}\hbar\frac{\partial}{\partial x}$ were very general, Jordan assumed further that any linear operator could be expressed that way, which meant that any mechanical observable could be constructed out of Q and P and that similarly any functional equation of the form (21) could be traded for a differential equation (Jordan acknowledged the possibility of the latter being of infinite order).

Jordan went next to discuss the realization of his axioms and gave some examples to show that indeed his generalized formalism covered all the previous ones. It is for instance easy to see how to recover from the general equations (21) the Schrödinger eigenvalue problem, or his time-dependent equation. The relationship with London's approach is clear as well. Jordan duely mentioned it in the begining of his paper, insisting however on the similarity of *formal* results, thus suggesting that his treatment was physically more elaborated.

Half a year later, Jordan submitted to the *Zeitschrift für Physik* a sequel to his first paper[68]. He aimed at sharpening and generalizing the results obtained previously also in the case where the spectra of the operators were discontinuous[69]. Jordan also acknowledged there an elaboration on his and Dirac's transformation theories published meanwhile by Hilbert, Nordheim and von Neumann, and some recent contributions of John von Neumann which yielded according to him another way of treating in a unified way the case of continuous as well as discontinuous spectra[70].

7 A work of a mathematician-physicist: John von Neumann's Hilbert space theory

The paper by David Hilbert, Lothar Nordheim and John von Neumann in the *Mathematischen Annalen*[71] was an outcome of Hilbert's lectures on

[68] Jordan 1927.

[69] As explained by Jordan in the introduction, associating to conjugated pairs of operators of which one has a discrete spectrum (without an accumulation point) the usual canonical commutation rules

$$\alpha\beta - \beta\alpha = -i\hbar$$

leads to a contradiction. As we have seen, this difficulty concerns in particular the quantization of action and angle variables, see Jordan 1927, p. 3.

[70] Interestingly, Jordan's attitude towards von Neumann's achievement seems rather devoid of enthusiasm. Although he praises von Neumann's mathematical achievement, he pinpoints some weaknesses in the presentation (the concept of canonicaly conjugated pairs and transformations), but most importantly, he considers von Neumann's starting points as not being sufficiently "natural" from the physical point of view, see Jordan 1927, p. 2.

[71] Hilbert, Nordheim and von Neumann 1927.

quantum theory given in the winter semester 1926/27, and elaborated by Nordheim. The general framework of the paper follows Jordan's account and the latter's axiomatic style (of course it must have delighted Hilbert). The authors rephrased Jordan's and Dirac's transformation theories using the theory of operators in a more mathematically oriented presentation, without however achieving this time as well full rigor. Essentially all the axioms introduced by Jordan were kept and special emphasis was devoted to the analysis of the reality conditions leading to the hermicity conditions on operators.

The paper ended with the recognition that further work was necessary in order to achieve full mathematical rigor. However, no further joint publication followed and John von Neumann took alone the task of a rigorous formulation of quantum theory. As we know, he actually did much more. Von Neumann's approach constitutes an original achievement combining physical insights with bold mathematical syntheses. Together with a foundational statement of a new mathematical field, the abstract theory of Hilbert spaces designed to express in as intrinsic way as possible the equivalence of wave and matrix mechanics (see below), it was as well an unquestionable contribution to the physical grounding of quantum theory: von Neumann's analysis of states of the theory and of the related issue of hidden variables exerted a seminal influence on subsequent works in quantum physics as well as in mathematics.

The first two papers[72] of John von Neumann, the «Mathematische Begründung der Quantenmechanik»[73], and the «Wahrscheinlichkeitstheoretischer Aufbau der Quantenmechanik»[74] presented quantum mechanics making essential and fully rigorous use of the (abstract) Hilbert space formalism. Together with a third paper, «Thermodynamik quantenmechanischer Gesamtheiten»[75], they subsequently served as base material for most of von Neumann's 1932 treatise, *Mathematische Grundlagen der Quantenmechanik*[76] translated into English in 1955 with the title *Mathematical Foundations of Quantum Mechanics*. Although his

[72] They were announced at the end of Hilbert, Nordheim and von Neumann 1927.
[73] von Neumann 1927a.
[74] von Neumann 1927b.
[75] von Neumann 1927c.
[76] von Neumann 1932.

achievement met a mixed reaction from pure physicists[77] it may still be considered today as one of the best, albeit idiosyncratic, expositions of the formalism.

