VON NEUMANN'S CONTRIBUTIONS TO QUANTUM THEORY

LÉON VAN HOVE

That von Neumann has been "par excellence" the mathematician of quantum mechanics is as obvious to every physicist now as it was a quarter of a century ago. Quantum mechanics was very fortunate indeed to attract, in the very first years after its discovery in 1925, the interest of a mathematical genius of von Neumann's stature. As a result, the mathematical framework of the theory was developed and the formal aspects of its entirely novel rules of interpretation were analyzed by one single man in two years time (1927–1929). Conversely, one could almost say in reciprocity, quantum mechanics introduced von Neumann into a field of mathematical investigation, operator theory, in which he achieved some of his most prominent successes.

Von Neumann's major contributions to quantum mechanics are his development of the mathematical framework of the theory and his formal study of quantum statistics, quantum measuring processes and their interrelations. Whereas the latter study was essentially complete in 1927 (except for the quantum ergodic theorem of 1929) the work on the mathematical foundations of quantum mechanics came to its culmination in 1929 with the spectral theorem for hypermaximal symmetric operators in Hilbert space. In the next two paragraphs we shall discuss these major contributions.

The mathematical framework of quantum theory. By the time von Neumann started his investigations on the formal framework of quantum mechanics this theory was known in two different mathematical formulations: the "matrix mechanics" of Heisenberg, Born and Jordan, and the "wave mechanics" of Schrödinger. The mathematical equivalence of these formulations had been established by Schrödinger, and they had both been embedded as special cases in a general formalism, often called "transformation theory," developed by Dirac and Jordan. This formalism, however, was rather clumsy and it was hampered by its reliance upon ill-defined mathematical objects, the famous delta-functions of Dirac and their derivatives. Although von Neumann himself attempted at first, in collaboration with Hilbert and Nordheim [1], to edify the quantum-mechanical

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formalism along similar lines, he soon realized that a much more natural framework was provided by the abstract, axiomatic theory of Hilbert spaces and their linear operators [2]. This mathematical formulation of quantum mechanics, whereby states of the physical system are described by Hilbert space vectors and measurable quantities by hermitian operators acting upon them, has been very successful indeed. Unchanged in its essentials it has survived the two great extensions which quantum theory was to undergo soon: the relativistic quantum mechanics of particles (Dirac equation) and the quantum theory of fields.

One might of course remark that Dirac's delta functions and their derivatives, although poorly defined at the time of their introduction, have been recognized since as bona fide mathematical entities in L. Schwartz' theory of distributions. This is quite true and moreover these functions have been used continually by physicists throughout the development of quantum theory, in particular in the last two decades for the study of scattering processes and of quantized fields. Delta functions have established themselves as the natural tool whenever operators with continuous spectra are to be considered. This does not affect in any way, however, the fact that the axiomatically defined separable Hilbert space is the suitable framework for the quantum-mechanical formalism as we know it today, and the recognition of this fact we owe to von Neumann.

An essential feature of the Hilbert space formulation of quantum theory is that the most important physical quantities as position, momentum or energy are represented by unbounded hermitian operators. Since the theoretical prediction of measurements makes essential use of the spectral resolution of the operators representing the physical quantities, von Neumann was, in his very first investigation [2], faced with the problem of extending to the unbounded case the known spectral theory of bounded hermitian operators. By 1929 he had brought this problem to a complete solution [3]. He introduced the all-important concept of hypermaximal symmetric operator, being the most general hermitian operator with a spectral resolution. This work, the results of which were reached independently by M. H. Stone [4], was for von Neumann the starting point of a long series of investigations on linear operators in Hilbert space.

Still another contribution of von Neumann to the mathematical foundation of quantum theory is worth mentioning here. He established the important theorem that (in the irreducible case and after a suitable reformulation) the canonical commutation rules $Q_jP_l-P_lQ_j =\hbar\, i\delta_{jl}$ determine the operators $Q_1, \cdots, Q_n, P_1, \cdots, P_n$ uniquely except for an arbitrary transformation [5]. Although rarely quoted as such, this theorem, which was already known to Dirac and Stone [6], is really fundamental for the understanding of many quantum-mechanical investigations where the theoretical analysis is exclusively based on the canonical commutation rules in their above form or in the equivalent field-theoretical form

