Von Neumann's work on Hilbert space quantum mechanics

It is mainly through the work of von Neumann that we think today of quantum mechanics as

non-commutative probability theory

This is explained in the lecture by recalling:

- Classical probability theory
- Hilbert space quantum mechanics as non-commutative probability theory
  (Hilbert lattice of projections, quantum states as σ additive measures on Hilbert lattice, Gleason's theorem, linear operators as non-commutative random variables)
- Von Neumann's contribution to the theory

Classical probability theory

$(X, \mathcal{S}, \mu)$	classical measure space
X	set
$\mathcal{S}$	Boolean algebra

$\mu: \mathcal{S} \to \mathbb{R}^+ \cup \infty$	σ-additive measure
	counting measure

$L^1(X, \mu)$	integrable functions
$p_g(A) = \int \chi_A g \mathrm{d}\mu$	probability measure
$g \in L^1(X, \mu)$	given by density function g
	w.r.t. counting measure μ
$(X, \mathcal{S}, p_g)$	probability measure space

Hilbert space Quantum Mechanics

$\|$

non-commutative probability theory

classical probability theory	$\Rightarrow$	quantum probability theory
	replace	
Boolean algebra $\mathcal{S}$	by	Hilbert lattice $\mathcal{P}(\mathcal{H})$
probability measure p	by	quantum state ϕ on $\mathcal{P}(\mathcal{H})$
random variables	by	linear operators
(bounded measurable functions)	by	(bounded linear operators)

$(\mathcal{B}, \vee, \wedge, \perp)$ is a Boolean algebra if it is an orthocomplemented distributive lattice with respect to the lattice operations $\vee$, $\wedge$ and $A \mapsto A^\perp$ orthocomplementation

Distributivity:

$$A \vee (B \wedge C) = (A \vee B) \wedge (A \vee C) \quad \text{for all } A, B, C$$

Stone's Theorem : A Boolean algebra is always isomorphic with a Boolean algebra of subsets of a set X
with respect to the set theoretical operations

$$\begin{aligned} A \wedge B &= \cap B \\ A \vee B &= A \cup B \\ A^\perp &= X \setminus A \end{aligned}$$

Hilbert lattice

$(\mathcal{P}(\mathcal{H}), \vee, \wedge, \perp)$

$\mathcal{P}(\mathcal{H})$ = set of all closed linear subspaces of a Hilbert space $\mathcal{H}$

$||$

$\mathcal{P}(\mathcal{H})$ = set of all projections on a Hilbert space $\mathcal{H}$

Lattice operations $\vee, \wedge, \perp$ defined by:

$$
\begin{aligned}
A \wedge B &= A \cap B \\
A \vee B &= \textit{closure of} \left[(A + B) = \{\xi + \eta : \xi \in A, \eta \in B\} \right] \\
A^{\perp} &= \{\xi \in \mathcal{H} : \langle \xi, \eta \rangle = 0 \ \forall \eta \in A\}
\end{aligned}
$$

Crucial difference between Boolean algebra and Hilbert lattice
(between classical physics and quantum physics):
A Hilbert lattice is not distributive, only orthomodular:
Orthomodularity:

$$If \quad A \leq B \text{ and } A^{\perp} \leq C \quad then \quad A \vee (B \wedge C) = (A \vee B) \wedge (A \vee C)$$

Failure of distributivity

$\Updownarrow$

non commutativity of product of projections

Proposition : If A, B are projections from a distributive sublattice of $\mathcal{P}(\mathcal{H})$ iff AB=BA

Hence the terminology:
non-commutative = non-distributive = non-classical = quantum

Non-commutative probability measures

Definition $\phi\colon \mathcal{P}(\mathcal{H}) \to [0,1]$ is a quantum probability measure (or quantum state) if

(1) $\phi(0) = 0 \qquad \phi(I) = 1$

(2) $\phi(\vee_i A_i) = \sum_i \phi(A_i)$ if $\left[A_i \perp A_j \ (\Leftrightarrow A_i \leq A_j^{\perp}) \ (i \neq j)\right]$

