Quantum Theory in Hilbert Space: a Review

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Contents

To prepare for philosophical aspects of quantum field theory, we begin with a review of mathematical quantum theory, with some interspersed Philosophical Remarks. Apart from these Remarks, the main themes here will be to build up to some intuition for the functional analysis ideas that underpin the algebraic approach, which we will often see applied to quantum field theory. We will also see some high points of quantum theory *per se*, such as Stone's theorem, Gleason's theorem and superselection.

The main books 'in the background' of this review are:
T. Jordan. *Linear Operators for Quantum Mechanics*: Chapters 1 to 5. Wiley 1969; Dover 2006.
E. Prugovecki. *Quantum Mechanics in Hilbert Space*: Parts III, IV. Academic 1981; Dover 2006.

We especially recommend for this review, and for foundations of quantum theory, as a whole:
N. Landsman. Foundations of Quantum Theory. Springer 2017: especially Chapters 5, 6,7,9,10.
Open access: downloadable at: https://link.springer.com/book/10.1007/978-3- 319-51777-3

We also recommend for the early history of mathematical quantum theory, Landsman's recent survey: 'Quantum theory and functional analysis', arxiv: 1911.06630.

1 Vector spaces and linear functionals

1: Vector spaces (over $\mathbb{R}$, or over $\mathbb{C}$). Inner products. For a vector space over $\mathbb{C}$, we write $(z\psi, w\phi) = z^* w(\psi, \phi)$. The Cauchy-Schwarz inequality: $|(\psi, \phi)| \leq ||\psi||.||\phi||$, with equality iff the vectors are linearly dependent.

2: *Hilbert space*:—
The convergence of vectors: $\psi_n \to \psi := ||\psi_n - \psi|| \to 0$ as $n \to \infty$. So infinite linear combinations of vectors are defined on analogy with $\Sigma_{n=1}^{\infty} \omega_n$ with $\omega_n \in \mathbb{C}$. The vector space is *complete* iff every Cauchy sequence converges. A *Hilbert space* is a complete inner product space. It is *separable* iff it has a countable (finite or denumerable) basis.

By the way: One similarly says that a *metric space* (X, d) (i.e. X is a set; $d : X^2 \to \mathbb{R}^+ := \{r \in \mathbb{R} \,|\, r \geq 0\}$ with $d(x, x) = 0, d(x, y) = d(y.x)$ and triangle inequality) is *complete* iff every Cauchy sequence converges. In fact, any metric space has a 'canonical completion'. We define an equivalence relation between Cauchy sequences of X. Roughly speaking: $\{x_n\} \sim \{x'_n\}$ iff $\{x_n\}$ and $\{x'_n\}$ are 'trying to converge to the same point that is trying to be in X'. The set of equivalence classes inherits the metric from (X, d) (I.e. in a representative-independent way); and (X, d) can be isometrically embedded in the set of equivalence classes.
Similarly: given an *incomplete* inner product space (sometimes called a 'pee-Hilbert space'), we can build its 'canonical completion' : which is a Hilbert space.

A subset of a vector space that is itself a vector space (so: closed under linear combination) is a *linear manifold*. A linear manifold that is closed, i.e. that contains the limit vector of every Cauchy sequence of vectors, is a *subspace*. For a finite-dimensional Hilbert space, every linear manifold is a subspace. A subspace of a separable Hilbert space is itself a separable Hilbert space.

Example: $l^2 := \{(x_1, x_2, ...) \mid x_n \in \mathbb{C}, \Sigma |x_n|^2 < \infty\}$ has an orthonormal basis $(1, 0, 0, ...), (0, 1, 0, 0, ...), ... =: \{\phi_n\}$. So each vector is $\Sigma\, x_n \phi_n$. The partial sums are $(x_1, x_2, ..., x_N, 0, 0, 0, ...)$, and these converge to $(x_1, x_2, ..., x_N, x_{N+1}, ...)$.

In general: each vector ψ has a unique expression in terms of an orthonormal basis $\{\phi_n\}$: $\psi = \Sigma\, (\phi_n, \psi)\phi_n$. One uses Schwarz, applied to partial sums, to show this .

Any two Hilbert spaces (over $\mathbb{R}$, or over $\mathbb{C}$) of equal dimension are isomorphic: ("just map one ortho-basis onto another"). So any infinite-dimensional separable Hilbert space can be identified with l^2.

Ortho-complements and projectors: if $\mathcal{M}$ is a subspace of a Hilbert space $\mathcal{H}$, then $\mathcal{M}^\perp := \{\psi \in \mathcal{H} \mid (\psi, \phi) = 0 \ \forall \phi \in \mathcal{H}\}$ is a linear manifold, indeed a subspace of $\mathcal{H}$. Every $\psi \in \mathcal{H}$ has a unique expression as a sum of two components in $\mathcal{M}$ and in $\mathcal{M}^\perp$ respectively: $\psi = \psi_{\mathcal{M}} + \psi_{\mathcal{M}^\perp}$.

3: *Spaces of functions*:—
Treating *spaces of functions* needs care, for two main reasons. We *want to* say: $\int \psi^*(x)\phi(x)\, dx$ is an inner product.
(1): But an inner product requires: $(\psi, \psi) \geq 0$ with equality only if $\psi = 0$. And there are many non-zero functions on, say $[0, 1]$, $\psi : [0, 1] \to \mathbb{C}$, with $\int_0^1 |\psi|^2 dx = 0$.
(2): Secondly, in Riemann (i.e. elementary) integration theory, there are Cauchy sequences that do not converge. Define $f_n : [0, 1] \to \{0, 1\} \subset \mathbb{R}$ by $f_n(x) := 1$ iff x is of the form $\frac{m}{2^{-n}}$, with m an integer between 0 and 2^n; and otherwise $f_n(x) := 0$. Then any two functions $f_n, f_{n'}$ differ at only finitely many points; and for every n, $\int f_n = 0$. But the limit of the sequence $\{f_n\}$ is the function f that takes the value 1 on every integer-multiple of a reciprocal of a power of 2, and is otherwise 0. f is not Riemann-integrable.

Both problems are solved by adopting Lebesque integration. We will not give details of this and the associated measure theory. But we note that the function f just defined (value 1 on every integer-multiple of a reciprocal of a power of 2, and otherwise 0) *is* Lebesque-integrable and $\int_{[0,1]} f dx = 0$: an intuitive result in that f takes value 1 on a 'merely' denumerable set of arguments.

For us, the benefits of adopting Lebesque integration can be summed up, in terms of our two problems: as follows ...

As to (1): We define an equivalence relation between functions on, say $[0,1]$, $\psi : [0,1] \to \mathbb{C}$: $f \sim f'$ iff f and f' are equal *almost everywhere* (a.e.), meaning 'equal everywhere except on a set of (Lebesque) measure 0'. Then the equivalence classes $[f]$ themselves form a vector space, in a natural way. For example, the equivalence class of the pointwise sum $f + g$ of two representative elements, $f \in [f]$ and $g \in [g]$, is independent of the representatives chosen. Besides, the equivalence classes $[f]$ of those functions f, whose square integral $\int |f|^2 dx$ is finite, form an inner product space in a natural way. That is: the inner product we intuitively want to have, viz. $\int f^*(x)g(x)\,dx$ is well-defined on the equivalence classes, since the integral is independent of the representatives f, g that are chosen. Thus returning to the original problem (1): the equivalence class of the zero-function, [0] is the unique vector with norm zero.

As to (2): This inner product space whose elements are equivalence classes (under: almost everywhere equality) of Lebesque-integrable functions f with finite square integral on, say $[0,1]$, i.e. $\int_0^1 |f|^2\,dx < \infty$, is *complete*. That is: it is a Hilbert space. Similarly for square-integrable functions on the whole real line. These spaces are called L^2 spaces. Thus we write, understanding the equivalence relation to be: almost everywhere equality:—

$$L^2([0,1]) := \{[\psi] \mid \psi : [0,1] \to \mathbb{C}, \int_0^1 |\psi|^2\,dx < \infty\} \;\; ; \;\; L^2(\mathbb{R}) := \{[\psi] \mid \psi : \mathbb{R} \to \mathbb{C}, \int_{\mathbb{R}} |\psi|^2\,dx < \infty\} \tag{1}$$

4: *Philosophical Remarks*:—
(A): We of course recognise $L^2(\mathbb{R})$ as the (rigorous version of) the quantum state-space of a spinless non-relativistic particle confined to the real line: the state-space with which we all first learnt wave mechanics. Since the classical configuration space of such a particle is $\mathbb{R}$, we see here the basic idea that the *state-space of a quantum system consists of assignments of complex amplitudes to the possible configurations of the corresponding classical system.* This will later lead to *quantization theory.* A general slogan, and notation, would be: "we replace a classical configuration space $\mathcal{Q}$ by its L^2 space: $L^2(\mathcal{Q})$".

(B): We already see here, in embryo, the *measurement problem*: "how can we extract—how does Nature deliver to us— a single classical fact, e.g. a particle being in a position $X \in \mathbb{R}$, from a function $\psi : \mathbb{R} \to \mathbb{C}$?" ... about which this document (this course?!) will be silent...

(C): Even if one sets aside the physical and philosophical measurement problem, the question arises: *'Why Hilbert space?'* That is: what motivations can be given for assuming the state space of a physical system is a Hilbert space?
Various research traditions make this precise, and offer an answer. Here is a glimpse of three:

(1): *Quantum logic.* This was initiated by Birkhoff and von Neumann in their 'Logic of Quantum Mechanics' (1936), and flourished especially in the 1960s (the Geneva school of J. Jauch) and later. Experimental 'Yes-No' propositions about a physical system are partially ordered by a sort of logical strength, endowed with logical operations of conjunction (and), disjunction (or) and negation (not), subject to certain (judiciously chosen!) conditions, to make them a *lattice*, (usually: an *orthomodular lattice*). This lattice is then shown in a representation theorem to be represented

by the lattice of subspaces/projectors of a Hilbert space, partially ordered by inclusion.

(2): *'Algebras of quantities': C*-algebras.* We have not yet discussed *quantities*. (In Section 2 below, we will review the usual treatment of them as self-adjoint operators on Hilbert space.) So we have not yet seen the quantum-classical contrast as a matter of quantum theory allowing non-commutation of quantities. But a good case can be made for thinking of a system as given primarily by an algebra of quantities: an algebra that is commutative for classical systems, but non-commutative for quantum systems. States are then introduced as mathematical superstructure on top of the algebra of quantities: namely, as linear expectation functionals—details below. The most developed version of this approach uses *C*-algebras*. More details later: here, we just note that in such an algebra, you can multiply any two elements even if they do not commute—an allowance about which you might well raise a philosophical eyebrow ... Then states on C*-algebras are shown to be representable in the traditional i.e. familiar ways—phase space for classical systems, Hilbert space for quantum systems. The buzzword is: *the GNS construction*, applying to commutative, respectively non-commutative, algebras.

(3): *Information-theoretic and operational approaches.* Inspired by studies of quantum non locality and Bell's theorem, and the rise of quantum information theory, with its protocols for eg. teleportation: various approaches take as primitive a set of probability distributions, for various quantities (normally with a finite discrete set of outcomes), on various *individual and joint* systems (normally finite-dimensional). Thus conditions like *no signalling/parameter independence* are prominent. Again, the Hilbert space formalism (normally finite-dimensional) is recovered with appropriate representation theorems. Example: D'Ariano, Chiribella and Perinotti, *Quantum Theory from First Principles*, CUP.

(D): The question 'Why should quantities be represented by self-adjoint operators?' also has a very different aspect or meaning, that is not touched on in the literature under (C). After all, there is nothing to prevent one associated experimental outcomes with complex, e.g. imaginary, numbers: 'I can paint '5i metres' on the dial of an apparatus measuring position!' In Section 2, we will report a helpful classification (due to Roberts) of the possibilities for a quantum physical quantity to be represented by an operator that is *not* self-adjoint.

(E): The pilot-wave theory is a noble tradition for solving the measurement problem. But it has been developed entirely using intuitive wave mechanics, not L^2 spaces.

5: *Linear functionals*:—
Given a vector space V over the field $\mathbb{R}$ or $\mathbb{C}$, the *dual space* V^* consists of the linear functionals $F : V \to \mathbb{R}$ (or $\mathbb{C}$). We recall that for a finite dimensional V, $\dim(V) = \dim(V^*)$; but there is no natural (canonical, i.e. basis-independent) isomorphism between them. But between V and its second dual V^{**}, there is a natural isomorphism.

