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*(Never) Mind your p’s and q’s: von Neumann versus Jordan on the Foundations of Quantum Theory**

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In early 1927, Pascual Jordan published his version of what came to be known as the Dirac-Jordan statistical transformation theory. Later in 1927 and partly in response to Jordan, John von Neumann published the modern Hilbert space formalism of quantum mechanics. Central to both formalisms are expressions for conditional probabilities of finding some value for one observable given the value of another. Beyond that Jordan and von Neumann had very different views about the appropriate formulation of problems in the new quantum mechanics. For Jordan, unable to let go of the connection to classical mechanics, the solution of such problems required the identification of sets of canonically conjugate variables. For von Neumann, not constrained by this analogy to classical physics, the identification of a maximal set of commuting operators with simultaneous eigenstates was all that mattered. In this talk we reconstruct the central arguments of these 1927 papers by Jordan and von Neumann, highlighting those elements that bring out the gradual loosening of the ties between the new quantum formalism and classical mechanics.

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Jordan and von Neumann on the Foundations of Quantum Theory

Pascual Jordan (1902–1980) **John von Neumann (1903–1957)**

Four different versions of quantum theory by the middle of 1926

matrix mechanics
(Heisenberg, Born, Jordan)

wave mechanics
(Schrödinger)

Already getting clear:

- Different versions predict the same results (Schrödinger)
- Formalism calls for probabilistic interpretation (Born)

Open questions:

- What is the underlying structure tying the different versions together?
- What is the general probabilistic interpretation of the unifying formalism?

q-number theory
(Dirac)

operator calculus
(Born, Wiener)

Late 1926/1927: Two unifying formalisms and their probabilistic interpretation

- **Jordan(-Dirac) statistical transformation theory.** Canonical transformations & conjugate variables central to formulation of the theory … **mind your *p*'s and *q*'s**

Conditional probability of finding **value *x*** for **observable** $\hat{x}$ given y for $\hat{y}$ $\Pr(\hat{x} = x | \hat{y} = y)$ = Square of probability amplitude $\varphi(x, y)$ satisfying generalization of time-independent Schrödinger equation.

- **Von Neumann's spectral theory of operators.**
Canonical transformations … *replaced by* … unitary transformations in Hilbert space
Conjugate variables … *replaced by*… maximal set of commuting operators
… **never mind your *p*'s and *q*'s**

Conditional probability of finding **value *x*** for **observable** $\hat{x}$ given y for $\hat{y}$ $\Pr(\hat{x} = x | \hat{y} = y)$ = Trace of product of projection operators onto eigenstates of $\hat{x}$ and $\hat{y}$ with eigenvalues x and y.

Sources

Articles (1927)

- Jordan, "Über eine neue Begründung [new foundation] der Quantenmechanik." 2 Pts. *Zeitschrift für Physik* (1927) [submitted December 18, 1926 & June 3, 1927] **NB I & II**

- Dirac, "The physical interpretation of the quantum dynamics." *Proceedings of the Royal Society* (1927) [submitted December 2, 1926]

- Hilbert, Von Neumann, and Nordheim, "Über die Grundlagen der Quantenmechanik." *Mathematische Annalen* (1928) [submitted April 6, 1927] **HvNN**

- Von Neumann, "Mathematische Begründung [foundation] der Quantenmechanik." *Göttingen Nachrichten* (1927) [submitted May 20, 1927] **MB**

- Von Neumann, "Wahrscheinlichkeitstheoretischer [probability-theoretic] Aufbau der Quantenmechanik." *Göttingen Nachrichten* (1927) [submitted November 11, 1927] **WA**

Sources

Books (1930s)

- Dirac, *Principles of Quantum Mechanics*. Oxford: Clarendon, 1930.
- Born & Jordan, *Elementare Quantenmechanik*. Berlin: Springer, 1930.
- Von Neumann, *Mathematische Grundlagen der Quantenmechanik*. Berlin: Springer, 1932.

  About Dirac's book (with footnotes to 1927 papers by Dirac and Jordan): "Dirac's method does not meet the demands of mathematical rigor in any way—not even when it is reduced in the natural and cheap way to the level that is common in theoretical physics … the correct formulation is not just a matter of making Dirac's method mathematically precise and explicit but right from the start calls for a different approach related to Hilbert's spectral theory of operators" (p. 2)

- Jordan, *Anschauliche Quantentheorie*. Berlin: Springer, 1936.

  Dirac-Jordan transformation theory: "the pinnacle of the development of quantum mechanics" (p. VI) & "the most comprehensive and profound version of the quantum laws." (p. 171)

Jordan, *On a New Foundation of Quantum Mechanics* I

Über eine neue Begründung der Quantenmechanik.

Von **P. Jordan** in Göttingen.