Von Neumann's first paper was essentially devoted to the study and application to quantum theory of the abstract Hilbert space structure, independently of the peculiarities of its specific realizations known then, namely the (Hilbert) l^2 space of sequences introduced by Hilbert in the framework of his generalization of Fredholm's results on integral equations, and the L^2 space of square-integrable functions[78]. Von Neumann's decision to develop an abstract theory of this structure was motivated by the desire both to overcome the shortcomings of the previous formulations, and to make natural the equivalence of matrix and wave formulations of wave mechanics. In what concerned the shortcomings, von Neumann characterized the situation in the following terms[79]:

> «Das Eigenwertproblem tritt in verschiedenen Erscheinungsformen auf: als Ew. pr. einer unendlichen Matrix (d. i. Transformieren derselben auf die Diagonalform), als solches einer Differentialgleichung. Indessen sind beide Formulierungen einander äquivalent: denn die Matrix (als lineare Transformation angesehen) entsteht aus dem Differential-Operator (der auf die «Wellenfunktion» angewandt, die linke Seite der Diff.-Gleichung ergibt), wenn man von der «Wellenfunktion» zu ihren Entwicklungskoeffizienten für ein vollständiges Orthogonalsystem übergeht. (Die Matrix vermittelt dann die entsprechende Transformation dieser Entwicklungskoeffizienten.)
>
> Beide Behandlungsweisen haben ihre Schwierigkeiten. Bei der Matrizen-Methode steht man eigentlich fast stets vor einem un-

[77] For instance, one can report this passage from a letter of Heisenberg to Pauli, dated 31 July 1928, where Heisenberg writes, presumably referring to von Neumann's *Thermodynamik quantenmechanischer Gesamtheiten*, «[...] wie in der von Dir so beschimpften Arbeit» (Hermann, von Meyenn and Weisskopf 1979, p. 466). Elsewhere however, Pauli speaks rather respectfully of von Neumann's physical ideas.
Jordan, as already mentioned, didn't like, on the other hand, the lack of "physical insight" of von Neumann's presentations. In general, it appears that von Neumann's approach was judged of little practical use for working physicists.

[78] See Dieudonné 1981, chapt. V, and Steen 1973 for detailed accounts.

[79] Von Neumann 1927a, pp. 151 – 153.

lösbaren Problem: die Energie-Matrix auf die Diagonalform zu transformieren. Dies ist ja nur möglich, wenn kein kontinuierliches Spektrum da ist, d. h. die Behandlungsweise ist einseitig (wenn auch in umgekehrtem Sinne als die klassische Mechanik): nur das Diskontinuierliche (gequantelte) tritt in ihr in Erscheinung (Das Wasserstoff-Atom – das auch ein kontinuierliches Spektrum besitzt – kann also da nicht korrekt behandelt werden). Man kann sich freilich helfen, indem man «kontinuierliche Matrizen» benützt, indessen ist dieses Verfahren (eigentlich ein simultanes Operieren mit Matrizen und Integralgleichungskernen) wohl nur sehr schwer mathematisch streng durchzuführen: muss man doch dabei Begriffsbildungen wie unendlich grosse Matrizen-Elemente oder unendlich nahe benachbarte Diagonalen einführen.