A quantum state is a σ-additive map from $\mathcal{P}(\mathcal{H})$ into $[0,1]$

ϕ is a complete analogue of a classical probability measure

Theorem (Gleason): If ϕ is a quantum state then there exists a positive, trace class operator ρ with $Tr(\rho) = 1$ such that

$$\phi(A) = Tr(\rho A) = \sum_i \langle \xi_i, \rho A \xi_i \rangle \tag{1}$$

and conversely, if ρ is a positive, trace class operator such that

∞ $Tr(\rho) = 1$ then (1) defines a quantum state ϕ

Tr is defined by

$$Tr(Q) = \sum_i \langle \xi_i, Q \xi_i \rangle \qquad \{\xi_i\} \text{ orthonormal basis in } \mathcal{H}$$

ρ is the analogue of the probability density function

Tr is the analogue of the counting measure

Gleason's theorem shows: ϕ can be extended

from projections $\mathcal{P}(\mathcal{H})$ to bounded operators $\mathcal{B}(\mathcal{H})$

Analogy: classical measure can be extended

from characteristic functions to integrable functions

The extension process is called: theory of integration

Conclusion: Gleason's theorem is a theorem in non-commutative integration

Recovering the standard notion of (vector) state as used in physics:

If $\rho = P_\xi$ = projection to $\xi \in \mathcal{H}$ (state vector) then

$$Tr(\rho Q) = \sum_i \langle \xi_i, Q P_\xi \xi_i \rangle = \langle \xi, Q P_\xi \xi \rangle = \langle \xi, Q\xi \rangle$$

$\langle \xi, Q\xi \rangle$ = the usual expectation value of observable Q in state ξ

Linear operators as non-commutative analogues of classical random variables

In the definition of random variable $f: X \to \mathbb{R}$ only the inverse function f^{-1} plays a role:

Definition $f: X \to \mathbb{R}$ is a random variable if $f^{-1}(d) \in \mathcal{S}$ (for all $d \in \mathcal{B}(\mathbb{R})$ = Boolean algebra of Borel sets of $\mathbb{R}$)

A (real valued) random variable f^{-1} is thus a Boolean algebra homomorphism from the Boolean algebra of Borel sets of real numbers into the Boolean algebra $\mathcal{S}$

$$f^{-1}: \mathcal{B}(\mathbb{R}) \to \mathcal{S}$$

The quantum analogue of real valued random variable is the Boolean algebra homomorphism from the Boolean algebra of Borel sets of real numbers into the Hilbert lattice $\mathcal{P}(\mathcal{H})$:

$$Q: \mathcal{B}(\mathbb{R}) \to \mathcal{P}(\mathcal{H})$$

Such a Q is called (understandably) a projection valued measure

Theorem (Spectral Theorem, von Neumann): There is a one-to-one correspondence between selfadjoint linear operators on a Hilbert space $\mathcal{H}$ and projection valued measures

Definition Q is a selfadjoint operator on $\mathcal{H}$ if $Q = Q^*$ (where Q^* is the adjoint of Q)

Definition If Q is densely defined with domain $D(Q)$ then there exists (uniquely) the adjoint Q^* of Q, an operator with domain $D(Q^*)$ such that

$$\langle \xi, Q\eta \rangle = \langle Q^*\xi, \eta \rangle \qquad \xi \in \mathcal{D}(Q^*), \quad \eta \in \mathcal{D}(Q)$$

Definition : Q_2 is an extension of Q_1 if

$$D(Q_1) \subseteq D(Q_2)$$

and

$$Q_1\xi = Q_2\xi \qquad \xi \in D(Q_1)$$

(Notation $Q_1 \subseteq Q_2$)

Definition: Q is symmetric if $Q \subseteq Q^*$

maximal symmetric if it is symmetric and there exists no symmetric operator Q' extending Q

closed if

if $\xi_n \to \xi$ and $Q\xi_n \to \eta$ then

$\xi \in D(Q)$ and $D\xi = \eta$

Proposition: If Q is selfadjoint, then

- its spectrum is a subset of the real numbers
- Q is maximal symmetric (but not conversely!)
- Q is closed

Proposition (Hellinger-Toeplitz Theorem) An everywhere defined closed operator is bounded

Corollary: A selfadjoint unbounded operator is not everywhere defined

All sorts of very tricky mathematical problems emerge if an operator is not everywhere defined – major difficulty in quantum mechanics and occurs frequently because the differential operators are not everywhere defined!