With the extra structure of an inner product space, there is a natural isomorphism between V and its dual V^*. (This underlies how in relativity theory, the metric raises and lowers indices.) Thus each ψ in an inner product space defines a linear functional F_ψ by:

$$F_\psi(\phi) := (\psi, \phi). \tag{2}$$

And if V is finite-dimensional, with $\{\phi_i\}$ an orthonormal basis: we assign to each $F \in V^*$, the vector $\psi_F := \Sigma_i F(\phi_i)^* \phi_i \in V$. Applying the definition in eq. 2 to this ψ_F yields F again. That is: for any vector $\phi = \Sigma_i (\phi_i, \phi)\phi_i$, we have:

$$F(\phi) = \Sigma_i (\phi_i, \phi) F(\phi_i) = (\psi_F, \phi). \tag{3}$$

To get a corresponding basis-independent correspondence for an infinite-dimensional inner product space, we must require the linear functionals to be *continuous*, defined in the obvious way.

Namely: that F is continuous iff: $\psi_n \to \psi$ implies that $F(\psi_n) \to F(\psi)$. Then we have the *Riesz representation theorem*:—
For every continuous linear functional F on a separable Hilbert space, there is a unique $\psi_F \in \mathcal{H}$, such that $F(\phi) = (\psi_F, \phi)$.

Of course, in Dirac notation the correspondence between linear functionals and vectors induced by the inner product is built in to the notation. The linear functional F_ψ is denoted by $\langle\psi|$, and the two sides of eq. 2 are written as $\langle\psi|\phi\rangle$.

2 Linear operators on a Hilbert space

1: Linear operators and matrices: the elements recalled ... On a suitable space of functions, a linear operator might be defined by

$$(A\psi)(x) := \frac{d\psi(x)}{dx} \quad ; \quad (A\psi)(x) := \int a(x,y)\psi(y)dy \tag{4}$$

We shall generally assume that all Hilbert spaces are separable.

2: *Bounded operators*:—
A linear operator A is *continuous* iff: $\psi_n \to \psi$ implies that $A(\psi_n) \to A(\psi)$. A linear operator A is *bounded* iff there is a positive number b such that for all ψ, $||A\psi|| < b||\psi||$. The infimum of such numbers is the *norm* of A, written $||A||$.

Theorem: A linear operator A is continuous iff it is bounded. (If $\mathcal{H}$ is finite-dimensional, then every linear operator is continuous, and so bounded.)

The norms of linear operators obey:

$$||A+B|| \leq ||A|| + ||B|| \; ; \; ||aA|| = |a|||A|| \; ; \; ||A|| = 0 \text{ iff } A = 0 \; ; \; ||AB|| \leq ||A||.||B|| \; . \tag{5}$$

The first three assertions follow straightforwardly from the same properties of the norm for vectors in $\mathcal{H}$. So we have a normed vector space of linear operators.

A bounded linear operator on a separable Hilbert spaces can be represented by a matrix.

3: *Inverses*:—
A linear operator A has an *inverse* if there is linear operator B with $AB = 1 = BA$. Theorem: A has an inverse iff: $\forall\psi, \exists!\phi$ with $\psi = A\phi$.

For a finite-dimensional $\mathcal{H}$, $\dim(\mathcal{H}) = n$, with $\{\phi_i\}$ any basis:— Each of the following is necessary and sufficient for A to have an inverse:

(i): there is no non-zero vector ϕ such that $A\phi = 0$;
(ii): the set $\{A\phi_1, ..., A\phi_n\}$ is linearly independent;
(iii): there is a linear operator B such that $BA = 1$;
(iv):the matrix corresponding to A has a non-zero determinant.

But for an infinite-dimensional $\mathcal{H}$, (i)-(iii) are not sufficient—even together. For consider the "right-shift" on l^2: $A : l^2 \to l^2$, with $A(x_1, x_2, x_3, ...) := (0, x_1, x_2, x_3, ...)$. Then (i) and (ii) hold. Also: define B as "delete the first component and left-shift": $B(x_1, x_2, x_3, ...) := (x_2, x_3, ...)$; then (iii) holds. But A has no inverse. For if $\psi = (x_1, x_2, x_3, ...)$ with $x_1 \neq 0$ then there is no ϕ such that $\psi = A\phi$.

4: *Unitaries*:—
A linear operator U is *unitary* iff: both (a) U has an inverse and (b) $||U\psi|| = ||\psi||$ for all ψ. (Incidentally: the example of the "right-shift" on l^2, just above, shows that for a infinite-dimensional $\mathcal{H}$, condition (a) is needed.)

Every unitary operator is bounded, with $||U|| = 1$.

Theorem: If U is unitary, then $(U\psi, U\phi) = (\psi, \phi)$ for all ψ, ϕ. Corollary: It follows that the unitary image of an ortho-basis is an ortho-basis.

A "partial converse to the Corollary": If U is bounded, and the U-image of some ortho-basis is an ortho-basis, then U is unitary.

5: *Adjoints and Hermitian operators*:—
Let A be bounded, and so continuous. Then for each $\psi \in \mathcal{H}$, the linear functional $F^{[\psi]}$ defined by

$$F^{[\psi]}(\phi) := (\psi, A\phi) \tag{6}$$

is continuous. And so, by the Riesz theorem (Section 1: 5), there is a unique vector, call it $A^\dagger(\psi)$ such that $F^{[\psi]}(\phi) := (A^\dagger(\psi), \phi)$.

$A^\dagger$ is trivially linear. Using the Schwarz inequality (applied to $||A^\dagger(\psi)||^2 = (\psi, AA^\dagger\psi)$, one has:

Theorem: If A is bounded, then $A^\dagger$ is bounded, and $||A^\dagger|| = ||A||$.

One checks that: $A^{\dagger\dagger} = A$; $(AB)^\dagger = B^\dagger A^\dagger$; $(aA)^\dagger = a^* A^\dagger$; $(A + B)^\dagger = A^\dagger + B^\dagger$.

A *bounded* linear operator A is *self-adjoint* or *Hermitian* iff $A^\dagger = A$. NB: for an infinite-dimensional $\mathcal{H}$, it is impossible to define an unbounded Hermitian operator on all vectors: see later. This means: $(\phi, A\psi) = (A\phi, \psi)$. That is: $(\phi, A\psi) = (\psi, A\phi)^*$. So for all ψ, we have: $(\psi, A\psi) \in \mathbb{R}$.

Example: On $L^2([0,1])$, we define $(A\psi)(x) := x\psi(x)$. This A is bounded with $||A\psi||^2 \leq ||\psi||^2$; and so $||A|| = 1$. And A is Hermitian, since $\int_0^1 \phi^*(x).x\psi(x)\,dx = \int_0^1 [x\phi(x)]^*.\psi(x)\,dx$.
But a "corresponding definition" on $L^2(\mathbb{R})$ is of course not bounded. But multiplying by a suitable "damping factor" gives a bounded and Hermitian operator on $L^2(\mathbb{R})$, e.g. we define $(V\psi)(x) := (\exp|x|)\psi(x)$.

Theorem: If A is bounded, and has a bounded inverse A^{-1}, then $(A^\dagger)^{-1}$ exists and $(A^\dagger)^{-1} = (A^{-1})^\dagger$.
Corollary: If A is bounded and Hermitian, and has a bounded inverse A^{-1}, then A^{-1} is Hermitian.

Hermitian operators are analogues of real numbers. As in: if A is bounded, then its real and imaginary parts defined by

$$\mathrm{Re}A := \frac{1}{2}(A + A^\dagger) \ ; \ \mathrm{Im}A := \frac{-i}{2}(A - A^\dagger) \tag{7}$$

are bounded and Hermitian; and $A = \mathrm{Re}A + \mathrm{Im}A$.

In the same way, unitary operators are analogues of complex numbers of absolute value one. We have:–
Theorem: A linear operator U is unitary iff $U^\dagger U = 1 = UU^\dagger$.

For bounded operators A, B, one readily checks using the adjoints that for any ortho-basis $\{\phi_n\}$, the representing matrix (c_{jk}) of the product $C := AB$ is the product of the representing matrices, that is: $c_{jk} = \Sigma_i a_{ji} b_{ik}$.

6: *Projection operators*:—
Recall from Section 1:2 that if $\mathcal{M}$ is a subspace of $\mathcal{H}$, then $\mathcal{M}^\perp := \{\psi \in \mathcal{H} \mid (\psi, \phi) = 0,\ \forall \phi \in \mathcal{H}\}$ is also a subspace; and every $\psi \in \mathcal{H}$ has a unique expression as a sum of the two components: $\psi = \psi_\mathcal{M} + \psi_{\mathcal{M}^\perp}$. So we define the projection/projector $E_\mathcal{M} : \mathcal{H} \to \mathcal{H}$, by $E_\mathcal{M}(\psi) := \psi_\mathcal{M}$.

Theorem: A bounded linear operator E is a projector iff $E^2 = E = E^\dagger$. (To prove the leftward implication, one defines the set $\mathcal{M}$ to be the range of E, shows it to be a subspace, and shows that for any vector ψ, $(1 - E)(\psi) \in \mathcal{M}^\perp$ etc.)

7: *Unbounded operators*:—
Example: The quantity *position* in the Schrödinger representation (of the canonical commutation relations; cf. later) on $L^2(\mathbb{R})$. We define $(Q\psi)(x) := x\psi(x)$. Then $||Q\psi||^2 \equiv \int_\mathbb{R} |x\psi(x)|^2\, dx$ can be arbitrarily larger than $||\psi||^2 \equiv \int_\mathbb{R} |\psi(x)|^2\, dx$. So Q is unbounded. In fact we have the following ...

Theorem: If a linear operator A is defined for all vectors, and if $(\phi, A\psi) = (A\phi, \psi)$ for all ϕ, ψ, then: A is bounded.

Quantum theory needs unbounded operators A with the algebraic Hermitian property, i.e. $(\phi, A\psi) = (A\phi, \psi)$ for all ϕ, ψ in the domain of A. So it needs operators A with domains of definition less than all of $\mathcal{H}$. Hence the jargon of: *dense domain*, and *extension*, of an operator.

If A has a dense domain, we can define $A^\dagger$. Namely:
$\mathrm{dom}(A^\dagger) := \{\psi \in \mathcal{H} \,|\, \text{there is a vector } \tilde{\psi} \text{ such that } \forall \phi \in \mathrm{dom}(A) : (\phi, \tilde{\psi}) = (A\phi, \psi)\,.\}$
Then we define $A^\dagger$ by $A^\dagger : \psi \in \mathrm{dom}(A^\dagger) \mapsto \tilde{\psi}$. This defines $A^\dagger(\psi)$ uniquely (because $\mathrm{dom}(A)$ is dense); and $A^\dagger$ is linear, and $\mathrm{dom}(A^\dagger)$ is a linear manifold.

We say that a linear operator A is *symmetric* iff: A has a dense domain, and $(\phi, A\psi) = (A\phi, \psi)$ for all ϕ, ψ in the domain of A. Then by the discussion just above, we conclude that: for all ψ in the domain of A, $A^\dagger(\psi)$ is defined, and $A^\dagger(\psi) = A(\psi)$. That is: $A^\dagger$ is an *extension* of A.
If in fact $A^\dagger = A$, then we say A is *self-adjoint* or *Hermitian*.

Example: We define Q on $L^2(\mathbb{R})$ by specifying that $\mathrm{dom}(Q)$: $=$. $\{\psi \mid \int_\mathbb{R} |x\psi(x)|^2\, dx < \infty\}$. This domain is dense. (For we can approximate an arbitrary $\psi \in L^2(\mathbb{R})$ by the "truncated" functions ψ_n ($n \in \mathbb{Z}$) that are defined to be equal to ψ on the interval $[-n, n]$, and to take the value 0 outside that interval. Clearly $\psi_n \to \psi$; and $x\psi_n(x)$ is square-integrable.) Then on this domain, we define: $(Q\psi)(x) := x\psi(x)$. Then Q is clearly symmetric, since $\int_\mathbb{R} \phi^*(x).x\psi(x)\, dx = \int_\mathbb{R} [x\phi(x)]^*.\psi(x)\, dx$. So $Q^\dagger$ is defined and extends Q. But is the domain of $Q^\dagger$ in fact larger than the domain of Q? In fact it is not larger: (cf. Jordan, p.31). So $Q^\dagger = Q$, and so Q is self-adjoint, aka: Hermitian.

A symmetric operator that cannot be extended to a larger domain is called *maximal symmetric*.
Theorem: Every self-adjoint operator is maximal symmetric; (but not conversely)

An unbounded operator cannot be continuous. The "next best thing to continuity" is being *closed*, as follows.
We say an operator A is *closed* iff: if (i) a sequence of vectors ψ_n in $\mathrm{dom}(A)$ converges to a vector ψ and (ii) the sequence of vectors $A(\psi_n)$ converges to a vector ϕ, then $\psi \in \mathrm{dom}(A)$ and $A\psi = \phi$.