Bei der Behandlung nach der Differential-Gleichungs-Methode waren zunächst die Wahrscheinlichkeits-Ansätze der Matrizen-Methode nicht vorhanden. [. . .] Dies wurde von Born und später von Pauli und Jordan nachgeholt, indessen ist das vollständige Verfahren, wie es von Jordan zu einem abgeschlossenen Systeme ausgebaut wurde, auch schweren mathematischen Bedenken ausgesetzt. Man kann nämlich nicht vermeiden, auch sog. uneigentliche Eigenfunktionen mit zuzulassen [. . .]; wie z. B. die zuerst von Dirac benützte Funktion δ(x), die die folgenden (absurden) Eigenschaften haben soll:

$$\delta(x) = 0, \quad \text{für} \quad x \neq 0$$

$$\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1$$

Eine besondere Schwierigkeit bei Jordan ist es, daß man nicht nur seine transformierenden Operatoren (deren Integral-Kerne die «Wahrscheinlichkeits-Amplituden» sind) berechnen muß, sondern auch den Variablen-Bereich, auf den transformiert wird (d. i. das Eigenwertspektrum).»

Von Neumann emphasized next what are the similar features of the eigenvalue problems met in matrix and wave mechanics[80]:

«[Die] Eigenwertprobleme der Quantenmechanik kommen in zwei hauptsächlichen Einkleidungen vor: als Eigenwertprobleme unendlicher Matrizen (oder was dasselbe ist, Bilinearformen), und als Eigenwertprobleme von Differentialgleichungen.

[80] Ibid, p. 154.

Wir wollen beide Erscheinungsformen für sich betrachten, und die gemeinsamen Merkmale hervorheben.

Betrachten wir zunächst die Matrizen-Formulierung. Hier liegt eine unendliche Matrix vor [...], und die Aufgabe ist, sie auf die Diagonalform zu transformieren (denn die Diagonalglieder sind dann die Energie-Niveaus. Nehmen wir an, daß das glatt geht (d. h. daß nur ein Punktspektrum da ist, [...]).

Wir nennen die Energie-Matrix

$$\mathbf{H} = \{h_{\mu\nu}\}, \quad (\mu, \nu = 1, 2, \dots);$$

sie ist als Hermiteisch anzunehmen, d. h.

$$h_{\mu\nu} = \bar{h}_{\nu\mu}.$$

Gesucht wird eine Transformations-Matrix

$$\mathbf{S} = \{s_{\mu\nu}\}, (\mu, \nu = 1, 2, \dots);$$

die das Folgende leistet: sie ist orthogonal, d. h.

$$\sum_{\rho=1}^{\infty} s_{\mu\rho}\bar{s}_{\nu\rho} = \begin{Bmatrix} 1, \mu = \nu \\ 0, \mu \neq \nu \end{Bmatrix}$$

und $\mathbf{S}^{-1}\mathbf{HS}$ hat die Diagonalform.

Wir nennen die Matrix $\mathbf{S}^{-1}\mathbf{HS}$ $\mathbf{W}$, die Diagonalglieder dieser (Diagonal-)Matrix seien $w_1, w_2, \dots$ Dann wird verlangt:

$$\mathbf{HS} = \mathbf{SW}$$

$$\sum_{\rho=1}^{\infty} h_{\mu\rho}s_{\rho\nu} = s_{\mu\nu}w_\nu$$

D. h. die ν-Spalte von $\mathbf{S}, s_{\nu 1}, s_{\nu 2}, \dots$, wird durch $\mathbf{H}$ in ihr w_ν-faches transformiert. Jede Spalte von $\mathbf{S}$ ist also eine Lösung des Eigenwertproblems: diejenigen Folgen $x_1, x_2, \dots$, ausfindig zu machen, die durch $\mathbf{H}$ in ein Vielfaches – etwa ins w -fache – von sich selbst transformiert werden [...].

Bei der Differentialgleichung-Formulierung ist die Situation noch klarer: es ist von Anfang an ein Eigenwertproblem gegeben. Es liegt ein Differentialoperator $\mathbf{H}$ vor [...] und man sucht eine Funktion ψ für die

$$\mathbf{H}\psi = w\psi$$

ist, d. h. die durch $\mathbf{H}$ in ein Vielfaches von sich selbst transformiert wird [...].