(Eingegangen am 18. Dezember 1926.)

Die vier bisher entwickelten Formen der Quantenmechanik: die Matrizentheorie, die Theorie von Born und Wiener, die Wellenmechanik und die Theorie der q-Zahlen, sind als Spezialfälle enthalten in einer allgemeineren formalen Theorie. Im Anschluß an einen Gedanken von Pauli kann diese neue Theorie auf einige einfache Grundpostulate statistischer Natur gegründet werden [1].

I. Teil.

§ 1. *Einleitung.* Nach Schrödinger ist einer Hamiltonschen Funktion $H(p, q)$ eine Schwingungsgleichung

$$\left\{H\left(\varepsilon \frac{\partial}{\partial y}, y\right) - W\right\} \varphi(y) = 0, \quad \varepsilon = \frac{h}{2\pi i} \tag{1}$$

zuzuordnen. Sie steht in Korrespondenz zur klassischen Hamilton-

Probability amplitudes.

Pauli's special case: $\psi_n(x)$ Schrödinger energy eigenfunction: $|\psi_n(x)|^2 dx$ gives conditional probability of finding value between x and $x + dx$ for position if the system is in n^{th} energy eigenstate.

Jordan's generalization: For any two quantities $\hat{x}$ and $\hat{y}$ with continuous spectra, there is a complex probability amplitude $\varphi(x, y)$ such that

$|\varphi(x, y)|^2 dx =$ conditional probability of finding a value between x and $x + dx$ for $\hat{x}$ if $\hat{y}$ has value y.

- Generalization to quantities with (partly) discrete spectra is only given in *Neue Begründung* II and turns out to be problematic.
- **From modern Hilbert space perspective:** $\varphi(x, y) = \langle x|y\rangle$
  E.g., $\psi_n(x) = \langle x|E_n\rangle$.

  Caution: neither Jordan nor Dirac—despite introducing the notation (x/y) in his 1927 paper—initially thought of these quantities as inner products of vectors in Hilbert space.

Jordan introduces postulates his probability amplitudes have to satisfy:

Obsession with axiomatization reflects Hilbert's influence.

Cf. Lacki, "The early axiomatizations of quantum mechanics: Jordan, von Neumann and the continuation of Hilbert's program." *Archive for History of Exact Sciences* 54 (2000): 279–318.

Postulate A. Introduction of probability amplitudes.

Postulate B. Symmetry: $\chi(\beta, q) = \varphi(q, \beta)^*$ Cf. Hilbert space: $\langle\beta|q\rangle = \langle q|\beta\rangle^*$

Probability density $|\chi(\beta, q)|^2$ of finding β for $\hat{\beta}$ given q for $\hat{q}$ **=** Probability density $|\varphi(q, \beta)|^2$ of finding q for $\hat{q}$ given β for $\hat{\beta}$

$$\Pr(\hat{\beta} = \beta \,|\, \hat{q} = q) \quad = \quad \Pr(\hat{q} = q \,|\, \hat{\beta} = \beta)$$

Jordan’s postulates (cont’d)

Postulate C. Interference of probabilities (NB I, 812). Amplitudes rather than probabilities themselves follow the usual **composition rules** of probability theory.

Let F_1 and F_2 be outcomes [*Tatsachen*] with amplitudes φ_1 and φ_2:

F_1 and F_2 mutually exclusive: $\varphi_1 + \varphi_2$ amplitude for $\boldsymbol{F_1}$ **OR** $\boldsymbol{F_2}$

F_1 and F_2 independent: $\varphi_1\varphi_2$ amplitude for $\boldsymbol{F_1}$ **AND** $\boldsymbol{F_2}$

Application of composition rules:

Let $\varphi(q, \beta)$ be the amplitude for finding q for $\hat{q}$ given β for $\hat{\beta}$;

$\chi(Q, q)$ " " Q for $\hat{Q}$ given q for $\hat{q}$;

$\Phi(Q, \beta)$ " " Q for $\hat{Q}$ given β for $\hat{\beta}$.

Then: $$\Phi(Q, \beta) = \int \chi(Q, q)\varphi(q, \beta)dq$$

Jordan’s postulates (cont’d)

Postulate C. Interference of probabilities (NB I, 812). Amplitudes rather than probabilities themselves follow the usual **composition rules** of probability theory.

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Application of composition rules:

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$\Phi(Q, \beta)$ " " Q for $\hat{Q}$ given β for $\hat{\beta}$.