$$A_j A_l^* - A_l^* A_j = \hbar \delta_{jl}, \qquad 2^{1/2} A_j = P_j - iQ_j.$$

Statistical aspects of quantum theory. In the course of his formulation of quantum mechanics in terms of vectors and operators of Hilbert space von Neumann also gave in complete generality the basic statistical rule of interpretation of the theory. This rule concerns the result of the measurement of a given physical quantity on a system in a given quantum state and expresses its probability distribution by means of a simple and now completely familiar formula involving the vector representing the state and the spectral resolution of the operator which represents the physical quantity [2]. This statistical rule, originally proposed by Born in 1926, was for von Neumann the starting point of a mathematical analysis of quantum mechanics in entirely probabilistic terms. The analysis, carried out in a paper of 1927 [7], introduced the concept of statistical matrix for the description of an ensemble of systems which are not necessarily all in the same quantum state. The statistical matrix (now often called ρ-matrix although von Neumann's notation was U) has become one of the major tools of quantum statistics and it is through this contribution that von Neumann's name became familiar to even the least mathematically minded physicists.

In the same paper von Neumann also investigates a problem which is still now the subject of much discussion, viz., the theoretical description of the quantum-mechanical measuring process and of the noncausal elements which it involves. Mathematically speaking von Neumann's study of this delicate question is quite elegant. It provides a clear-cut formal framework for the numerous investigations which were needed to clarify physically the all-important implications of quantum phenomena for the nature of physical measurements, the most essential of which is Niels Bohr's concept of complementarity.

The results of the paper just discussed were immediately used by the author to lay the foundation for quantum thermodynamics [8]. He gave the quantum analogue

$$S = -k \operatorname{Sp} (\rho \ln \rho), \qquad \rho \text{ statistical matrix,}$$

of the well known classical formula for the entropy

$$S = -k \int f \ln f d\omega, \qquad f \text{ distribution function in phase space.}$$

He further wrote down the density matrix for a canonical ensemble at temperature T:

$$\rho = Z^{-1} \exp(-H/kT), \quad Z = \mathrm{Sp}\,[\exp(-H/kT)],$$

H being the Hamilton operator. Two years later von Neumann came back to quantum thermodynamics with a contribution to a much more difficult problem: the formulation and proof of an ergodic theorem for quantum systems [9]. The basic principle of this work is to define quantum analogues of cells in phase space by considering sets of quantum states for which all macroscopic quantities have given values within a certain inaccuracy. One further considers the unitary transformation u relating these quantum states to the eigenstates of the hamiltonian. The ergodicity is then established for "almost every" value of the transformation u. Although the latter restriction is a rather unsatisfactory one from the physical standpoint, one must consider von Neumann's ergodic theorem as one of the very few important contributions to a most difficult subject which even now is far from complete clarification.

Most of the work we have briefly reviewed has been republished by the author, in greatly expanded form, as a book which rapidly became and still is the standard work on the mathematical foundations of quantum mechanics [10]. Von Neumann devoted in his book considerable attention to a point which had not been discussed in the 1927 papers and which was later the subject of much controversy. It is the question of the possible existence of "hidden variables," the consideration of which would eliminate the noncausal element involved in the measuring process. Von Neumann could show that hidden parameters with this property cannot exist if the basic structure of quantum theory is retained. Although he mentioned the latter restriction explicitly,[1] his result was often quoted without due reference to it, a fact which sometimes gave rise to unjustified criticism in the many discussions devoted through the years to the possibility of an entirely deterministic reformulation of quantum theory.

Other contributions. As von Neumann's complete bibliography will reveal, he wrote quite a few other papers on questions of quantum mechanics, often in collaboration with physicists, especially with Wigner. Most of these papers deal with technical matters and the

[1] See e.g. ref. 10, p. 109, line 17 and foll.

importance of the major contributions discussed above is so eminent that, in comparison, the other papers' scope is modest. There is only one broad subject which we would like to mention here, because von Neumann, obviously giving it considerable thought, returned to it several times in 1934 and 1936 (in collaboration with Jordan, Wigner and Garrett Birkhoff). It is the question of the algebraic and logical structure of quantum mechanics, where the hope has existed to reach through abstract analysis possible generalizations of the accepted theory. Nobody knows whether such a hope is justified, but it is undoubtedly a natural one and it has appealed to many other people, giving one more example of the power and originality of von Neumann's thinking.

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INSTITUTE FOR THEORETICAL PHYSICS OF THE UNIVERSITY,
UTRECHT, NETHERLANDS