> Was ist der gemeinsame Grundzug aller dieser Fälle ? Offenbar der: Jedesmal ist eine Mannigfaltigkeit von gewissen Größen gegeben (nämlich die aller Zahlenfolgen $x_1, x_2, \ldots$, bezw. die aller Funktionen ψ von zwei Winkeln ϑ, φ, oder von einer Koordinate q, oder von drei Koordinaten x, y, z), und ein linearer Operator $\mathbf{H}$ in dieser Mannigfaltigkeit. Jedesmal wird nach allen Lösungen des zu $\mathbf{H}$ gehörigen Eigenwertproblems gesucht, d. h. nach allen (reellen) Zahlen w, zu denen es ein nichtverschwindendes Element f dieser Mannigfaltigkeit gibt, so daß
>
> $$\mathbf{H}f = wf$$
>
> gilt. Diese Eigenwerte w repräsentieren dann die Energieniveaus.
>
> Es ist nun unsere Aufgabe, von dieser einheitlichen Formulierung zu einem einheitlichen Problem zu gelangen. Dies werden wir ausführen, indem wir nachweisen, daß alle soeben angeführten Mannigfaltigkeiten (sowie überhaupt alle, zu denen man durch die heute üblichen Fragestellungen der Quantenmechanik geführt werden kann), im wesentlichen miteinander identisch sind; d. h. daß sie alle aus einer einzigen Mannigfaltigkeit durch bloße Umbenennung gewonnen werden können. »

Now, the execution of the program just outlined is not as easy as could be initially expected: the similarity of both eigenvalue problems is trickier as could appear at first sight. This is because in the Schrödinger approach, the eigenvalue problem can, at a closer inspection, hardly be written in a form really similar to that of matrix mechanics. In his 1932 treatise, where he gives the topic an exhaustive treatment, von Neumann explains first that, indeed, there is a well-defined class of 'continuous' mathematical problems analogous to matrix theory eigenvalue equation for the columns of the transformation matrix:

$$\sum_\nu h_{\mu\nu} x_\nu = \lambda x_\mu \quad (\mu = 1, 2, \ldots) \tag{22}$$

These are the integral equations defined, for a continuous kernel $h(q_1, \ldots, q_k; q'_1, \ldots, q'_k)$ analogous to the discrete $h_{\mu\nu}$,

$$\int_\Omega \cdots \int_\Omega h(q_1, \ldots, q_k; q'_1, \ldots, q'_k) \phi(q'_1, \ldots, q'_k) \mathrm{d}q'_1 \ldots \mathrm{d}' q_k = \lambda \phi(q_1, \ldots, q_k), \tag{23}$$

that have been investigated extensively in mathematics, and can in fact be handled in far reaching analogy to the problem (22).

However, he continues, the wave equation of Schrödinger[81],

> "unfortunately [...] does not have this form, or, rather, it can only be brought into this form if a function $h(q_1, \dots, q_k; q'_1, \dots, q'_k)$ can be found for the differential operator
>
> $$H = H(q_1, \dots, q_k; -i\hbar\frac{\partial}{\partial q_1}, \dots, -i\hbar\frac{\partial}{\partial q_k})$$
>
> such that
>
> $$\mathbf{H}\phi(q_1, \dots, q_k) = \int_\Omega \dots \int_\Omega h(q_1, \dots, q_k; q'_1, \dots, q'_k)\phi(q'_1, \dots, q'_k)dq'_1 \dots d'q_k$$
>
> identically (i. e., for all $\phi(q_1, \dots, q_k)$). This $h(q_1, \dots, q_k; q'_1, \dots, q'_k)$, if it exists, is called the "kernel" of the functional operator **H** , and **H** itself is then called an "integral operator".
>
> Now such a transformation is generally impossible, i. e., differential operators **H** are never integral operators."