Then: $\Phi(Q, \beta) = \int \chi(Q, q) \varphi(q, \beta) dq$

Modern perspective: Set $\varphi(q, \beta) = \langle q|\beta\rangle$. Hilbert space structure ensures that composition rules hold:

$$\langle Q|\beta\rangle = \int dq \langle Q|q\rangle\langle q|\beta\rangle \qquad \textbf{Completeness}$$

Jordan's postulates (cont'd)

Definition: $\hat{p}$ is the **conjugate momentum** of $\hat{q}$ **IF** amplitude of finding p for $\hat{p}$ given q for $\hat{q}$ is $\rho(p, q) = e^{-ipq/\hbar}$. Special case of Heisenberg's uncertainty principle *avant la lettre*: "For a given value of $\hat{q}$ all possible values of $\hat{p}$ are *equiprobable*" (NB I, 814)

NBI submitted December 18, 1926; uncertainty paper submitted March 23, 1927. Max Jammer, *The Conceptual Development of Quantum Mechanics* (1966): uncertainty principle "had its origin in the Dirac-Jordan transformation theory"(p. 326) & "Heisenberg derived his principle from the Dirac-Jordan transformation theory"(p. 345). See also Mara Beller, *Quantum Dialogue* (1999), Ch. 4.

Postulate D. Conjugate variables. For every $\hat{q}$ there is a conjugate momentum $\hat{p}$.

Special probability amplitude $\rho(p, q) = e^{-ipq/\hbar}$ trivially satisfies

$$\left(p + \frac{\hbar}{i}\frac{\partial}{\partial q}\right)\rho(p, q) = 0 \qquad \left(\frac{\hbar}{i}\frac{\partial}{\partial p} + q\right)\rho(p, q) = 0$$

Equations for other probability amplitudes (e.g., time-independent Schrödinger equation for $\varphi(x, E) \equiv \psi_n(x) = \langle x|E_n\rangle$) obtained through **canonical transformations.**

Lacki, "The puzzle of canonical transformations in early quantum mechanics." *SHPMP* 35 (2004): 317–344.

Duncan & Janssen (HQ2): "From canonical transformations to transformation theory, 1926–1927: The road to Jordan's *Neue Begründung*." *SHPMP* 40 (2009): 352–362.

Canonical transformations and probability amplitudes (cont'd)

(1) Canonical transformation S: $\varphi(q, \beta) \to \Phi(Q, \beta)$: $\Phi(Q, \beta) = S\, \varphi(q, \beta)\big|_{q = Q}$

(2) Composition rule for probability amplitudes: $\Phi(Q, \beta) = \int dq\, \chi(Q, q)\varphi(q, \beta)$

Requires that S can be represented as (NB I, 829): $S \ldots = \int dq\, \chi(Q, q)\ldots.$

Dual role of $\chi(Q, q)$ etc.
- Probability amplitude
- 'Matrix' (integral kernel) for canonical transformation

Jordan's basic strategy in setting up his statistical transformation theory:

Properties of canonical transformations connecting pairs of conjugate variables ensure that postulated composition rules for probability amplitudes hold.

Canonical transformations and probability amplitudes (cont'd)

(1) Canonical transformation S: $\varphi(q, \beta) \rightarrow \Phi(Q, \beta)$: $\Phi(Q, \beta) = S\, \varphi(q, \beta)\big|_{q\,=\,Q}$

(2) Composition rule for probability amplitudes: $\Phi(Q, \beta) = \int dq\ \chi(Q, q)\varphi(q, \beta)$

Requires that S can be represented as (NB I, 829): $S\ \ldots = \int dq\ \chi(Q, q)\ldots.$

From a modern Hilbert space perspective: $\Phi(Q, \beta) = \langle Q|\beta\rangle$ & $\varphi(q, \beta) = \langle q|\beta\rangle$; both (1) and (2) are given by the completeness relation:

$$\langle Q|\beta\rangle = \int dq\ \langle Q|q\rangle\langle q|\beta\rangle.$$

The role of canonical transformations in the Dirac-Jordan theory is taken over by unitary transformations between different orthonormal bases in Hilbert space. The structure of Hilbert space ensures that composition rules for probability amplitudes hold.

Jordan, *On a New Foundation of Quantum Mechanics* II

Über eine neue Begründung der Quantenmechanik. II.

Von **P. Jordan**, z. Z. in Kopenhagen.

(Eingegangen am 3. Juni 1927.)

Es wird eine vereinfachte und verallgemeinerte Darstellung der in I. entwickelten Theorie gegeben. Eine Verallgemeinerung war insofern nötig, als dort nur die Theorie stetiger quantenmechanischer Größen vollständig entwickelt wurde, während die unstetigen, „gequantelten" Größen nicht genauer untersucht wurden. Es zeigt sich, daß die kanonische Vertauschungsregel $pq - qp = h \cdot (2\pi i)^{-1}$ nur bei stetigen Größen p, q besteht; es ist z. B. nicht richtig, für eine gequantelte Wirkungsvariable J zu setzen $Jw - wJ = h \cdot (2\pi i)^{-1}$; auch gilt keinerlei derartige Gleichung in der Theorie des Magnetelektrons. Dagegen bewährt sich allgemein, bei stetigen und bei unstetigen Größen, die in I. gegebene Definition kanonisch konjugierter Größen; sie liefert auch die Theorie des ruhenden Magnetelektrons.