Theorem: If $\mathrm{dom}(A)$ is dense, then $A^\dagger$ is closed. So every self-adjoint operator is closed.

It is natural to ask: *'What are the conditions for a symmetric operator to be self-adjoint?'*
As just noted, being maximally symmetric is not sufficient. What about being symmetric and closed? This also turns out to be not sufficient. But in paragraph 4 of the next Section, we will get an answer: an answer that relates to Philosophical Remark (D) in paragraph 4 of Section 1: about the idea that a quantity can be represented by an operator that is *not* self-adjoint.

3 Diagonalizing operators

We assume a complex separable Hilbert space.

1: *Eigenvalues and eigenvectors*:—
The definition of eigenvalue and of eigenvector is exactly the same for an infinite-dimensional Hilbert space, as for the finite-dimensional case. The following elementary but important results are derived exactly as for the finite-dimensional case:

1: If T is a linear operator with an inverse T^{-1}, then A and TAT^{-1} have the same eigenvalues.

2: The eigenvalue of a Hermitian, respectively unitary, operator is real, respectively of absolute value 1.

3: Two eigenvectors of a Hermitian, or of a unitary, operator, corresponding to different eigenvalues are orthogonal.

Let A be Hermitian or unitary. Let $a_1, a_2, ..., a_k, ...$ be its eigenvalues, with eigenspaces $\mathcal{M}_1, \mathcal{M}_2, ..., \mathcal{M}_k, ...$ Then the orthogonal sum $Eig(A) := \oplus_k \mathcal{M}_k$ is the subspace of $\mathcal{H}$ spanned by eigenvectors of A. Of course, for a finite-dimensional complex Hilbert space, $Eig(A) = \mathcal{H}$. This is the *spectral decomposition* or *eigen-decomposition* of the operator A.

We say that a subspace $\mathcal{M} < \mathcal{H}$ *reduces* the linear operator A iff both $\mathcal{M}$ and $\mathcal{M}^\perp$ are invariant under A. This turns out to be equivalent to A commuting with the projector onto $\mathcal{M}$:

Theorem: Let $E_\mathcal{M}$ be the projector onto $\mathcal{M}$. Then $\mathcal{M}$ reduces A iff $E_\mathcal{M} A = A E_\mathcal{M}$ iff $(1-E_\mathcal{M})A = A(1 - E_\mathcal{M})$.

Theorem: Let A be Hermitian or unitary: then $Eig(A)$ reduces A. So a Hermitian or unitary operator splits in to two separate parts: one part acting on $Eig(A)$, and represented there, with respect to an eigenbasis, as a diagonal matrix; the other part acting on $Eig(A)^\perp$.

2: *Eigenvalue decomposition*:—
We will generalise the spectral decomposition of a Hermitian or unitary operator A to the infinite-dimensional case, i.e. address the question of how A acts on $Eig(A)^\perp$. We begin by rewriting in a suggestive way the spectral decomposition of a Hermitian operator A for the finite-dimensional case.

So let A's real eigenvalues be, in ascending order: $a_1 < a_2 < ... < a_k < ... < a_m$, with corresponding eigenspaces $\mathcal{M}_k$. Let I_k be the projector on to $\mathcal{M}_k$. Then the spectral decomposition of A is just

$$A = \Sigma_{k=1}^m \, a_k I_k \equiv \oplus_{k=1}^m \, a_k I_k \tag{8}$$

Now we define for each real number x, $E_x := \oplus_{a_k < x} I_k$. So: $E_x = 0$ for $x < a_1$, and $E_x = 1$ for $x > a_m$. And if $x < y$, then $E_x E_y = E_x = E_y E_x$, i.e. $E_x \leq E_y$.

For each $x \in \mathbb{R}$, we also define $dE_x := E_x - E_{x-\varepsilon}$ with ε chosen so small that there is no a_j such that $x - \varepsilon < a_j, x$.

So dE_x is not zero only when x is an eigenvalue a_k; and in that case $dE_x = I_k$.

So for $\Sigma_{k=1}^m I_k = 1$, we can write: $\int_\mathbb{R} dE_x = 1$. And for $A = \Sigma_{k=1}^m \, a_k I_k$, we can write: $A = \int_\mathbb{R} x \, dE_x$.

Besides: $(\phi, E_x \psi)$ is a complex function of $x \in \mathbb{R}$ that is continuous from the right, but which jumps in value by $(\phi, I_k \psi)$ at $x = a_k$. So we have (a sordinary Riemann integrals):

$$(\phi, \psi) = \int_\mathbb{R} d(\phi, E_x \psi) \;\; ; \;\; (\phi, A\psi) = \int_\mathbb{R} x \, d(\phi, E_x \psi) \, . \tag{9}$$

Similarly, for a unitary operator U in the finite-dimensional case. Its eigenvalues are $u_k \equiv e^{i\theta_k}$, where in ascending order: $0 < \theta_1 < \theta_2 < ... < \theta_k < ... < \theta_m \leq 2\pi$. Then we define for each real

number x, $E_x := \oplus_{\theta_k<x} I_k$. So we can write:

$$U = \int_0^{2\pi} e^{ix} dE_x \;\; ; \;\; (\phi, U\psi) = \int_0^{2\pi} e^{ix}\, d(\phi, E_x\psi)\; . \tag{10}$$

3: *Spectral decomposition:*—
A family of projectors $\{E_x\}_{x\in\mathbb{R}}$ is called a *spectral family* iff:
(i) if $x \leq y$ then $E_x \leq E_y$, i.e. $E_xE_y = E_x = E_yE_x$;
(ii) continuity from the right: for all ψ and for all x: if $\varepsilon > 0$, then $E_{x+\varepsilon}\psi \to E_x\psi$, as $\varepsilon \to 0$;
(iii) for all ψ: $E_x\psi \to 0$ as $x \to -\infty$, and $E_x\psi \to \psi$ as $x \to +\infty$. The main theorem is then...

The Spectral Theorem: For each self-adjoint operator, there is a unique spectral family $\{E_x\}_{x\in\mathbb{R}}$ such that for all $\psi, \phi \in \mathcal{H}$:

$$(\phi, A\psi) = \int_{\mathbb{R}} x\, d(\phi, E_x\psi) \;\; ; \quad \text{so we write} \quad A = \int_{\mathbb{R}} x\, dE_x\, . \tag{11}$$

This obviously generalizes eq. 8. Similarly for unitary operators U, with $E_x = 0$ for $x \leq 0$, and $E_x = 1$ for $x > 2\pi$:

$$(\phi, U\psi) = \int_0^{2\pi} e^{ix}\, d(\phi, E_x\psi) \;\; ; \quad \text{so we write} \quad U = \int_0^{2\pi} e^{ix}\, dE_x\, . \tag{12}$$

Example: "Position" on $L^2([0,1])$. We define E_x on $L^2([0,1])$ as "chopping the function off above x". That is: $(E_x\psi)(y) := \psi(y)$ for $y \leq x$, and $(E_x\psi)(y) := 0$ for $y > x$. Then

$$||E_{x+\varepsilon}\psi - E_x\psi)||^2 = \int_x^{x+\varepsilon} |\psi(y)|^2\, dy \;\to 0, \quad \text{as } \varepsilon \to 0\, . \tag{13}$$

and $\{E_x\}_{x\in\mathbb{R}}$ is a spectral family. Now define A on $L^2([0,1])$ by $(A\psi)(x) := x\psi(x)$. Then A is bounded and self-adjoint. For all $\psi, \phi \in \mathcal{H}$, we have

$$\int_{\mathbb{R}} x\, d(\phi, E_x\psi) = \int_{\mathbb{R}} x\; d \int_0^1 \phi(y)^*(E_x\psi)(y)\, dy = \int_{\mathbb{R}} x\; d \int_0^x \phi(y)^*\psi(y)\, dy = \int_0^1 \phi(x)^* x\psi(x)\, dx = (\psi, A\phi)\, . \tag{14}$$

So $\{E_x\}_{x\in\mathbb{R}}$ gives the spectral decomposition of A.

This $\{E_x\}_{x\in\mathbb{R}}$ is continuous from the left, as well as from the right. We have

$$(\psi, E_x\phi) - (\psi, E_{x-\varepsilon}\phi) \equiv \int_{x-\varepsilon}^{x} \psi^*(y)\phi(y) dy \;\to 0, \quad \text{as } \varepsilon \to 0\, . \tag{15}$$

We say that $\{E_x\}_{x\in\mathbb{R}}$ *jumps in value at* x if for some vector ψ, $(E_x - E_{x-\varepsilon})\psi$ does *not* converge to 0, as $\varepsilon \to 0$. Otherwise, we say that $\{E_x\}_{x\in\mathbb{R}}$ *is continuous* at x.

So in the above example, $\{E_x\}_{x\in\mathbb{R}}$ is continuous at all x, since A has no eigenvalues/eigenvectors. Similarly of course for position on $L^2(\mathbb{R})$.

Theorem: Let A be a self-adjoint operator with spectral decomposition $A = \int_{\mathbb{R}} x\, dE_x$. Then $\{E_x\}_{x\in\mathbb{R}}$ jumps in value at a iff a is an eigenvalue of A. And with I_a the projector onto the eigenspace fo a, we have: $E_xI_a = 0$ for $x < a$; and $E_xI_a = I_a$ for $x \geq a$; and for any ψ, $E_a\psi - E_{a-\varepsilon}\psi \to I_a\psi$, as $\varepsilon \to 0$.

Accordingly, we define:—
(1): the *spectrum* of $A := \mathrm{sp}(A) := \{x \in \mathbb{R} \,|\, E_x \text{ increases}\} \equiv \{x \in \mathbb{R} \,|\, x \notin \text{ interval } (a,b) \text{ on which } E_x \text{ is constant}\}$;

(2): the *point spectrum* of $A := \{x \in R \,|\, E_x \text{ jumps}\} \equiv \{x \in R \,|\, x \text{ is an eigenvalue of } A\}$;
(3): the *continuous spectrum* of $A := \{x \in R \,|\, E_x \text{ increases continuously}\}$.

Theorem:: A self-adjoint operator is bounded iff its spectrum is bounded.

We say that self-adjoint operator A is *positive* iff for all ψ, $(\psi, A\psi) \geq 0$.

Theorem::A self-adjoint operator is positive iff its spectrum is non-negative.

4: *Philosophical remarks*:—
(A): We return to the Philosophical Remark (D) in paragraph 4 of Section 1: the idea that a quantum physical quantity can be represented by an operator that is *not* self-adjoint. Cf. B. Roberts (2018): 'Observables, disassembled', *Studies in History and Philosophy of Modern Physics* **63**, 150– 162. (Preprint: http://philsci-archive.pitt.edu/14449/). On p. 153, Roberts reports that being self-adjoint is a "two out of three" property. That is:
A closed, densely-defined linear operator A is self-adjoint if it satisfies *any two* of the following three properties:

(1): A is *normal*. That is: $AA^\dagger = A^\dagger A$;
(2): A is symmetric: $(\phi, A\psi) = (A\phi, \psi)$ for all ϕ, ψ in the (dense) domain of A.
(3): A has real Spectrum, where we define 'Spectrum' in a more general way than we did 'spectrum' above: namely as the set $\text{Spec}(A) := \{z \in \mathbb{C} \,|\, (A - z.\mathbb{I}) \text{ has no inverse}\}$. So the condition is: $\text{Spec}(A) \subset \mathbb{R}$.

This yields four ways that a closed, densely-defined linear operator A can *fail to be* self-adjoint: having just one of the above three properties, or having none of them. Roberts then explores each of these four ways, finding for each of them: conceptual issues and circumstances in which it is a reasonable notion of physical quantity.

(B): It would be hard to over-emphasise the importance of the spectral theorem, summed up in the second equation of eq. 11: $A = \int_{\mathbb{R}} x \, dE_x$. As we said: this obviously generalizes eq. 8: which is central to the quantum theory using finite dimensional Hilbert spaces. But there are two ways that thinking of the integrand x as position can be misleading. Hence our use of scare quotes around "Position" in Paragraph 3's example on $L^2([0, 1])$.

The first point returns us to (A). It is that because we think of the eigenvalues in the spectral theorem as the possible values of the quantity, as the system's "score" for the quantity: we tend to think that the mathematical fact that x in the spectral theorem, i.e. in eq. 11 for *any* operator, must be real, forces on us the conclusion that "scores" for physical quantities must be real. (This thought is probably reinforced by the facts that (i) the quantum particle on the line is so entrenched as the basic example in wave mechanics, and (ii) a classical particle's position is a real number.)