The action of the Hamiltonian differential operator on the wave function is in general impossible to express as that of an integral operator, interpreting the kernel as related to a continuous matrix and the wave function as a countinuous column vector. To force the analogy can only be pursued, observes von Neumann, at the price of introducing the singular delta-function, and its derivatives (with their help a kernel for the Hamiltonian can indeed be constructed). This is the path followed by Dirac, but that von Neumann prefers to discard, because of its lack of rigor, and because he sees a different way out. For this, one has to remember the Riesz-Fischer $l^2 \equiv L^2$ isomorphy theorem[82]. Indeed[83]:

> "The method sketched [above] resulted in an analogy between the "discrete" space of index values $Z = (1, 2, \dots)$ and the continuous state space Ω of the mechanical system (Ω is k-dimensional, where k is the number of classical mechanical degrees of freedom). That this cannot be achieved without some violence to the formalism

[81] I am quoting from the English translation of von Neumann's 1932 treatise (von Neumann 1955).

[82] For a history of this result, see Dieudonné 1981.

[83] von Neumann 1955, pp. 28 – 33.

and to mathematics is not surprising. The spaces Z and Ω are in reality very different, and every attempt to relate the two must run into great difficulties.

What we do have, however, is not a relation of Z to Ω , but only a relation between the functions in these two spaces, i. e., between the sequences $x_1, x_2, \ldots$ which are the functions in Z, and the wave functions $\phi(q_1, \ldots, q_k)$ which are the functions in Ω. These functions, furthermore, are the entities which enter most essentially into the problems of quantum mechanics.

In the Schrödinger theory, the integral

$$\int\limits_{\Omega} \cdots \int\limits_{\Omega} |\phi(q_1, \ldots, q_k)|^2 \, \mathrm{d}q_1 \ldots \mathrm{d}q_k$$

plays an important role – it must $= 1$, in order that ϕ can be given a physical interpretation [...]. In matrix theory, on the other hand [...], the vector $x_1, x_2, \ldots$ plays the decisive role. The condition of the finiteness of $\sum_\nu |x_\nu|^2$ in the sense of the Hilbert theory of such eigenvalue problems [...], is always imposed on this vector [...] We call the totality of such functions F_z and F_Ω respectively.

Now the following theorem holds: F_z and F_Ω are isomorphic (Fischer and F. Riesz) [...].

We do not intend to pursue any investigation at this point as to how this correspondence is to be established, since this will be of great concern to us in the next chapter. But we should emphasize what its existence means: Z and Ω are very different, and to set up a direct relation between them must lead to great mathematical difficulties. On the other hand, F_z and F_Ω are isomorphic, i. e., identical in their intrinsic structure (they realize the same abstract properties in different mathematical forms) – and since they (and not Z and Ω themselves) are the real analytical substrata of the matrix and wave theories, this isomorphism means that the two theories must always yield the same numerical results. That is, this is the case whenever the isomorphism lets the matrix

$$\mathbf{H} = \mathbf{H}(\mathbf{Q}_1, \ldots, \mathbf{Q}_k; \mathbf{P}_1, \ldots, \mathbf{P}_k)$$

and the operator

$$\mathbf{H} = H(q_1, \ldots, q_k; -\mathrm{i}\hbar\frac{\partial}{\partial q_1}, \ldots, -\mathrm{i}\hbar\frac{\partial}{\partial q_k})$$

correspond to one another. Since both are obtained by the same algebraic operations from the matrices $\mathbf{Q}_l, \mathbf{P}_l$ $(l = 1, \ldots, k)$ and the functional operators

$$q_l, -\mathrm{i}\hbar\frac{\partial}{\partial q_l}, (l = 1, \ldots, k)$$

respectively, it suffices to show that $q_l \ldots$ corresponds to the matrix $\mathbf{Q}_l$ and $-\mathrm{i}\hbar\frac{\partial}{\partial q_l}$ to the matrix $\mathbf{P}_l$.