Die vorliegende Abhandlung ist, wie der Titel anzeigt, eine Fortsetzung zu einer früheren Arbeit, die wir hier als I. zitieren[1]. Es wird jedoch nur eine ungefähre Kenntnis der Überlegungen von I. vorausgesetzt. Die Wiederaufnahme der Betrachtungen von I. schien deshalb geboten, weil dort nur die Theorie solcher Größen vollständig entwickelt war, deren mögliche Werte eine kontinuierliche Mannigfaltigkeit bilden: für alle „gequantelten" Größen (Energien, Quantenzahlen) ist die Theorie zunächst nicht anwendbar. Der gleichen Beschränkung unterliegen die mit I. im wesentlichen gleichbedeutenden Ergebnisse von Dirac[2]. Daß diese Beschränkung sehr einschneidend, und daß die notwendige Verallgemeinerung der Theorie nicht trivial ist, werden wir bald erkennen.

Problems with Jordan's reliance on canonical transformations

- **Canonical transformations need not be unitary and thus need not preserve Hermiticity**. In NB I Jordan introduced something called the *Ergänzungsamplitude* to allow non-Hermitian quantities in his formalism. When he dropped the *Ergänzungs-amplitude*, he had to restrict the class of canonical transformations to unitary ones.

- **Definition of conjugate variables loosened to the point where it loses almost all contact with classical origins**. For $\hat{p}$'s and $\hat{q}$'s with continuous spectra, Jordan's definition is equivalent to standard one, $[\hat{p}, \hat{q}] = \hbar/i$. Not true for $\hat{p}$'s and $\hat{q}$'s with discrete spectra. Example: spin components $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$, dealt with in NB II. For Jordan, $\hat{\alpha}$ and $\hat{\beta}$ are conjugate variables if:

  (1) $\varphi(\alpha, \beta) = \langle\alpha|\beta\rangle = e^{-i\alpha\beta/\hbar}$ flat ('mutually unbiased') probability distribution

  (2) $\int d\beta\varphi(\alpha, \beta)\varphi(\alpha', \beta)^* = \int d\beta\langle\alpha|\beta\rangle\langle\beta|\alpha'\rangle = \delta(\alpha-\alpha')$ orthogonality/completeness

  But:
  - (2) is true for any two variables $\hat{\alpha}$ and $\hat{\beta}$.
  - (1)&(2) are true for bona fide conjugate variables, but also for, say, $\hat{\sigma}_x$ and $\hat{\sigma}_y$.

- **Other than in classical mechanics, the relevant quantities in quantum mechanics cannot always be sorted neatly into pairs of $\hat{p}$'s and $\hat{q}$'s**. Example: Hamiltonian dependent on all three spin components.

Hilbert, von Neumann, and Nordheim, *On the Foundations of Quantum Mechanics*

Über die Grundlagen der Quantenmechanik.

Von

D. Hilbert, J. v. Neumann und L. Nordheim in Göttingen.

§ 1.

Einleitung.

Die neuere Entwicklung der Quantenmechanik, die an die Arbeiten von Heisenberg[1]), Born und Jordan einerseits und Schrödinger[2]) andererseits anknüpft, hat es ermöglicht, das ganze Gebiet der Atomerscheinungen unter einen einheitlichen Gesichtspunkt zusammenzufassen und die wichtigsten Beobachtungsergebnisse zu erklären, so daß man kaum noch zweifeln kann, in ihr einen Gedankenkomplex von gleicher Bedeutung wie etwa die klassische Mechanik oder Elektrodynamik gefunden zu haben. Bei dieser hohen Bedeutung der Quantenmechanik ist es ein dringendes Bedürfnis, ihre Prinzipien so klar und allgemein wie möglich zu erfassen. Hier hat nun Jordan[3]) im Anschluß an eine Idee von Pauli[4]) eine Formulierung und Begründung der Theorie gegeben, die von großer Allgemeinheit ist und dem physikalischen Charakter der zu grunde liegenden Erscheinungen sehr gut angepaßt erscheint. Unabhängig von Jordan ist Dirac[5]) zu ähnlichen Anschauungen gelangt.

Exposition of Jordan's transformation theory based on Hilbert's lectures on quantum mechanics, Göttingen 1926/27 (see Tilman Sauer, Ulrich Majer (eds.). *David Hilbert's Lectures on the Foundations of Physics, 1915–1927*. Berlin: Springer, 2009).