But that is a *petitio principii*, i.e. it is begging the question. It is only because of choosing a self-adjoint operator that the integrand in the spectral theorem is real. After all: consider the e^{ix} integrand in the spectral theorem for unitaries, i.e. in eq. 12.

The second point is about the way that *space and time apparently get different treatments in quantum theory*. Thus it is often said that in non-relativistic quantum theory: position is a dynamical variable, namely represented by the self-adjoint operator $Q : \psi(x) \mapsto x\psi(x)$ as we have discussed; but that time is not such a variable—indeed, there is no self-adjoint operator representing time. (Indeed, there is a line of argument, originating from Pauli, that there cannot be such an operator.) And people often go on to say that in a relativistic theory, space and time should get similar treatments: which indeed they do, in quantum field theory—namely, by *both* space and time being parameters/indices of the fields, as in $\widehat{\psi}(x, t)$, i.e. *neither* space nor time being operators.

All this folklore is ... true enough as far as it goes. But there are many subtleties hereabouts! Here we just pick out some main points of J. Hilgevoord (2002), 'Time in quantum mechanics', *American Journal of Physics* **70**, 301-306.

He emphasizes that we must of course distinguish:

(a) space and time coordinates, i.e. labels (x, y, z) of spatial points, or (x, y, z, t) of spacetime point-events: which labels can then function as coordinates of point-sized systems or physical events; from:

(b) position as a dynamical variable of a system, especially of a point-particle (subject to equations of motion, whose values determine those of other quantities e.g. energy).

Then Hilgevoord's point is that the (a) vs. (b) contrast is valid in both classical and quantum theory, and in both relativistic and non-relativistic theories. And thus the folklore's emphasis on quantum theory having a position operator *matches* classical physics' having position as a dynamical variable of a point-particle. Since the latter is written as q (especially in Hamiltonian mechanics), and is thus notationally well-distinguished from the spatial coordinate x (or (x, y, z)), Hilgevoord points out (p. 303) that in wave mechanics, a much less confusing notation for the wave function would be $\psi(q)$, rather than the usual (universal! ... and followed herein!) $\psi(x)$ or $\psi(\mathbf{x})$. We can only agree! Recall our first Philosophical Remark (A) in Paragraph 4 of Section 1: that the arguments of the complex-valued wave function are to be classical configurations, i.e. values of the dynamical variables q, not "mere" spatial positions in the (Lucretian!) "void".

Besides, it follows that, contrary to the suggestion of the folklore, some good sense *can* be made of a "time observable", i.e. time as a physical quantity—just like position is in its guise as a dynamical variable. Thus Hilgevoord says (p. 302):

> But do physical systems exist that have a dynamical variable that resembles the time coordinate t in the same way as the position variable q of a point particle resembles the space coordinate x? The answer is yes! Such systems are *clocks*. A clock stands, ideally, in the same simple relation to the universal time coordinate t as a point particle stands to the universal space coordinate x. We may generally define an ideal clock as a physical system describable by a dynamical variable that, under time translations, behaves similarly to the time coordinate t.

For more on *time observables*, cf. B. Roberts (2014),'A general perspective on time observables', *Studies in History and Philosophy of Physics* **47**, 50-54, http://philsci-archive.pitt.edu/10600/. (A large collection of research articles is Muga, G., Sala Mayato, R. and Egusquiza I., ed.s (2008) *Time in Quantum Mechanics*, Springer: two volumes.)

We just make a broad philosophical remark:— Physics—science!—aims to describe, indeed predict, how the values of variables vary as a function of . . . the values of other variables! Thus it is perfectly legitimate, even useful, to ask, for a body that is accelerating what is the position q as a function of the momentum p, i.e. to ask for q *not* as a function of time.

But agreed; it is a deep fact about physics (the world?!) that in classical and quantum physics, and relativistic and non-relativistic physics, and in an Hamiltonian or Lagrangian framework: it is vastly useful and tractable to describe the values of (most, if not all) dynamical variables as a function of . . . a single *external* time. (Here, *external* means, at least: not interacting with the system under investigation.) But as the Hilgevoord quote (and other papers, e.g. by Paul Busch) brings out: this external time need not be some unphysical idealization: it can be a dynamical variable of an appropriate clock system.

And for the *time-energy uncertainty principle*, note that:

(i) a philosopher's introduction is at: J. Butterfield, 'Time in quantum physics', http: //philsci-archive.pitt.edu/9287/;

(ii) a critique of widespread folklore that the principle explains particle creation by temporary violations (and briefer, the larger the violation) of energy conservation (!), is at: B. Roberts and J. Butterfield (2020), 'Time-energy uncertainty does not create particles', http://philsci-archive.pitt.edu/17443/

Finally, there is another aspect of how space and time are treated in quantum theory: the nature of localization—especially the subtleties in relativistic quantum theories: e.g. *Newton-Wigner localization*. We discuss this later, under quantum field theory.

5: *Functions of an Operator*:—
Let A be a self-adjoint operator, with spectral decomposition $A = \int_{\mathbb{R}} x\, dE_x$. Let f be a complex-valued function on the real line: $f : \mathbb{R} \to \mathbb{C}$. We define the operator $f(A)$, by

$$(\phi, f(A)\psi) := \int_{\mathbb{R}} f(x)\, d(\phi, E_x\psi)\ ; \tag{16}$$

which for f continuous can be taken as an ordinary Riemann integral. Then we have:
(1): for $f(x) = x$, $f(A) = A$;
(2): for $f(x) = 1$, $f(A) = 1$, since $\int_{\mathbb{R}} d(\phi, E_x\psi) = (\phi, \psi)$;
(3): $(f + g)(A) = f(A) + g(A)$ and $(cf)(A) = c(f(A))$;
(4): we define $(fg)(x) := f(x)g(x)$, so that $(\phi, (fg)(A)\psi) := \int_{\mathbb{R}} (fg)(x)\, d(\phi, E_x\psi) = \int_{\mathbb{R}} f(x)g(x)\, d(\phi, E_x\psi)$, and then we compute that

$$\int_{\mathbb{R}} f(x)g(x)\, d(\phi, E_x\psi) = \int_{\mathbb{R}} f(x)\, d \int_{-\infty}^{x} g(y)\, d(\phi, E_y\psi) = \int_{\mathbb{R}} f(x)\, d_x \int_{-\infty}^{+\infty} g(y)\, d_y(E_x\phi, E_y\psi) = \tag{17}$$

$$\int_{-\infty}^{+\infty} f(x)\, d(\phi, E_x g(A)\psi) = (\phi, f(A)g(A)\psi)\ . \tag{18}$$

So we conclude that $(fg)(A) = f(A)g(A)$, and thus that functions of the operator A commute with each other.

So (5): polynomial functions are defined in the natural way. If $f(x) = c_0 + c_1x + c_2x^2 + ... + c_nx^n$, then $f(A) = c_0 + c_1A + c_2A^2 + ... + c_nA^n$.

(6) If we define $(f^*)(x) := (f(x))^*$, then we compute that

$$(\phi, [f(A)]^\dagger\psi) = (\psi, f(A)\phi)^* = \int_{-\infty}^{+\infty} f(x)^* d(\psi, E_x\phi)^* = \int_{-\infty}^{+\infty} (f^*)(x) d(\phi, E_x\psi)\ ; \tag{19}$$

so that $[f(A)]^\dagger = (f^*)(A)$. So if f is a real-valued function, $f; \mathbb{R} \to \mathbb{R}$, $f(A)$ is also self-adjoint. And if $f^*f = 1$, then $f(A)$ is a unitary operator since $[f(A)]^\dagger f(A) = 1 = f(A)[f(A)]^\dagger$.

(7): $f(A)$ is positive if $f(x) \geq 0$ on the spectrum of A. For just consider: $(\phi, f(A)\phi) = \int_{-\infty}^{+\infty} f(x) d||E_x\phi||^2$. Similarly, we deduce:
(8): $f(A)$ is bounded if $|f(x)|$ is bounded on the spectrum of A.

6: *Stone's Theorem* :—
Given a self-adjoint operator $H = \int_{-\infty}^{+\infty} x dE_x$, we define for all $t \in \mathbb{R}$: $(\phi, U_t\psi) := \int_{-\infty}^{+\infty} e^{itx} d(\phi, Ex\psi)$. Then U_t is an operators, viz. $U_t = e^{itH}$ and U_t is unitary since $(e^{itx})^*.e^{itx} = 1$ (cf. the end of (6) above). Evidently, $U_0 = 1$; and since $e^{itx}e^{it'x} = e^{i(t+t')x}$, we have $U_tU_{t'} = U_{t+t'}$. The converse of this is...

Stone's Theorem: Suppose that for all $t \in \mathbb{R}$, U_t is a unitary operator, such that:
(i): for all vectors ϕ, ψ: $(\phi, U_t\psi)$ is a continuous function of t
(ii): $U_0 = 1$ and $U_tU_{t'} = U_{t+t'}$: so the family $\{U_t\}_{t\in\mathbb{R}}$ is a *unitary representation* of the group $(\mathbb{R}, +)$.

Then: there is a unique a self-adjoint operator H such that $U_t = e^{itH}$ for all $t \in \mathbb{R}$, and

(1): the domain of H is $\{\psi \in \mathcal{H} \mid \frac{1}{it}(U_t - 1)\psi$ converges as $t \to 0\}$; and then the limit vector is $H\psi$;

(2): if a bounded operator commutes with all of the U_t, then it commutes with H.

Using (1), we infer: If $U_t\psi \in \mathrm{dom}(H)$, then: $\frac{1}{i\Delta t}(U_{\Delta t} - 1)U_t\psi) \ \to \ HU_t\psi$, as $\Delta t \to 0$. That is:

$$\frac{1}{i\Delta t}(U_{t+\Delta t} - U_t)\psi \ \to \ HU_t\psi \,, \ \text{as } \Delta t \to 0 \tag{20}$$

which we write as the "Schrödinger equation":

$$-\, i\frac{d}{dt}(U_t\psi) = HU_t\psi \,. \tag{21}$$

7: *Functions of commuting operators*:—

Theorem: Let A be self-adjoint with spectral decomposition $A = \int x dE_x$; and let B be bounded, self-adjoint and $AB = BA$. Then $BE_x = E_x B$.

Proof: If A has pure point spectrum, $A = \Sigma_k \, a_k I_k$, the proof is elementary. If A is unbounded, one needs a more careful statement to deal with issues about domains. Indeed: if two self-adjoint operators A_1, A_2 are both unbounded, then we take $E^1_x E^2_y = E^2_y E^1_x$ for all $x, y \in \mathbb{R}$ to be the *definition* of $[A_1, A_2] = 0$.

Given $f : \mathbb{R}^2 \to \mathbb{C}, (x, y) \mapsto f(x, y)$, we define $f(A_1, A_2)$ for two commuting self-adjoint operators A_1, A_2 by

$$(\phi, f(A_1, A_2)\psi) = \int_{\mathbb{R}} \int_{\mathbb{R}} f(x, y) \, d_x d_y (\phi, E^1_x E^2_y \psi) \ , \quad \text{for all} \quad \phi, \psi \in \mathcal{H} \,. \tag{22}$$

Sums, scalar multiples, and products of such functions are defined in the obvious way. One shows that:

$[f(A_1, A_2)]^\dagger = (f^*)fA_1, A_2)$; so that real functions f define self-adjoint operators $f(A_1, A_2)$ and functions f for which $f^* f = 1$ define unitary operators $f(A_1, A_2)$;

$f(A_1, A_2)$ is positive if $f(x, y) > 0$ on the cartesian product of the spectra of A_1 and A_2 ;

$f(A_1, A_2)$ is bounded if $f(x, y)$ is bounded on the cartesian product of the spectra of A_1 and A_2.

Compare items (5) to (8) at the end of Paragraph 5 above.