Now nothing further was required of the $\mathbf{Q}_l, \mathbf{P}_l$ $(l = 1, \ldots, k)$ than that they satisfy the commutation rules [...]:

$$\mathbf{P}_l\mathbf{Q}_k - \mathbf{Q}_k\mathbf{P}_l = \left\{ \begin{array}{c} 0, l \neq k \\ -ih, l = k \end{array} \right\}$$

But the matrices corresponding to the $q_l, -\mathrm{i}\hbar\frac{\partial}{\partial q_l}$ will certainly do this, because the functional operators $q_l, -\mathrm{i}\hbar\frac{\partial}{\partial q_l}$ possess the properties mentioned, and these are not lost in the isomorphic transformation to F_z .

Since the systems F_z and F_Ω are isomorphic, and since the theories of quantum mechanics constructed on them are mathematically equivalent, it is to be expected that a unified theory, independent of the accidents or the formal framework selected at the time, and exhibiting only the really essential elements of quantum mechanics, will then be achieved, if we do this: Investigate the intrinsic properties (common to F_z and F_Ω) of these systems of functions, and choose these properties as a starting point."

We witness now the birth of the "abstract Hilbert space"[84]:

"The system F_z is generally known as "Hilbert space". Therefore, our first problem is to investigate the fundamental properties of Hilbert space, independent of the special form of F_z and F_Ω. The mathematical structure which is described by these properties (which in any specific special case are equivalently represented by calculations within F_z and F_Ω , but for general purposes are easier to handle directly than by such calculations, is called "abstract Hilbert space".

We wish then to describe the abstract Hilbert space, and then to prove rigorously the following points:

[84] Ibid.

> 1. That the abstract Hilbert space is characterized uniquely by the properties specified, i. e., that it admits of no essentially different realizations.
>
> 2. That its properties belong to F_z as well as F_Ω. [...] When this is accomplished, we shall employ the mathematical equipment thus obtained to shape the structure of quantum mechanics."

The study of this structure with the intention to apply it to express the essential structure of quantum mechanics makes indeed the content of von Neumann's *Mathematische Begründung der Quantenmechanik*[85]. Von Neumann gathers and completes there first some basic results on orthogonal systems and related expansions. He introduces then linear operators and, in a most idiosyncratic move, finally trades the eigenvalue problem for the spectral theory of self-adjoint operators. In particular, he generalizes Born's interpretation of $|\psi|^2$ as a probability of the observable "position" for an arbitrary product of commuting physical quantities. Doing so, von Neumann wanted to improve what he judged as inconsequent ways of presenting and using the formalism. Von Neumann's criticism concerned the phase arbitrariness of the eigenfunctions and in general the arbitrary choice of basis in the eigenspaces which he judged unphysical since eventually the final probabilities do not depend on them. As he states on p. 153:

> «Ein gemeinsamer Mangel aller dieser Methoden ist aber, daß sie prinzipiell unbeobachtbare und physikalisch sinnlose Elemente in die Rechnung einführen: [...]. Die als Schlußresultate erscheinenden Wahrscheinlichkeiten sind zwar invariant, es ist aber unbefriedigend und unklar, weshalb der Umweg durch das nichtbeobachtbare und nicht-invariante notwendig ist.
>
> In der vorliegenden Arbeit wird versucht, eine Methode anzugeben, die diesen Mißständen abhilft, und, wie wir glauben, den heute vorhandenen statistischen Standpunkt in der Quantenmechanik einheitlich und konsequent zusammenfaßt. »

Using the projectors of the resolution of unity associated to a given Hermitian operator one can indeed bypass the wave function stage and then dispense with the intermediate unphysical features.

[85] von Neumann 1927a.

For completeness, let me still report that in his next paper, the «Wahrscheinlichkeitstheoretischer Aufbau. . . »[86], von Neumann introduces the concept of the "statistical operator" associated with an ensemble, better known today as the density matrix. The main result of the paper is, given a physical quantity $\mathcal{R}$ with its associated operator R, the statistical formula

$$Exp(\mathcal{R}) = Tr(UR) \tag{24}$$

where Exp is the expectation value of $\mathcal{R}$ when one considers measurements on a collective (ensemble) of systems characterized by the statistical operator U. This formula, the conditions of its validity as well as its interpretation were to be later at the core of much of the controversy surrounding the problem of hidden variables, but the latter was however not yet considered in the paper[87]. It was to be fully discussed in von Neumann's 1932 treatise, where the formula (24) was derived again along the lines of the paper, but within a much more epistemologically loaded context. This goes however beyond our present concern.