Hilbert, Von Neumann, and Nordheim, "Über die Grundlagen der Quantenmechanik." *Mathematische Annalen* (1928) [submitted April 6, 1927, before *Neue Begründung* II]

- Jordan-Dirac way of subsuming wave mechanics under matrix mechanics:

$$\hat{q}f(q) = qf(q) \longrightarrow \hat{q}f(q) = \int dq' q' \delta(q-q') f(q')$$

$$\hat{p}f(q) = \frac{\hbar}{i}\frac{\partial}{\partial q} f(q) \longrightarrow \hat{p}f(q) = \int dq' \left(\frac{\hbar}{i}\frac{\partial}{\partial q'}\delta(q-q')\right) f(q')$$

'Matrices' $\hat{q}_{qq'}$ and $\hat{p}_{qq'}$ → **integral kernels** $q'\delta(q-q')$ & $\frac{\hbar}{i}\frac{\partial}{\partial q'}\delta(q-q')$

- Authors emphasize that the theory is mathematically unsatisfactory. "We hope to return to these questions on some other occasion." Footnote: "Cf. a paper which will soon appear in the *Göttingen Nachrichten*, "Mathematical Foundation of Quantum Mechanics" by J. v. Neumann" (HvNN, 30)

  Suggests that von Neumann just cleaned up Jordan-Dirac theory mathematically. In fact, von Neumann took an entirely different approach.

Von Neumann's *Mathematical Foundations of Quantum Mechanics*

Mathematische Begründung der Quantenmechanik.

Von

J. v. Neumann, Göttingen.

Vorgelegt von M. Born in der Sitzung vom 20. Mai 1927.

Einleitung.

I. Die von Heisenberg, Dirac, Born, Schrödinger und Jordan [1]) gegebenen Formulierungen der „Quantenmechanik" haben viele ganz neuartige Begriffsbildungen und Fragestellungen aufgeworfen, von denen wir die Folgenden hervorheben möchten:

α. Es hat sich gezeigt, daß das Gebaren eines atomaren Systems irgendwie mit einem gewissen Eigenwertproblem zusammenhängt — wie dasselbe zu formulieren ist, soll noch später, in § XII berührt werden — insbesondere sind die Werte der das System beschreibenden charakteristischen Größen die Eigenwerte selbst.

β. Hierdurch wurde die lange gesuchte Verschmelzung des Kontinuierlichen (klassisch-mechanischen) und des Diskontinuierlichen (gequantelten) in der Welt der Atome befriedigenderweise erreicht: ein Eigenwertspektrum kann ja sowohl kontinuierliche als auch diskontinuierliche Teile besitzen.

Von Neumann's take on unifying matrix mechanics and wave mechanics à la Jordan & Dirac

Eigenvalue problems in matrix mechanics (1) and wave mechanics (2):

(1) Find square-summable infinite sequences $\mathbf{x} = (x_1, x_2, \ldots)$ such that $\mathbf{Hx} = E\mathbf{x}$.

(2) Find square-integrable functions $f(x)$ such that $\hat{H}f(x) = Ef(x)$

How to unify (1) and (2)? Jordan-Dirac solution (from von Neumann's perspective):

'Space' Z of discrete values of the index of x_i	Space Ω of continuous values of the argument of $f(x)$	$\rightarrow$	Instantiations of more general space R
$\sum_{i=1}^{\infty}$	$\int_{\Omega} dx$	$\rightarrow$	'Integrals' over R
H_{ij}	$H_{xx'}$	$\rightarrow$	'R components' of 'matrix' of $\hat{H}$

von Neumann: analogy between Z and Ω "very superficial, as long as one abides by the usual standards of mathematical rigor" (MB, 11; similar statement in intro 1932 book).

Von Neumann's approach to unifying matrix mechanics and wave mechanics

Appropiate analogy is not between Z and Ω but between

space of square-summable sequences over Z	**and**	**space of square-integrable functions over Ω**

Notation: 1927 paper: H_0 and H (Fraktur);

1932 book: F_Z and F_Ω;

Modern notation: l^2 and L^2.

<u>Note</u>: in 1927 paper, von Neumann says l^2 is known as 'Hilbert space'; in a 1926 paper. Fritz London had called L^2 'Hilbert space' (see Lacki 2004, Duncan & Janssen 2009).

Basis for unification: **isomorphism of l^2 and L^2**

Based on "long known mathematical facts" (MB, 12):

Parseval $l^2 \to L^2$ [mapping $\{x_i\} \in l^2$ onto $f(x) \in L^2$]; Riesz-Fischer (1907) $L^2 \to l^2$.

Von Neumann introduces abstract Hilbert space $\overline{H}$.