Example: the Schrödinger representation of position in $\mathbb{R}^3$. Consider $L^2(\mathbb{R}^3) \ni \psi(\mathbf{x}) \equiv \psi(x_1, x_2, x_3)$; with inner product $(\phi, \psi) = \int_{\mathbb{R}^3} \phi^*(\mathbf{x})\psi(\mathbf{x}) \, d\mathbf{x}$. For $r = 1, 2, 3$, we define the self-adjoint operator Q_r by $Q_r\psi(\mathbf{x}) = x_r\psi(\mathbf{x})$. Then in the spectral decomposition

$$Q_r = \int_{\mathbb{R}} x \, dE^r_x \tag{23}$$

the projectors E^r_x are defined by :$(E^r_x\psi)(\mathbf{y}) = \psi(\mathbf{y})$ for $\mathbf{y}$ with $y_r \leq x$, and $(E^r_x\psi)(\mathbf{y}) = 0$ for $\mathbf{y}$ with $y_r > x$. Then one has

$$(f(Q_1, Q_2, Q_3)\psi)(\mathbf{x}) \ = \ f(x_1, x_2, x_3)\psi(\mathbf{x}) \ . \tag{24}$$

8: *Complete sets of commuting operators* :—

Let $A_1, A_2, ..., A_N$ be mutually commuting self-adjoint operators with pure point spectra; each with their spectral decomposition, $r = 1, 2, ..., N$

$$A_r = \Sigma_k \, a^{(r)}_k I^{(r)}_k \,. \tag{25}$$

Then for all r, s and $j.k$, we have: $I_k^{(r)} I_j^{(s)} = I_j^{(s)} I_k^{(r)}$. And for any $j, k, ...l$, the product $I_j^{(1)} I_k^{(2)} ... I_l^{(N)}$ is a projector. Namely, the projector onto the subspace of simultaneous eigenvectors with corresponding eigenvalues, i.e. the space of vectors ψ with $A_1\psi = a_j^{(1)}\psi$, $A_2\psi = a_k^{(2)}\psi, ..., A_N\psi = a_l^{(N)}\psi$. Some of these projectors may be zero: corresponding to combinations of eigenvalues that are not, in philosophical jargon!, *co-possible* or *compossible*.

These subspaces are orthogonal, i.e.

$$I_j^{(1)} I_k^{(2)} ... I_l^{(N)} I_{j'}^{(1)} I_{k'}^{(2)} ... I_{l'}^{(N)} = \delta_{jj'}\delta_{kk'}...\delta_{ll'}\, I_j^{(1)} I_k^{(2)} ... I_l^{(N)} \tag{26}$$

and complete, i.e.

$$\Sigma_j \, \Sigma_k \, ... \Sigma_l \; I_j^{(1)} I_k^{(2)} ... I_l^{(N)} = 1 \, . \tag{27}$$

If none of these projects onto a subspace of dimension larger than one, we say that $\{A_1, A_2, ..., A_N\}$ is a *complete set* of commuting operators. Then choosing eigenvectors of length one, and labelling them with their eigenvalues, i.e. choosing an *orthonormal eigenbasis*, we can write in Dirac notation:

$$I_j^{(1)} I_k^{(2)} ... I_l^{(N)} \; = \; |a_j^{(1)} a_k^{(2)} ... a_l^{(N)}\rangle\langle a_j^{(1)} a_k^{(2)} ... a_l^{(N)}| \tag{28}$$

Theorem: Let $A_1, A_2, ..., A_N$ be mutually commuting self-adjoint operators with pure point spectra. This is a complete set iff: every bounded operator B that commutes with all the $A_1, A_2, ..., A_N$ is a function of them: $B = f(A_1, A_2, ..., A_N)$.

The orthonormal eigenbasis $\{|a_j^{(1)} a_k^{(2)} ... a_l^{(N)}\rangle\}$ gives a *spectral representation* of $A_1, A_2, ..., A_N$ and of the functions $f(A_1, A_2, ..., A_N)$ as diagonal matrices:

$$\langle \, a_j^{(1)} a_k^{(2)} ... a_l^{(N)} \, | \, f(A_1, A_2, ..., A_N)\psi \, \rangle = f(a_j^{(1)} a_k^{(2)} ... a_l^{(N)}) \, \langle \, a_j^{(1)} a_k^{(2)} ... a_l^{(N)} \, | \, \psi \, \rangle \, . \tag{29}$$

9: *Philosophical Remarks*:—
The selection of a self-adjoint operator with pure point spectrum, and so of a complete family of orthogonal eigenspaces, is at the heart of not just

(i) the mathematics; but also:
(ii) the physics; and
(iii) the interpretation/philosophy

of quantum theory. Besides, the main issues are already clear in the case of finite dimensional Hilbert spaces. (Indeed, they are clear for real Hilbert spaces: for which, of course, 'self-adjoint' is replaced by 'symmetric' in the sense of elementary matrix theory, i.e. the matrix elements a_{ij} obey: $a_{ij} = a_{ji}$. Of course, this is not the sense we defined above!)

As to (i), the mathematics: we here note just:
Recall Philosophical Remark (C) (1), about quantum logic, in Paragraph 4 of Section 1. That is: the lattice $\mathcal{L}$ of projectors (equivalently: subspaces) of Hilbert space. Selecting a complete family of orthogonal eigenspaces, $\{E_i\}$ say, amounts to picking a sublattice of L: one that is *Boolean*. More precisely: a complete family of orthogonal eigenspaces (equivalently: projectors) is the set of atoms (smallest, logically strongest, least-in-the-partial-order—but non-zero—elements) of a Boolean sublattice of $\mathcal{L}$. The other elements of the sublattice are given by all the possible sums (orthogonal sums, $\oplus$) of these atoms. Roughly speaking: 'Boolean' means that the distributive laws, of intersection $\cap$ over $+$, and vice versa, hold. That is with E, F, G being three subspaces, $E, F, G < \mathcal{H}$, the laws are:

$$E \cap (F + G) = (E \cap F) + (E \cap G) \; ; \;\; \text{and} \;\; E + (F \cap G) = (E + F) \cap (E + G) \tag{30}$$

These equations are easily proved for E, F, G mutually orthogonal (as are the atoms); cf. elementary projector algebra. But they also hold for the various possible sums of atoms. And they are very easily

disproved for E, F, G 'skew'. Just take three mutually skew rays in the Euclidean plane $\mathcal{H} = \mathbb{R}^2$. Then the first equation of eq. 30 would read: $E = 0$, and the equation of eq. 30 would read: $E = \mathcal{H}$. Both of which are false.

We say that *roughly speaking* 'Boolean' means that the distributive laws hold: because we are here neglecting conditions about the behaviour of the complement, i.e. the unary operation on subspaces, $E \mapsto E^{\perp}$, or equivalently for projectors, $E \mapsto 1 - E$.

Three final remarks about this lattice-theoretic perspective:

(1): Since a function f is in general many-one, i.e. two arguments can map to the same value, a self-adjoint operator B being a function of another A, i.e. $B = f(A)$, means that the sublattice of $\mathcal{L}$ that is defined, as sketched above, by B (with B's eigenspaces as its atoms) will be a sublattice of the sublattice defined by A. In short: *coarse-graining*.

Note also that B can be a function of two operators A, C that do *not* commute: i.e. . $B = f(A) = g(C)$ with $[A, C] \neq 0$. This point will be crucial in the discussion of FUNC and of 'no go' theorems against 'hidden variable' supplementations of orthodox quantum theory, that we discuss under interpretation/philosophy below. For it means that imposing conditions on the assignment of values to the operator B (and perhaps some other operator with which B commutes) can have consequences for the values of operators A and C that do *not* commute.

(2): Later, when we discuss states i.e. probability distributions for the values of quantities (and so for the values 1 and 0 for projectors), this Booleanness of the sub-lattice will secure there being a classical (Kolmogorov) probability space for the distribution to be defined on.

(3): When we consider the algebraic approach to quantum theory, Booleanness of a lattice will correspond to the abelianness of the algebra of quantities. The rough picture, here stated only for bounded operators, is:

(3A): Although the elements of an algebra 'go beyond' projectors, by including also self-adjoint operators (indeed, arbitrary real linear combinations of projectors: which can then be spectrally resolved), and then also skew-adjoint operators, the projectors are the building blocks of the algebra; and so the abelianness of the algebra is caught by the mutual commutation of the projectors.

(3B): The commutation of projectors $[E, F] = 0$ is equivalent to a neat lattice-theoretic expression of their ranges (1-eigenspaces). If we now write E, F for the ranges, it is (using $\oplus$ to signal that the summands are orthogonal):

$$E = (E \cap F) \oplus (E \cap F^{\perp}) \; ; \quad \text{and} \quad F = (E \cap F) \oplus (E^{\perp} \cap F) \; . \tag{31}$$

As to (ii), the physics: we note:
The selection of such an operator can be interpreted as choosing to measure the quantity it represents, i.e. choosing an experimental context. And the non-commutation of two operators represents it being impossible to measure them both simultaneously with arbitrary accuracy. *Recall Bohr on mutually exclusive experimental contexts!* Cf. e.g. his essay in P.A. Schilpp ed. *Albert Einstein: Philosopher-Scientist*

Later, after we introduce states, we will make simultaneous measurability more rigorous. As we will see: this can be done *without* committing us to a version of the Projection Postulate or a similar "collapse of the wave-packet". For the moment, we just note that for a finite dimensional (indeed real or complex) Hilbert space, it is natural to define:

(the quantities represented by) two self-adjoint operators A and B are *co-measurable*
along the following lines:

'a measurement of one quantity does not disturb a pre-existing value of the other quantity'.
And it is natural to make 'pre-existing value' more precise in terms of an outcome/result ("pointer-reading") from an immediately preceding measurement process. That is: we imagine a measurement

of A yields some outcome/eigenvalue a; then an immediately succeeding measurement B yields some outcome/eigenvalue b; and then an immediately succeeding *second* measurement A is done and yields some outcome/eigenvalue a'. In this scenario with its three successive acts of measurement, it is natural to define:

'measuring B does not disturb the measurement of A'

as follows:

'Whatever are the outcomes/eigenvalues a, b of the first two measurements (and whatever probabilities our theory may ascribe to them), the third measurement (i.e. the final = second measurement A) is bound/certain to give the same outcome/eigenvalue as the first one did: $a' = a$'.

So let us say that A and B are *co-measurable* iff: measuring B does not disturb the measurement of A in this operational sense, *and vice versa*; that is: also, measuring A does not disturb the measurement of B (i.e. in an obvious notation, we must have: $b' = b$).

Then it is easy to connect this definition of co-measurability to *commutation of operators* for finite dimensional Hilbert space, *if* we also say that measurement processes are described by the elementary Projection Postulate, i.e. the postulate that a measurement of the system, in any state (vector) ψ, for the quantity represented by A

(i) projects the system's state instantaneously into the eigenspace of the eigenvalue obtained as the measurement's outcome; and then of course

(ii) re-normalizes the state by dividing it by its own length.

Thus, the Projection Postulate says there is an instantaneous state transition, which is, in a notation adapted from the above discussion:

$$\psi \mapsto \frac{E^A_a \psi}{||E^A_a \psi||} \tag{32}$$

The connection, for finite dimensional Hilbert space, of the above definition of co-measurability, understood with this Projection Postulate, to commutation of operators is the readily proved equivalence:

Theorem: Two self-adjoint operators, with pure point spectra $A = \Sigma\, a_j E^A_j$ and $B = \Sigma\, b_k E^B_k$ are co-measurable in this sense iff they commute, i.e. $[A, B] = 0$. (Of course, this latter condition is equivalent to all pairs of spectral projectors sommuting: i.e. $[E^A_j, E^B_k] = 0$, for all j, k.)

As to (iii), the interpretation/philosophy: we note:

The orthodox view in the quantum textbooks (a kind of 'precipitate' of Bohr, Dirac, Heisenberg, von Neumann; 'Copenhagen') is of course that a quantum system in state ψ only has values for those physical quantities of which ψ is an eigenstate/eigenvector (the value being the corresponding eigenvalue). (These quantities are sometimes called ψ's *eigenquantities*.)

In particular, the lack of common eigenstates for non-commuting quantities like position and momentum (suppressing here their having continuous spectra...) means that no system has a value for both position and momentum. Thus we are faced with the measurement problem, i.e. the appalling possibility that this lack of values, though it seems acceptable in the atomic realm which is after all unvisualizable etc etc, could propagate to the macro-realm—and so conflict with the supreme success of classical physics' ascription to systems of values for both position and momentum. (Cf. Schrödinger's amazing 'cat' paper of 1935!) . . .

So it is natural to propose that we supplement the orthodox quantum state: we are to ascribe values beyond the orthodox eigenvalues. The natural hope is that there are states that ascribe to every self-adjoint operator an element of its spectrum, subject to natural conditions. What natural conditions? The obvious one (sometimes called 'FUNC') is that if A is ascribed a value a, then $f(A)$ is ascribed the value $f(a)$. (After all, we often envisage measuring $f(A)$ by measuring A and

applying f to the outcome.) But even if we consider only operators with pure point spectrum on a finite dimensional Hilbert space, there are problems.

That is: there are *'no-go' theorems* that such an assignment, for all the self-adjoint operators, satisfying FUNC for them all, is *impossible*. Indeed, it is provably impossible even for some judiciously—the aspiring solver of the measurement problem might say: 'unfortunately!'—chosen *finite* sets of projectors on all Hilbert spaces of (complex) dimension 3 or more (i.e. $\mathbb{C}^3, \mathbb{C}^4, \ldots$).