8 An epilogue: From a formal calculus to a full-fledged 'regulative' theory

Von Neumann's 1927 papers were the culmination of a year of efforts from physicists to clarify the mathematical structure of quantum mechanics. As we saw, they did it groping for solutions to specific problems related to quantization in different sets of variables, that is problems arising directly within their physical (theoretical) practice. This led to the insight of transformation theory, and even if it was the mathematician von Neumann who provided the last word in terms of formal rigor, it is not out of place to consider his motivations as quite physical. This observation and the story that I sketched above, provide, it seems to me, the necessary counterpoint to the narrow (if not partial) account of Dieudonné that I discussed in the introduction. Moreover, and closer

[86] von Neumann 1927b.

[87] However, von Neumann did point out that, since for any pure state φ there does exist a Hermitian operator of which φ is not an eigenstate, the associated distribution of values will have dispersion. von Neumann 1927b, p. 222.

to the intention of the editors of this volume, the parallel development of both fields of functional analysis and quantum mechanics with the common underlying issue of properly recognizing and taking advantage of the underlying linear structure, illustrates in my opinion strikingly the complex and stirring links between physics and mathematics. It is appropriate then to end this survey with a reflection on Hilbert and his readiness to marvel at the harmony that physics and mathematics have often displayed along the history of their mutual developments. The Hilbert, Nordheim and von Neumann 1927 paper was to be Hilbert's last publication devoted to physics. Not much is known on what was his further thinking on quantum theory. Some situations are reported where Hilbert expresses his loss of touch with respect to a field in rapid (and complex) development[88], but this appears to be all. It is true that Hilbert was nearing his end, and the last years of his life were rather devoted to pursue his commitment to the fundaments of mathematics[89]. It should finally be noted that in one of his last papers, «Naturerkennen und Logik»[90], where one can find his famous adjunction «Wir müssen wissen, Wir werden wissen», Hilbert did not even bother to mention the most recent formal developments that led to von Neumann's formalism. Commenting on the recent glorious developments of physics, he praised, along with the relativity theory, the discoveries of what one would call today the old quantum theory, but strangely enough did not devote a single line to the new formalism of quantum mechanics. How much this hints at Hilbert's caution with respect to a theory he possibly considered provisional is hard to tell[91]. Nearing to a century of quantum mechanics, we know today that quantum mechanics has fully lived up to its promises and is still going strong with no alternative in sight. In what concerns its basic formal principles and its role as a 'regulative' theory providing rules for the quantization of systems, quantum mechanics witnessed since the early thirties essentially no changes, even not complements. The relativistic equations (Dirac and Klein-Gordon), the understanding of symmetries remarkably implemented in quantum theory because of the linear nature

[88] See Reid 1970, p. 183.
[89] See Reid 1970, also Szanton 1992.
[90] Hilbert 1930.
[91] See Lacki 2000 for some further thoughts.

of the state space, the quantization of fields, all these developments are of course milestones of 20th century theoretical physics, but they do not introduce major changes in the scheme achieved in 1926/27. The possibility of its being overthrown by 'another' theory appears, *from present perspective*, unlikely[92]. But be it as it may, whatever is to come will not fundamentally change the strong links that have been established again, on the occasion of the discovery of its formalism, between physics and mathematics. Even if quantum mechanics should finally turn out as not the *very* last word on the reality of microphenomena, it will stay in science as a powerful resource for stimulating first rank mathematical research.

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[92] This statement purports to the formalism of quantum mechanics: I am not venturing to make any bids concerning the issue of the ongoing debate on its interpretation, where many conflictual positions have been proposed with fluctuating popularity over time.

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