This settled the issue of the equivalence of wave mechanics and matrix mechanics: anything that can be done in wave mechanics, i.e., in L^2, has a precise equivalent in matrix mechanics, i.e., in l^2 (discrete spectra, continuous spectra, a combination of both)

Von Neumann's introduction of probabilities in *Mathematische Begründung*

Possible route:

- Von Neumann could have just identified Jordan's probability amplitudes $\varphi(x, y)$ as inner products $\langle x|y\rangle$ of vectors in Hilbert space. But actually he never does.

- Von Neumann's objections:
    - $\varphi(x, y)$ only determined up to a phase factor: "It is true that the probabilities appearing as end results are invariant, but it is unsatisfactory and unclear why this detour through the unobservable and non-invariant is necessary" (MB, 3). Jordan defends his use of amplitudes against von Neumann's criticism in NB II, 20.
    - Jordan's basic amplitude $\rho(p, q) = e^{-ipq/\hbar}$—eigenfunctions of momentum from Schrödinger perspective—not part of Hilbert space.

Von Neumann's actual route:

- Basic task (following Jordan): what is the probability of finding x for $\hat{x}$ given y for $\hat{y}$.

- Derive an expression for such conditional probabilities in terms of projection operators associated with spectral decomposition of operators for the observables $\hat{x}$ and $\hat{y}$.

Von Neumann's derivation of formula for conditional probabilities

[in Dirac notation & using same notation for observable and operator representing observable]

- Let A be a finite Hermitian matrix with non-degenerate discrete spectrum with eigenvalues a_i and eigenvectors $|a_i\rangle$ (normalized).

- Introduce projection operator $\hat{P}_{a_i} = |a_i\rangle\langle a_i|$ onto eigenstate $|a_i\rangle$
    - von Neumann's term: "Einzeloperator" or "E. Op." (MB, 25).
    - Von Neumann didn't think of projection operators as constructed out of bras and kets (just as Jordan didn't think of probability amplitudes as constructed out of bras and kets).
    - There is no phase ambiguity in $\hat{P}_{a_i}$.

- Spectral decomposition of A:

$$A = \sum_i a_i |a_i\rangle\langle a_i|$$

- Von Neumann generalized this result to arbitrary self-adjoint operators (bounded/ unbounded; degenerate/non-degenerate, continuous/discrete spectrum).

Von Neumann's derivation of formula for conditional probabilities (cont'd)

Consider (MB, 43): probability of finding the system in some region K if we know that its energy is in some interval I that includes various eigenvalues of its energy:

$$\sum_I \int_K |\psi_n(x)|^2 dx \qquad \text{with } I \text{ shorthand for "all } n \text{ for which } E_n \text{ lies in } I\text{"}$$

Introduce projection operators

$$\hat{F}(K) \equiv \int_K |x\rangle\langle x| dx \qquad \hat{E}(I) \equiv \sum_I |E_n\rangle\langle E_n|$$

Rewrite probability, using $\psi_n(x) = \langle x|E_n\rangle$:

$$\sum_I \int_K |\psi_n(x)|^2 dx = \sum_I \int_K \langle x|E_n\rangle\langle E_n|x\rangle dx$$

Insert $\hat{1} = \sum_\alpha |\alpha\rangle\langle\alpha|$, with $\{|\alpha\rangle\}$ some orthonormal basis of Hilbert space

$$\sum_\alpha \sum_I \int_K \langle x|\alpha\rangle\langle\alpha|E_n\rangle\langle E_n|x\rangle dx = \sum_\alpha \langle\alpha|\left(\sum_I |E_n\rangle\langle E_n| \int_K |x\rangle\langle x| dx\right)|\alpha\rangle = \mathrm{Tr}(\hat{E}(I)\hat{F}(K))$$

Von Neumann’s derivation of formula for conditional probabilities (cont’d)

Probability that the position is in region K if the energy is in interval I:

$$\sum_I \int_K |\psi_n(x)|^2 dx = \mathrm{Tr}(\hat{E}(I)\hat{F}(K))$$

Since $\mathrm{Tr}(\hat{E}\hat{F}) = \mathrm{Tr}(\hat{F}\hat{E})$:

$$\mathrm{Pr}(\text{Position in } K | \text{Energy in } I) = \mathrm{Pr}(\text{Energy in } I | \text{Position in } K)$$

Von Neumann’s analogue (MB, 44) of Jordan’s postulate B: $\chi(\beta, q) = \varphi(q, \beta)^*$.

Von Neumann's lone reference to canonical transformations

"Our expression for prob. is invariant under canonical transformations. What we mean by a canonical transformation is the following [defines unitary operator $\hat{U}$: $\hat{U}^{-1} = \hat{U}^{\dagger}$] The canonical transf. now consists in replacing every lin. op. $\hat{R}$ by $\hat{U}\hat{R}\hat{U}^{\dagger}$." (MB, 46–47)

Note: $\mathrm{Tr}(\hat{U}\hat{E}\hat{U}^{\dagger}\hat{U}\hat{F}\hat{U}^{\dagger}) = \mathrm{Tr}(\hat{E}\hat{F})$ ($\hat{U}^{\dagger}\hat{U} = \hat{1}$ and cyclic property of the trace).