These theorems are mostly associated with the names of Gleason (a theorem of 1957), and Kochen and Specker (a joint paper of 1967). But beware: what is usually called 'Gleason's theorem' is a *positive* result. It is a representation theorem for probability distributions on the set of all subspaces (projectors) of a Hilbert space. We will state it later, when we discuss states rigorously. The no-go theorem is a *corollary* to this positive result.

The history has various ironies: one might say, sadnesses. For:

First: One can prove this corollary directly. And J S Bell did so in his paper, 'The problem of hidden variables in quantum mechanics', published in *Reviews of Modern Physics*, in 1966. This paper was written in 1963: *before* Bell proved the Bell inequalities—which he did, and published, in 1965. (The publication delay was due to the typescript being lost in the back of a filing cabinet at the offices of *Reviews of Modern Physics*!) And the 1966 paper was written as a *defence* of the programme of supplementing the orthodox quantum state, not as an argument against it. For Bell proved the corollary, i.e. no-go theorem, as part of an analysis urging that the assumptions of it were *eminently deniable*.

Second: Indeed, he pointed out in his 1966 paper that the assumptions are denied by the pilot-wave theory: which he considered tenable, indeed *eminently reasonable*, despite having a manifest non-locality in its guidance equation for a bipartite system. That is, in the traditional and best-developed non-relativistic version of the theory: the deterministic spatial trajectory of one part of such a system (one point-particle, according to the pilot-wave theory) is sensitive to where in space the other point-particle is: instantaneously sensitive, in the manner of action-at-a-distance, though without any fall-off with distance as one has in Newtonian gravitation.

Third: In fact, Bell's 1966 paper ends by making this point: that the pilot-wave theory is manifestly non-local. He also there stresses that, of course, Bohm in 1952 was well aware of this non-locality; and he ends by raising the question whether any supplementation of quantum theory must be in some way non-local. (A footnote added in proof then mentions his previously published 1965 paper as having answered this question, for one notion of non-locality. Not so much a case of backwards causation *a la* science fiction, but merely a disordered filing cabinet ...)

Fourth: Gleason's *positive* theorem—the representation theorem for probability distributions on the set of all subspaces (projectors) of a Hilbert space—generalizes a theorem of von Neumann, in his 1932 book. Historically, this latter theorem was very influential in persuading physicists between ca 1932 and ca 1966 that this sort of supplementation of quantum theory could not work. It is standardly called von Neumann's 'no hidden variables theorem'.

Here again, Bell's 1966 paper is gold. For it articulates the Achilles heel of von Neumann's theorem. Namely: von Neumann assumes that, whatever the advocate of hidden variables envisages as a state, they should accept that states ascribe expectations to self-adjoint operators, subject to the following linearity condition. Namely: a state ascribes as the expectation $\mathrm{Exp}(A+B)$ of the sum of self-adjoint operators A, B, the sum of their individual expectations. So $\mathrm{Exp}(A + B) = \mathrm{Exp}(A) + \mathrm{Exp}(B)$.

Bell points out that any advocate of hidden variables, i.e. of postulated dispersion-free states (i.e. states ascribing values to all quantities) can, indeed should!, deny this condition. In a judo-like manoeuvre ('use your opponent's momentum to defeat them!'), Bell invokes the Bohrian idea that if A and B do not commute, and so cannot be measured together, one cannot measure $A + B$ by measuring both A and B and adding the outcomes. So although $A + B$ is self-adjoint, and

can in general be measured, doing so will require some other experimental arrangement, different from both that for A and that for B. Agreed: *quantum states*—whether vector states as discussed so far, or density matrices, to be discussed later—*do* obey this linearity condition, even if A and B do not commute. But, says Bell, that is a peculiarity of the quantum formalism, and by no means a compulsory feature of states as ascriptions of expectation values. (Cf 1966, Section III, p. 449, column 1. Incidentally, Einstein pointed out the same Achilles heel to Bargmann in conversation in the 1940s ...)

Beware: the entire algebraic approach to quantum theory will blithely endorse von Neumann's assumption. As we say in England: 'swallow it, hook line and sinker' . . . We will return to this irony . . .

Fifth: Finally, there is a further irony in relation to the first one above, about Bell's 1966 paper proving the relevant corollary of Gleason's positive theorem. This final irony is that the main drift of the Kochen-Specker paper of the following year (1967) is also to prove this corollary. This paper is rightly lauded. Its merits include: . . .

(a) It connects the corollary to the quantum logic, lattice-theory, approach sketched above. The non-Boolean lattice of projectors with its delicately interlaced Boolean sub-lattices, is treated in a kindred manner to differential geometry's treatment of a manifold with its delicately interlaced charts. In particular, the operations, like taking the sum of two projectors, are *partial*. They are restricted to the summands being both in some Boolean sub-lattice. Thus the buzzword: *partial Boolean algebra*. . . .

(b) It exhibits a specific finite set of projectors to which the values 1 and 0 cannot be assigned without violating the (apparently natural) assumptions like FUNC, above. It even relates these projectors to a specific quantum system (orthohelium). . . .

(c) It is mathematically elegant and has engendered an enormous literature, pursuing e.g. the physical idea of 'contextuality', and mathematical fields like topos theory ...
But the Kochen-Specker paper falls in the quantum logic tradition. It does not discuss, as Bell does, that the apparently natural assumptions are in fact deniable . . .

10: *Complete (sets of commuting) operators, with continuous spectra* :—
For operators $A_1, A_2, ..., A_N$ with *continuous* spectra, the *definition* of a complete set is given by the condition in the Theorem at the end of Paragraph 8, above: viz. that every bounded operator B that commutes with all the $A_1, A_2, ..., A_N$ is a function of them: $B = f(A_1, A_2, ..., A_N)$. In fact, the Schrödinger representation of position is, by itself, a complete set. That is: if on $L^2(\mathbb{R})$, we define the self-adjoint operator Q by $(Q\psi)(x) = x\psi(x)$, then:

Theorem: every bounded operator B that commutes with Q is a function of Q.

We briefly connect with the Dirac notation which brings out the analogy with a complete set of commuting operators, with pure point spectra. Thus we write:

$$\langle\, x \,|\, \psi \,\rangle = \psi(x) \;\text{ and }\; \langle\, x \,|\, Q\psi \,\rangle = x\langle\, x \,|\, \psi \,\rangle \;\text{ and }\; \langle\, x \,|\, f(Q)\psi \,\rangle = f(x)\langle\, x \,|\, \psi \,\rangle \,. \tag{33}$$

Of course, Q has no eigenvectors. (For if $x\psi(x) = a\psi(x)$, then $\psi(x) = 0$ for $x \neq a$, and so: $||\psi||^2 = 0$.) But we use delta functions, so that writing

$$a\delta(x–a) = x\delta(x–a) \tag{34}$$

"justifies" our writing

$$Q|\, a \,\rangle = a|\, a \,\rangle \;\text{ and }\; \langle\, a \,|\, \psi \,\rangle = \psi(a) = \int_{\mathbb{R}} \delta(x–a)\psi(x)\, dx \,. \tag{35}$$

And similarly

$$\psi(x) = \int_{\mathbb{R}} \psi(a)\delta(x–a)\, da \;\text{ "justifies" }\; |\, \psi \,\rangle = \int_{\mathbb{R}} \langle\, a \,|\, \psi \,\rangle |\, a \,\rangle\, da \,; \tag{36}$$

so that any vector ψ can be "thought of" as a linear combination of delta-functions Thus delta-functions are like an orthonormal basis of eigenfunctions.

We similarly use delta-functions to express operators, especially their spectral resolutions. Thus for each $a \in \mathbb{R}$, let us define the 'dyad' $|\,a\,\rangle\langle\,a\,|$ by its action

$$(\,|\,a\,\rangle\langle\,a\,|\,\psi\,)(x) := \psi(a)\delta(x–a) \quad \text{i.e.} \quad (|\,a\,\rangle\langle\,a\,|)\,\psi := \langle\,a\,|\,\psi\,\rangle|\,a\,\rangle\,. \tag{37}$$

Then with E_x in the spectral family for Q, we can write for all ψ: $(E_x\psi)(y) \equiv \int_{-\infty}^{x} \psi(a)\delta(y–a)\,da = \int_{-\infty}^{x} (|\,a\,\rangle\langle\,a\,|\,\psi)(y)\,da$. So we can write

$$E_x = \int_{-\infty}^{x} |\,a\,\rangle\langle\,a\,|\,da \;\text{ ; and similarly }\; Q \equiv \int_{\mathbb{R}} x\,dE_x = \int_{\mathbb{R}} x\,|\,x\,\rangle\langle\,x\,|\,dx\,. \tag{38}$$

In the same way, the three operators Q_r on $L^2(\mathbb{R}^3) \ni \psi(\mathbf{x}) \equiv \psi(x_1, x_2, x_3)$, defined at the end of Paragraph 7 by $(Q_r\psi)(\mathbf{x}) = x_r\psi(\mathbf{x})$ are a complete set of commuting operators, with pure continuous spectra. On analogy with eq. 33 to 38, writing $\mathbf{Q} := (Q_1, Q_2, Q_3)$, we write:

$$\langle\,\mathbf{x}\,|\,\psi\,\rangle = \psi(\mathbf{x}) \;\text{ and }\; \langle\,\mathbf{x}\,|\,\mathbf{Q}\psi\,\rangle = \mathbf{x}\langle\,\mathbf{x}\,|\,\psi\,\rangle \;\text{ and }\; \langle\,\mathbf{x}\,|\,\mathbf{f}(\mathbf{Q})\psi\,\rangle = \mathbf{f}(\mathbf{x})\langle\,\mathbf{x}\,|\,\psi\,\rangle\,. \tag{39}$$

The operators Q have no eigenvectors. But we again use delta functions, and write $|\,\mathbf{a}\,\rangle$ for $\delta(\mathbf{x}–\mathbf{a})$; so that writing

$$\mathbf{a}\delta(\mathbf{x}–\mathbf{a}) = \mathbf{x}\delta(\mathbf{x}–\mathbf{a}) \tag{40}$$

"justifies" our writing

$$Q|\,\mathbf{a}\,\rangle = \mathbf{a}|\,\mathbf{a}\,\rangle \;\text{ and }\; \langle\,\mathbf{a}\,|\,\psi\,\rangle = \psi(\mathbf{a}) = \int_{\mathbb{R}} \delta(\mathbf{x}–\mathbf{a})\psi(\mathbf{x})\,\mathbf{dx}\,. \tag{41}$$

And similarly

$$\psi(x) = \int_{\mathbb{R}} \psi(\mathbf{a})\delta(\mathbf{x}–\mathbf{a})\,\mathbf{da} \;\text{ "justifies" }\; |\,\psi\,\rangle = \int_{\mathbb{R}} \langle\,\mathbf{a}\,|\,\psi\,\rangle|\,\mathbf{a}\,\rangle\,\mathbf{da}\,; \tag{42}$$

so that any vector ψ can be "thought of" as a linear combination of delta-functions Thus delta-functions are like an orthonormal basis of eigenfunctions.

We similarly use delta-functions to express operators. So we write

$$E_x^{(r)} = \int_{a_r \le x} |\,\mathbf{a}\,\rangle\langle\,\mathbf{a}\,|\,d\mathbf{a} \;\text{ ; and similarly }\; \mathbf{Q} = \int_{\mathbb{R}^3} \mathbf{x}\,|\,\mathbf{x}\,\rangle\langle\,\mathbf{x}\,|\,d\mathbf{x}\,. \tag{43}$$

11: *Fourier transforms, and the spectral representation of* $i\vec{\nabla}$:—

11.A: **Basics**:— We again consider $L^2(\mathbb{R}^3) \ni \psi(\mathbf{x}) \equiv \psi(x_1, x_2, x_3)$; with inner product $(\phi, \psi) = \int_{\mathbb{R}^3} \phi^*(\mathbf{x})\psi(\mathbf{x})\,d\mathbf{x}$. For $r = 1, 2, 3$, we define the operator P_r by

$$(P_r\psi)(\mathbf{x}) := -i\frac{\partial}{\partial x_r}\psi(\mathbf{x})\,; \;\text{ or, writing } \mathbf{P} := (P_1, P_2, P_3) :\; (\mathbf{P}\psi)(\mathbf{x}) := -i\nabla\psi)(\mathbf{x})\,. \tag{44}$$

These operators P_r are self-adjoint. For they have the symmetric property $(\phi, P_r\psi) = (P_r\phi, \psi)$ (integration by parts), and they have dense domain, so that $P_r^\dagger$ is defined; and one can show that $P_r^\dagger = P_r$; cf. Paragraph 7 of Section 2.