Definition: If Q is a symmetric operator then n^+ and n^- defined below are called the defect indices of T:

$$n^+ = \dim \left[Range(Q + iI) \right]^\perp \tag{2}$$

$$n^- = \dim \left[Range(Q - iI) \right]^\perp \tag{3}$$

Theorem[von Neumann, 1928]:

- A symmetric operator Q is maximal symmetric if and only if one of its defect indices is zero
- Q is selfadjoint if and only if both of its defect indices are zero

There is a very tight formal structural correspondence between concepts in classical probability theory and quantum probability theory, an analogy that goes beyond the correspondence mentioned sofar:

$$
\begin{array}{rcl}
p & \longleftrightarrow & \phi \\
\mu \text{ counting measure} & \longleftrightarrow & Tr \\
\text{probability density} & \longleftrightarrow & \rho \\
\text{random variable} & \longleftrightarrow & Q
\end{array}
$$

The correspondence is summarized in the next 3 slides

Classical probability theory	Quantum probability theory
$(X, \mathcal{S}, \mu)$ classical measure space	$(\mathcal{H}, \mathcal{P}(\mathcal{H}), Tr)$ Hilbert space QM
$\mathcal{S}$ Boolean algebra	$\mathcal{P}(\mathcal{H})$ orthomodular lattice
μ counting measure	Tr functional
$L^1(X, \mu)$ integrable functions	$\mathcal{T}(\mathcal{H})$ trace class operators

$L^\infty(X,\mu)$	$\mathcal{B}(\mathcal{H})$
essentially bounded functions	bounded operators
(bounded) random variables	(bounded) observables
$g \in L^1(X,\mu)$, $g \geq 0$, $\int g \mathrm{d}\mu = 1$	$\rho \in \mathcal{T}(\mathcal{H})$, $\rho \geq 0$, $Tr(\rho) = 1$
probability density	density matrix ((*normal*) state)
$\mathcal{S} \ni A \mapsto p_g(A) = \int \chi_A g \mathrm{d}\mu \in [0,1]$	$\mathcal{P}(\mathcal{H}) \ni A \mapsto Tr(\rho A) \in [0,1]$
$\int gf \mathrm{d}\mu$, $g \in L^1(X,\mu)$	$Tr(\rho A)$, $\rho \in \mathcal{T}(\mathcal{H})$
expectation value of $f \in L^\infty(X,\mu)$	expectation value of $A \in \mathcal{B}(\mathcal{H})$
with respect to p_g	in state ρ

$L^1(X,\mu)$ Banach space	$\mathcal{T}(\mathcal{H})$ Banach space
$\Vert g\Vert_1 = \int \vert g\vert \mathrm{d}\mu$	$\Vert\rho\Vert_{Tr} = Tr(\vert\rho\vert)$
$L^\infty(X,\mu)$ Banach space	$\mathcal{B}(\mathcal{H})$ Banach space
$\Vert f\Vert_\infty = ess.sup.f$	$\Vert A\Vert = sup_{\Vert\xi\Vert\leq 1}\Vert A\xi\Vert$
$L^1(X,\mu)^* = L^\infty(X,\mu)$ duality	$\mathcal{T}(\mathcal{H})^* = \mathcal{B}(\mathcal{H})$ duality
$\phi \in L^1(X,\mu)^*$	$\phi \in \mathcal{T}^*$
$\phi(g) = \int fg\mathrm{d}\mu$	$\phi(\rho) = Tr(\rho A)$
for some $f \in L^\infty(X,\mu)$	for some $A \in \mathcal{B}(\mathcal{H})$
$L^\infty(X,\mu)^* \supset L^1(X,\mu)$	$\mathcal{B}(\mathcal{H})^* \supset \mathcal{T}(\mathcal{H})$
$L^\infty(X,\mu) \ni f \mapsto \int gf\mathrm{d}\mu$, $g \in L_1(X,\mu)$	$\mathcal{B}(\mathcal{H}) \ni A \mapsto Tr(\rho A)$
$\Vert\cdot\Vert_\infty$-cont. functional	$\Vert\cdot\Vert$ (op.norm) cont. functional

Interpretation of classical probability theory + analogy between classical and quantum probability theory suggests the following physical interpretation of the mathematical formalism of Hilbert space quantum mechanics $(\mathcal{H}, \mathcal{P}(\mathcal{H}), \mathcal{B}(\mathcal{H}), \rho)$:

$\mathcal{P}(\mathcal{H})$	set of random quantum events
$\xi \in \mathcal{H}$	state vector ξ describes physical states
	states = probability measures
	represent ensembles
pure state	represents indecomposable ensemble
$\rho \in \mathcal{T}$	representation of general physical state
(mixed state)	(decomposable ensemble)
Q selfadjoint operator	physical quantity (observable)
spectrum of Q	possible values of Q
$Tr(\rho Q)$	expectation value (average) of observable
	in state (ensemble) ρ

Von Neumann's contribution to establishing Hilbert space QM:

- Creating the notion of abstract Hilbert space (generalized from l^2 and L^2)
- Isolating the set of projections as a crucial entity BUT
  – von Neumann never defined orthomodularity explicitly
  – he analyzed lattice theoretic properties of projections only after he had abandoned Hilbert space quantum mechanics (1935-1936) in favor of operator algebraic approach (see later)
  – von Neumann saw conceptual problems with interpreting $\mathcal{P}(\mathcal{H})$ as algebraic structure representing random events (see later)
- Introducing the notion of density operator (first as statistical operator (a not normalized positive operator U), later as trace-one operator)

- Introducing the trace functional as counting measure ("a priori probability")
- Introducing the notion of projection valued measure (Spektralschar)
- Proving Spectral Theorem
- Analyzing unbounded operators, clarifying the difference between selfadjoint, symmetric and maximal symmetric operators

Major works of von Neumann containing his results on the mathematical foundations of quantum mechanics:

References

[1] D. Hilbert, L. Nordheim, J. von Neumann: Über die Grundlagen der Quantenmechanik (1926)
Mathematische Annalen **98** (1927) 1-30

[2] J. von Neumann: Mathematische Begründung der Quantenmechanik
Göttinger Nachrichten (1927) 1-57

[3] J. von Neumann: Wahrscheinlichkeitstheoretischer Aufbau der Quantenmechanik
Göttinger Nachrichten (1927) 245-272

[4] J. von Neumann: Thermodynamik quantenmechanischer Gesamtheiten
Göttinger Nachrichten (1927) 245-272

[5] J. von Neumann: Allgemeine Eigenwertstheorie Hermitescher Funktionalopertoren
Mathematische Annalen **102** (1927) 49-131

[6] J. von Neumann: Die Eindeutigkeit des Schrödingerschen Operatoren
Mathematische Annalen **104** (1931) 570-578

[7] J. von Neumann: *Mathematische Grundlagen der Quantenmechanik* (Dover Publications, New York, 1943) (first American Edition; first edition: Springer Verlag, Heidelberg, 1932; first English translation: Princeton University Press, Princeton, 1955.)

Von Neumann on his book on the mathematical foundations of quantum mechanics:

The subject-matter is partly physical-mathematical, partly, however, a very involved conceptual critique of the logical foundations of various disciplines (theory of probability, thermodynamics, classical mechanics, classical statistical mechanics, quantum mechanics). This philosophical-epistemological discussion has to be continuously tied in and quite critically synchronised with the parallel mathematical-physical discussion. It is, by the way, one of the essential justifications of the book, which gives it a content not covered in other treatises, written by physicists or by mathematicians, on quantum mechanics."

(von Neumann to Cirker, October 3, 1949)

Uniqueness of Schrödinger representation of
Heisenberg's commutation relation :

$$QP - PQ = I \quad \text{(on a dense subset of} \quad \mathcal{H}) \tag{4}$$

Difficulty: Q and P cannot be bounded

$$\Rightarrow$$

All the usual domain problems arise

A specific example of Q, P satisfying (**??**)
is the Schrödinger representation defined by

$$(Qf)(x) = xf(x) \qquad (Pf)(x) = -if'(x) \qquad f \in L^2(\mathbb{R}, \mu) \tag{5}$$

Are there other examples?

First trick in

can be viewed as the infinitesimal form of a commutation relation and, accordingly, it can be reformulated in terms of the one parameter groups U, V of unitary operators determined by Q, P as infinitesimal generators:

$$U(a)V(b) = e^{iab}V(b)U(a) \quad a, b \in \mathbb{R} \tag{6}$$