Note: von Neumann's definition of canonical transformations makes no reference whatsoever to sorting quantities into sets of conjugate variables.

Jordan's response in *Neue Begründung* II: "A formulation that applies to both continuous and discrete quantities in the same way has recently been given by von Neumann … His investigations, however, still need to be supplemented. In particular, a definition of canonically conjugated quantities is missing; moreover, von Neumann did not cover the theory of canonical transformations at any length" (NB II, 2).

Von Neumann's *Probability-theoretic Construction of Quantum Mechanics*

Wahrscheinlichkeitstheoretischer Aufbau der Quantenmechanik.

Von

J. v. Neumann, Berlin.

Vorgelegt von Max Born in der Sitzung vom 11. November 1927.

Einleitung.

I. Die neuere Entwicklung der Quantenmechanik hat bekanntlich zum Entstehen zweier prinzipiell verschiedener Auffassungsweisen ihrer Resultate geführt, die als „Wellentheorie" und „Transformations-" oder „Statistische Theorie" bezeichnet werden. Die letztere ist es, die uns hier haupfsächlich beschäftigen soll.

Die statistische Theorie ist von Born, Pauli und London angebahnt und von Dirac und Jordan zum Abschluß gebracht worden [1]). Sie ermöglicht hauptsächlich die Beantwortung von Fragen folgender Art:

Gegeben ist eine gewisse physikalische Größe in einem bestimmten physikalischen Systeme. Welche Werte kann sie annehmen? Welche sind die a priori Wahrscheinlichkeiten dieser Werte? Wie ändern sich diese Wahrscheinlichkeiten, falls die Werte gewisser anderer (vorher gemessener) Größen angegeben werden?

Von Neumann’s re-introduction of probabilities in *Wahrscheinlichkeitstheoretischer Aufbau*

Goals

- Clarify relation between quantum probability concepts and ordinary probability theory. Look at expectation values of quantities in large ensembles of systems.
- Derive Born rule from a few *seemingly* innocuous assumptions about expectation values and essentials of the Hilbert space formalism

“The method hitherto used in statistical quantum mechanics was essentially *deductive*: the square of the norm of certain expansion coefficients of the wave function or of the wave function itself was *fairly dogmatically* set equal to a probability, and agreement with experience was verified afterwards. A systematic derivation of quantum mechanics from empirical facts or fundamental probability-theoretic assumptions, i.e., an *inductive* justification, was not given” (WA, 246, our emphasis).

Von Neumann's *Wahrscheinlichkeitstheoretischer Aufbau*

System S. Ensemble of copies of system: $\{S_1, S_2, S_3, \ldots\}$

Quantity $\hat{a}$. Expectation value of $\hat{a}$: $\mathbf{E}(\hat{a})$

Assumptions about the function $\mathbf{E}$:

A Linearity: $\mathbf{E}(\alpha\hat{a} + \beta\hat{b} + \ldots) = \alpha\mathbf{E}(\hat{a}) + \beta\mathbf{E}(\hat{b}) + \ldots$

- Footnote. Consider example of one-dimensional harmonic oscillator [von Neumann considers 3D case]. "The three quantities

$$\left[\ \frac{\hat{p}^2}{2m},\ \ \frac{1}{2}m\omega\hat{q}^2,\ \ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega\hat{q}^2\ \right]$$

  have very different spectra: the first two both have a continuous spectrum, the third has a discrete spectrum. Moreover, no two of them can be measured simultaneously. Nevertheless, the sum of the expectation values of the first two equals the expectation value of the third" (WA, 249).

- Same assumption crucial for no-hidden variable proof in von Neumann's 1932 book.

B If $\hat{a}$ never takes on negative values, then $\mathbf{E}(\hat{a}) \geq 0$.

Assumptions about the function $\mathbf{E}$ (cont'd):

"… in conjuction with not very far going material and formal assumptions" (WA, 246)

C Linear assignment of operators $\hat{S}, \hat{T}, \ldots$ on Hilbert space to quantities $\hat{a}, \hat{b}, \ldots$:

If $\hat{S}, \hat{T}, \ldots$ represent quantities $\hat{a}, \hat{b}, \ldots$, then $\alpha\hat{S} + \beta\hat{T} + \ldots$ represents $\alpha\hat{a} + \beta\hat{b} + \ldots$

D If operator $\hat{S}$ represents quantity $\hat{a}$, then $f(\hat{S})$ represents $f(\hat{a})$

Using assumptions (A)–(D), von Neumann shows (modern notation):

$\mathbf{E}(\hat{S}) = \mathrm{Tr}(\hat{\rho}\hat{S})$ with $\hat{\rho}$ a density operator (positive Hermitian operator).