The spectral representation of these operators is given by Fourier transforms of the spectral representation of the operators Q_r, $(Q_r\psi)(\mathbf{x}) = x_r\psi(\mathbf{x})$, discussed at the end of Paragraph 10. The main theorem is:

Theorem: For any $\psi(\mathbf{x}) \in L^2(\mathbb{R}^3)$, the sequence of vectors χ_n, $n \in \mathbb{Z}$, defined by

$$\chi_n(\mathbf{k}) := (2\pi)^{-\frac{3}{2}} \int_{-n}^{n} dx_1 \int_{-n}^{n} dx_2 \int_{-n}^{n} dx_3 \ \exp(-i\mathbf{k}\cdot\mathbf{x})\,\psi(\mathbf{x}) \tag{45}$$

converges to a limit vector $F\psi$ such that $||F\psi||^2 = ||\psi||^2$. $F\psi$ is the *Fourier transform* of ψ. Besides, the sequence of vectors

$$\psi_n(\mathbf{x}) := (2\pi)^{-\frac{3}{2}} \int_{-n}^{n} dk_1 \int_{-n}^{n} dk_2 \int_{-n}^{n} dk_3 \ \exp(i\mathbf{k}\cdot\mathbf{x})\,(F\psi)(\mathbf{k}) \tag{46}$$

converges to ψ.

A vector ψ is in the domain of P_r iff $k_r(F\psi)(\mathbf{k})$ is square-integrable: in which case (cf. integration by parts with boundary term vanishing)

$$(FP_r\psi)(\mathbf{k}) = k_r(F\psi)(\mathbf{k}) \tag{47}$$

Accordingly, we write

$$(F\psi)(\mathbf{k}) = (2\pi)^{-\frac{3}{2}} \int \exp(-i\mathbf{k}\cdot\mathbf{x})\,\psi(\mathbf{x})\ d\mathbf{x} \tag{48}$$

and

$$\psi(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int \exp(i\mathbf{k}\cdot\mathbf{x})\,(F\psi)(\mathbf{k})\ d\mathbf{k}\,. \tag{49}$$

Since F preserves norm and has an inverse, it is *unitary*, and so preserves inner products; cf. Paragraph 4 of Section 2. So we have

$$\int (F\phi)(\mathbf{k})^*(F\psi)(\mathbf{k})\ d\mathbf{k} \ = \ \int \phi(\mathbf{x})^*\psi(\mathbf{x})\ d\mathbf{x}\,. \tag{50}$$

We write the inverse of F as

$$(F^{-1}\phi)(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int \exp(i\mathbf{k}\cdot\mathbf{x})\,\phi(\mathbf{k})\ d\mathbf{k}\ ;\ \text{i.e. as:}\ \ (F^{-1}\phi)(\mathbf{x}) = (F\phi)(-\mathbf{x})\ . \tag{51}$$

Eq. 61 implies that

$$(P_r\psi)(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int k_r \exp(i\mathbf{k}\cdot\mathbf{x})\,(F\psi)(\mathbf{k})\ d\mathbf{k}\ ; \tag{52}$$

and that in three dimensions

$$-i\nabla(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int \mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{x})\,(F\psi)(\mathbf{k})\ d\mathbf{k}\,. \tag{53}$$

Writing $(Q_r\psi)(\mathbf{x}) = x_r\psi(\mathbf{x})$, eq. 47 then implies

$$FP_r = Q_rF\ ;\ \text{i.e.:}\ \ \mathbf{P} = F^{-1}\mathbf{Q}F\,. \tag{54}$$

This now implies how to express the spectral decomposition of P_r in terms of that of $Q_r = \int x\, dE_x^{(r)}$; as follows. One checks that $\{F^{-1}E_x^{(r)}F\}$ is a spectral family, because F is unitary and $\{E_x^{(r)}\}$ is a spectral family, Then using $F^{-1} = F^\dagger$, we compute:

$$(\phi, P_r\psi) = (\phi, F^\dagger Q_r F\psi) = (F\phi, Q_rF\psi) = \int x\, d(F\phi, E_x^{(r)}F\psi) = \int x\, d(\phi, F^{-1}E_x^{(r)}F\psi)\ . \tag{55}$$

So the spectral decomposition of P_r is:

$$P_r = \int x \, dF^{-1} E_x^{(r)} F \, . \tag{56}$$

11.B: **Completeness**:— We can now repeat for momentum, $\mathbf{P} := (P_1, P_2, P_3)$, the discussion of complete commuting operators and their functions, that we had for position $\mathbf{Q} := (Q_1, Q_2, Q_3)$. Cf. the end of Paragraph 7 (especially eq. 22 to 24), and the end of Paragraph 10 (especially eq. 39 to 43).

Thus we recall eq. 22's definition of a function $f(A_1, A_2)$ of two commuting operators A_1, A_2 in terms of inner products $(\phi, E_x^{(1)} E_y^{(2)} \psi)$. Thus functions of the three two commuting operators P_1, P_2, P_3 are defined by integrals with respect to inner products

$$(\phi, \, (F^{-1} E_x^{(1)} F . F^{-1} E_y^{(2)} F . F^{-1} E_z^{(3)} F) \, \psi) = (F\phi, E_x^{(1)} E_y^{(2)} E_z^{(3)} F \psi) \, . \tag{57}$$

So for any function $f; \mathbb{R}^3 \to \mathbb{C}$, the operator $f(\mathbf{P}) = f(P_1, P_2, P_3)$ is determined by inner products:

$$(\phi, \, (f(\mathbf{P})) \, \psi) = \int \int \int f(x, y, z) dx dy dz (F\phi, E_x^{(1)} E_y^{(2)} E_z^{(3)} F\psi) \equiv (F\phi, \, f(Q_1, Q_2, Q_3) \, F\psi) = (\phi, \, F^{-1} f(\mathbf{Q}) F \, \psi) \tag{58}$$

So

$$f(\mathbf{P}) = F^{-1} f(\mathbf{Q}) F \, . \tag{59}$$

Comparing this with eq.s 47 and 61 respectively, we deduce:

$$(F f(\mathbf{P}) \psi)(\mathbf{k}) = f(\mathbf{k}) (F\psi)(\mathbf{k}) \tag{60}$$

and

$$(f(\mathbf{P})\psi)(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int f(\mathbf{k}) \, \exp(i\mathbf{k} \cdot \mathbf{x}) \, (F\psi)(\mathbf{k}) \, d\mathbf{k} \, . \tag{61}$$

We can also repeat for momentum, $\mathbf{P}$, the discussion in Paragraph 10 (especially the beginning) that position illustrates the result that a bounded operator that commutes with a complete set of operators is a function of them. Thus since Q_1, Q_2, Q_3 is a complete set of operators, so is P_1, P_2, P_3. For if B is a bounded operator that commutes with the three operators $\mathbf{P}$, then FBF^{-1} is a bounded operator that commutes with the three operators $F\mathbf{P}F^{-1} = \mathbf{Q}$. So there is a function f of three variables such that $FBF^{-1} = f(\mathbf{Q})$. And so, eq. 59 implies:

$$B = F^{-1} f(\mathbf{Q}) F = f(\mathbf{P}) \, . \tag{62}$$

Philosophical Remark:— This last paragraph is a template for the later discussions (especially in the algebraic approach) of *unitary equivalence*: i.e. the idea that a single unitary operator U "carries" each operator A in an algebra of operators $\mathcal{A} \ni A$ to an element of another algebra: $UAU \in \mathcal{A}' := U\mathcal{A}U$. Later, it will be important that for a quantum system with infinitely many degrees of freedom, i.e. a quantum field or a quantum statistical mechanical system in the limit of infinitely many components (e.g. an infinite lattice), one can need—in order to describe the various possible physical behaviours of the system—unitarily *inequivalent* algebras. (But in a certain precise sense: a finite system does not need unitarily inequivalent algebras.)

11.C: **Delta functions etc.**:— **Yet to do...**

4 Operator algebras

1: *Irreducible sets of operators, and Schur's Lemma*:—
We recall from Paragraph 1 of Section 3 that a subspace $\mathcal{M} < \mathcal{H}$ *reduces* the linear operator A iff both $\mathcal{M}$ and $\mathcal{M}^\perp$ are invariant under A; and this is equivalent to A commuting with the projector $E_\mathcal{M}$ onto $\mathcal{M}$.

Thus we say that a set of operators is *reducible* if there is a proper subspace, i.e. a subspace other than the zero subspace or all of $\mathcal{H}$, that reduces every operator in the set; otherwise the set is *irreducible*. So $\mathcal{M}$ reduces a set of operators iff $\mathcal{M}$ and $\mathcal{M}^\perp$ are *invariant* under every operator in the set. We also say that a set of operators is *symmetric* if it is closed under taking adjoints. It is easy to prove:

Theorem: If $\mathcal{M}$ is invariant under a symmetric set of operators, then $\mathcal{M}$ reduces the set. That is: $\mathcal{M}^\perp$ is also invariant.

Theorem: *Schur's Lemma*: A symmetric set of bounded or Hermitian operators is irreducible iff: multiples of the identity $c\mathbb{1}$ are the only bounded operators that commute with all operators in the set.

Proof sketch:
(1): The leftward implication follows from the theorem just cited from Paragraph 1 of Section 3: One proves the contrapositive, as follows: if $\mathcal{M}$ reduces the set, then $E_\mathcal{M}$ commutes with every element of it, and so by assumption is a multiple of the identity.
(2): The rightward implication uses previous work straightforwardly, by considering the cases of (a) a projector, (b) a bounded Hermitian operator and (c) a bounded non-Hermitian operator; as follows.

(a): Any projector E commuting with every element of the set is onto a subspace that reduces the set. Since the set is irreducible, E is a multiple of the identity, so $E = \mathbb{1}$ or $E = \mathbb{0}$.

(b): If B is a bounded Hermitian operator commuting with every element of the set, then a short argument shows that every spectral projector E_x of B commutes with every element of the set. So $E_x = \mathbb{1}$ or $E_x = \mathbb{0}$. That is: there is some real number $b \in \mathbb{R}$, such that $E_x = \mathbb{0}$ for $x < b$, and $E_x = \mathbb{1}$ for $x \geq b$. So for any vectors ϕ, ψ

$$(\phi, B\psi) = \int_\mathbb{R} x\, d(\phi, E_x\psi) = b(\phi, \psi) = (\phi, b\psi)\ ; \tag{63}$$

so $B\psi = b\psi$ for all ψ. So $B = b\mathbb{1}$.

(c): If B is a bounded non-Hermitian operator commuting with every element A of the set, then since the set is symmetric i.e. closed under taking adjoints, B commutes with $A^\dagger$, i.e. $BA^\dagger = A^\dagger B$. Taking the adjoint: $AB^\dagger = B^\dagger A$. That is: $B^\dagger$ commutes with every element A of the set. Therefore, so do Re B and Im B: since they are bounded Hermitian operators, part (b) implies that they are multiples of the identity. Therefore, $B \equiv \text{Re } B + i\ \text{Im } B$ is also a multiple of the identity.

2: *Functions of non-commuting operators; von Neumann algebras*:—
A set of bounded operators is called a *symmetric ring* or *symmetric algebra* or **-algebra* iff it is closed under: scalar multiplication, addition, product (i.e. composition of operators, even if they do not commute) and taking adjoints. An obvious example is: all the bounded functions of a set of commuting Hermitian operators. Any such example is of course commutative/abelian, i.e. the product is commutative.

Our governing question is now: *Given a set of non-commuting Hermitian operators, which bounded operators should be considered functions of them?*
We certainly want: all operators we can get by scalar multiplication, addition and product, starting from bounded functions of each individual Hermitian operator. This gives a symmetric ring of

bounded operators, each of them a polynomial of bounded functions of the individual Hermitian operator.

But it is natural to include some sort of limit. For reasons we shall see shortly, the natural notion is *weak limit*. We say that a bounded operator B is the *weak limit* of a set of bounded operators iff: $\forall \psi_1, \ldots, \psi_n, \forall \phi_1, \ldots, \phi_n, \forall n \in \mathbb{N}, \forall \varepsilon > 0:$ there is A in the set such that

$$\forall k = 1, ..., n \quad |(\phi_k, A\psi_k) - (\phi_k, B\psi_k)| < \varepsilon : \tag{64}$$

Thus the idea is: any finite collection of matrix-elements of B can be approximated arbitrarily well by an element A of the set.

Hence we define the *weak closure* of a set of bounded operators; and such a set being *weakly closed*. And we say that any weakly closed, symmetric ring of bounded operators is a *von Neumann algebra*, also known as a *W*-algebra*.