Density operator for pure ("rein") or uniform ("einheitlich") ensemble (WA, Sec. IV)

$$\hat{\rho} = \hat{P}_{\varphi} = |\varphi\rangle\langle\varphi| \quad \text{projection operator onto state } |\varphi\rangle$$

Conclusions (von Neumann's free lunches)

- Pure dispersion-free states (or ensembles) correspond to unit vectors in Hilbert space.

  Essence of von Neumann's later no-hidden variable proof (1932 book, Ch. 4, p. 171).

  Criticized by Bell: questioned linearity assumption $\mathbf{E}(\alpha\hat{a} + \beta\hat{b}) = \alpha\mathbf{E}(\hat{a}) + \beta\mathbf{E}(\hat{b})$.

  John. S. Bell, "On the Problem of Hidden Variables in Quantum Mechanics" *Rev. Mod. Phys*. 38 (1966): 447–452.

  Cf. Guido Bacciagaluppi and Elise Crull, "Heisenberg (and Schrödinger, and Pauli) on hidden variables." *SHPMP* 40 (2009) 374–382.

- The expectation value of a quantity $\hat{a}$ represented by the operator $\hat{S}$ in a uniform ensemble is given by the Born rule: $\mathbf{E}(\hat{S}) = \mathrm{Tr}(\hat{\rho}\hat{S}) = \mathrm{Tr}(|\varphi\rangle\langle\varphi|\hat{S}) = \langle\varphi|\hat{S}|\varphi\rangle$

  Crucial input for this result: inner-product structure of Hilbert space (absent in more general spaces such as Banach spaces).

Specifying states by measuring a complete set of commuting operators

- Knowledge of (the structure of an ensemble for) a given system (specification of a state) is provided by the results of measurements performed on the system (WA, 260).

- Consider the simultaneous measurement of a complete set of commuting operators and construct the density operator for an ensemble in which the corresponding quantities have values in certain intervals.

- Show that such measurements fully determine the state and that the density operator is the one-dimensional projection operator onto the corresponding state vector.

<u>Concrete example</u>: bound states of hydrogen atom.

State uniquely specified:
- principal quantum number n (eigenvalue of $\hat{H}$)
- orbital quantum number l (eigenvalue of $\hat{L}^2$),
- magnetic quantum number m_l (eigenvalue of $\hat{L}_z$)
- spin quantum number m_s (eigenvalue of $\hat{\sigma}_z$)

A single Hermitian operator can be constructed with a non-degenerate spectrum and eigenstates in one-to-one correspondence with the (n, l, m_l, m_s) states (von Neumann shows that this is true in general).

Summary: (Never) mind your *p*'s and *q*'s

Solving problems in quantum mechanics calls for identification of appropriate sets of canonical variables.

$\Pr(\hat{x} = x | \hat{y} = y)$ given by the square of probability amplitudes $\varphi(x, y)$ satisfying certain composition rules.

Probability amplitudes double as integral kernels of canonical transformations which ensures that composition rules hold

Solving problems in quantum mechanics calls for identification of maximal sets of commuting operators.

$\Pr(\hat{x} = x | \hat{y} = y)$ given by the trace of projection operators onto eigenstates of $\hat{x}$ and $\hat{y}$ with eigenvalues x and y.

Trace formula invariant under unitary transformations.

Coda: from quantum statics/kinematics to quantum dynamics

Both Jordan and von Neumann consider conditional probalities

$$\Pr(\hat{A} \text{ value } a \,\big|\, \hat{B} \text{ value } b) \;\; \text{or} \;\; \Pr(\hat{A} \text{ value in interval } I \,\big|\, \hat{B} \text{ value in interval } J).$$

Type of experiment considered: (1) prepare state in which $\hat{B}$ has value b (pure state) or value in interval J (mixed state); (2) measure $\hat{A}$.

In other words, this is all about **quantum statics/kinematics**

What happens to the prepared state after measurement (**quantum dynamics**)?

von Neumann (WA, 271–272, conclusion): "A system left to itself (not bothered by any measurements) has a completely causal time evolution [governed by the Schrödinger equation]. In the face of experiments, however, the statistical character is unavoidable: for every experiment there is a state adapted [*angepaßt*] to it in which the result is uniquely determined (the experiment in fact produces such states if they were not there before); however, for every state there are "non-adapted" measurements, the execution of which demolishes [*zertrümmert*] that state and produces adapted states according to stochastic laws" (first published statement of the measurement problem, paper submitted November 11, 1927).