The reason that admitting weak limits of operators is natural lies in how it gives a generalization to non-commuting operators of the following theorem for commuting ones. (This theorem should be compared with the Theorem in Paragraph 8 of Section 3 that: a set of commuting Hermitian operators, all with pure point spectra, is complete iff every bounded operator commuting with all of them is a function of them.)

Theorem: A bounded operator B is a function of the commuting Hermitian operators $A_1, \ldots, A_n$ iff: B commutes with every bounded operator that commutes with $A_1, \ldots, A_n$.

We define the *commutant* S' of a set S of operators to be the set of bounded operators that commute with all of S. Similarly S'' is the *double commutant*. So this theorem says: A bounded operator B is a function of the commuting Hermitian operators $A_1, \ldots, A_n$ iff $B \in \{A_1, \ldots, A_n\}''$.

Von Neumann's *double commutant* theorem generalizes this to the non-commuting case—by taking weak limits; as follows.

Theorem: Given a set S of Hermitian operators, the double commutant S'' is a von Neumann algebra. It is the weak closure of the symmetric ring of polynomials generated by bounded functions of each element of S.

S'' is called the von Neumann algebra *generated* by S. It is the smallest von Neumann algebra containing S.

Combining this theorem with Schur's lemma, we get:
If S is a symmetric set of bounded or Hermitian operators, and is irreducible, then $S' = \{c\mathbb{1} : c \in \mathbb{C}\}$. And so $S'' = \mathcal{B}(\mathcal{H}) :=$ the set of all bounded operators on $\mathcal{H}$.

Example: $\{\mathbf{Q}, \mathbf{P}\}$ is an irreducible set of Hermitian operators on $L^2(\mathbb{R}^3)$. So $\{\mathbf{Q}, \mathbf{P}\}'' = \mathcal{B}(L^2(\mathbb{R}^3))$.

The introduction of weak limits prompts a brief review of rival operator topologies, explained in terms of their associated notion of convergence.

3: *Operator topologies*:—
We begin with the uniform operator topology. It is relatively *fine*, aka: *strong*. That is: convergence in the uniform operator topology is a logically strong condition. So NB: requiring closure in it is a relatively *weak* condition.

- *Uniform convergence.* $\{A_n\}$ converges to A in $\mathcal{H}$'s uniform operator topology iff $||A_n - A|| \to 0$ as $n \to \infty$; i.e. iff $\sup_{(\psi|,\psi)=1} |(A_n - A)\psi| \to 0$ as $n \to \infty$.
- *Strong convergence.* $\{A_n\}$ converges to A in $\mathcal{H}$'s strong operator topology iff, for all $\psi \in \mathcal{H}$:

$(A_n - A)\psi \to 0$ as $n \to \infty$.

- *Weak convergence.* $\{A_n\}$ converges to A in $\mathcal{H}$'s weak operator topology iff, for all $\psi, \phi \in \mathcal{H}$: $(\phi, (A_n - A)\psi) \to 0$ as $n \to \infty$.

Strong and weak convergence are forms of *pointwise*, "vector by vector", convergence. Generally: uniform entails strong, which entails weak convergence. But *not* conversely; as the next two examples show.

Example of strong, but not uniform, convergence:
Let $\{\phi_k\}$ be an orthobasis and E_n the projector onto the subspace spanned by $\{\phi_1, ..., \phi_n\}$. Then the sequence $\{E_n\}$ converges to the identity strongly but not uniformly. For $\{E_n\}$ is a *Cauchy sequence* in the strong topology. That is: $\forall\psi, \forall\varepsilon, \exists N, \forall n > m > N : ||(E_n - E_m)\psi|| < \varepsilon$. That is: for each fixed ψ, the component on ψ in $\mathrm{ran}(E_n)^\perp$ tends to zero.

But not uniformly! Clearly $||E_n - E_m|| = 1$ for $n \neq m$.

Example of weak, but not strong, convergence:
Let $\{\phi_k\}$ be an orthobasis and let $A_n : \mathcal{H} \to \mathcal{H}$ be the "n-shift": $A_n(\phi_k) := \phi_{k+n}$. Then the sequence $\{A_n\}$ converges weakly to zero, but not strongly.

But if $\dim(\mathcal{H}) < \infty$, then all three topologies (notions of convergence) are equivalent.

5 States

We recall the Philosophical Remarks in Paragraph 9 of Section 3, stressing the classical vs. quantum contrast, essentially as a matter of commutative vs. non-commutative algebras (in particular: commutative vs. non-commutative projectors/subspaces). This contrast will have echoes for our notion of a state. A bit more precisely: quantum states will "look classical" (to a large extent...but not totally!) when one considers their restrictions to commutative sub-algebras of the total algebra of quantities.

1: *Density matrices and traces*:—
A *density matrix* ρ (also often written W) is a positive self-adjoint operator such that if $\{\psi_k\}$ is an orthobasis, then $\Sigma_k(\psi_k, \rho\psi_k) = 1$.

Theorem: A density matrix ρ has a pure point spectrum, and so can be written in Dirac notation as $\rho = \Sigma_k\, w_k\, |\psi_k\rangle\langle\psi_k|$ with $w_k \geq 0$ and $\Sigma_k\, w_k = 1$.

Theorem: If ρ is a density matrix, B is bounded and $\{\psi_k\}, \{\phi_j\}$ are two orthobases, then the four series: $\Sigma_k\,(\psi_k, \rho B\psi_k)$, $\Sigma_k\,(\phi_k, \rho B\phi_k)$, $\Sigma_k\,(\psi_k, B\rho\psi_k)$, $\Sigma_k\,(\phi_k, B\rho B\phi_k)$: are all absolute convergent and equal.

Hence we define the *trace* of ρB by $\mathrm{Tr}(\rho B) := \Sigma_k\,(\psi_k, \rho B\psi_k)$, independent of the choice of orthobasis; and similarly for $\mathrm{Tr}(B\rho)$. The case $B = \mathbb{1}$ then gives $\mathrm{Tr}(\rho) = 1$. In fact: a positive self-adjoint operator ρ is a density matrix iff it has an orthobasis of eigenvectors $\{\psi_k\}$ and $\Sigma_k\,(\psi_k, \rho\psi_k) = 1$.

If ρ is a density matrix with an orthobasis of eigenvectors $\{\psi_k\}$, then: $\mathrm{Tr}(\rho B) = \Sigma_k\, w_k\,(\psi_k, B\psi_k)$.

From this last, we note:

(a): See Paragraph 2 below, for the obvious physical interpretation in terms of "ignorance" or a "mixed beam" of systems with proportion w_k in the state ψ_k.

(b): If B is self-adjoint, then $\mathrm{Tr}(\rho B)$ is real.

(c): If B is self-adjoint and positive, then $\mathrm{Tr}(\rho B) \geq 0$.

(d): If the projectors E_k are mutually orthogonal so that $\Sigma_k\, E_k$ is a projector, then: $\mathrm{Tr}(\rho(\Sigma_k\, E_k))$

$= \Sigma_k \ \mathrm{Tr}(\rho E_k)$. Intuitively, this is a "additivity of probability for exclusive alternatives": it is a natural generalization of classical measure theory on *Boolean algebras*.This *countable additivity on mutually orthogonal projectors* will later, in Paragraph 4, be the sole main assumption of *Gleason's representation theorem for states*.

(e): The linearity of Trace implies that: for all complex numbers $c \in \mathbb{C}$: $\mathrm{Tr}(\rho.cB) = \mathrm{c\ Tr}(\rho B)$; and fo all bounded operators A, B, $\mathrm{Tr}(A + B) = \mathrm{Tr}(A) + \mathrm{Tr}(B)$.

Philosophical Remark:— Notice that the linearity in (e) applies even when A, B do not commute. This linearity is what you expect of "averaging", and as we will see in Paragraph 2, the trace will provide average/expectation values of quantities. But: when A, B do not commute, and so cannot be co-measured, this sort of linearity is not an *a priori* requirement. Recall the last part, viz. (iii), of the Philosophical Remarks in Paragraph 9 of Section 3: about Bell's 1966 critique of von Neumann—and indeed Gleason ...

2: *Density matrices for the intuitive, 'ignorance-interpretation' of a mixture—and for the Projection Postulate*:
This Paragraph uses Dirac notation ... If the system is not known to be in state $|\psi\rangle$, but only known to be one of the states, $|\psi_i\rangle$, with respective probabilities w_i (with $\Sigma_i w_i = 1$): then the statistics for any quantity will of course be given by the w_i-weighted average of the elementary Born-rule probabilities prescribed by the various $|\psi_i\rangle$.

Think of a beam of systems, prepared by "a ham-fisted lab assistant" who cannot prepare all particles in the beam in the very same state $|\psi\rangle$. This situation is well represented by (i) to (iii):—

(i) Thinking of the state as the real linear combination, with weights w_i, of the projectors $|\psi_i\rangle \ \langle\psi_i|$; i.e. the state is $\rho := \Sigma_i \ w_i \ |\psi_i\rangle \ \langle\psi_i|$. This is a real linear combination of projectors, and so is self-adjoint.

(ii) NB: The $|\psi_i\rangle$ need not be orthogonal; nor need they be eigenstates of a given quantity, or even of some preferred handful of quantities you have in mind. Nevertheless, ρ is a self-adjoint and trace 1 operator. Being self-adjoint, it has a spectral decomposition: which will in general *not* be the form in which we have introduced it, viz. as corresponding to the different possibilities for what is in the individual case, the familiar (vector) state

(iii) Extracting the statistics by a trace formula. If E^q is the spectral projector of the measured quantity, Q say, for eigenvalue q, then the probability of getting q for a measurement of Q on a system (think: randomly selected member of a beam) in state $\rho := \Sigma_i \ w_i \ |\psi_i\rangle \ \langle\psi_i|$ is: $\mathrm{Tr}(E^q.\rho)$. This is equal to $\Sigma_i \ \ w_i \ ||E^q(|\psi_i\rangle)||^2$. That is: the w_i-weighted average of the elementary Born-rule probabilities. And with the usual correspondence between probabilities of individual results and expectations, the linearity of trace, applied to the spectral projection of $Q = \Sigma_a \ q_a E^{q_a}$, implies: the expected/average value of Q is

$$\Sigma_a \ q_a \mathrm{Tr}(E^{q_a}.\rho) \equiv \mathrm{Tr}[\Sigma_a \ q_a \ (E^{q_a}.\rho)] \equiv \mathrm{Tr}[Q.\rho] \tag{65}$$

(iv) Jargon: Any self-adjoint and trace 1 operator is called a *statistical operator*, or (especially when represented as a matrix!), a *density matrix*. The familiar (vector) state $|\psi\rangle$ is equally well represented as the special case of a density matrix: i.e. one-dimensional projector. For indeed: $||E^q(|\psi\rangle)||^2 = \mathrm{Tr}(E^q.|\psi\rangle \ \langle\psi|)$.

(v) This is the usual, intuitive, 'ignorance-interpretable' idea of a *mixture*. It is usual, for *any* probabilistic theory, to think of forming heterogeneous ensembles ("mixed beams"); so that a beam that mixes states α_i in proportions w_i (with $\Sigma_i w_i = 1$) is represented by the mixed state $\Sigma_i w_i \alpha_i$. Think: any convex combination of probability distributions is itself a probability distribution. More Jargon: A state that cannot be thus expressed except in the degenerate sense, i.e. some $w_i = 1$ and the rest are zero, is called *pure*. Otherwise a state/ensemble/beam is *mixed* or a *mixture*.

(vi) There are very similar ideas in the mixed states of classical statistical mechanics (i.e.

non-Dirac probability distributions on phase space). Indeed: it is in quantum statistical mechanics that most people first meet the density matrix. For the elementary equilibrium state (Gibbs state) for a system with Hamiltonian H, at inverse temperature $\beta := 1/kT$ is: $\rho := \frac{1}{Z}\exp(-\beta H)$, where $\frac{1}{Z}$ is the normalization factor, $Z := \mathrm{Tr}[\exp(-\beta H)]$. (Of course, differentiating this Z reveals much physics!). And this is indeed a statistical operator! For $\exp(-\beta H)$ is self-adjoint (since a real function of a self-adjoint operator!), and the $\frac{1}{Z}$ implies the trace is 1.

(vii) The density matrix idea also represents neatly the *projection postulate*: i.e. the orthodox idea that on measurement, there is a *'collapse of the wave packet'*. The idea is that the initial superposition of eigenstates of the measured quantity Q, say $|\psi\rangle := \Sigma_i c_i|\psi_i\rangle$ collapses, if the individual case of the measurement yields the ith eigenvalue, to: that eigenstate lying in the eigenspace corresponding to the eigenvalue obtained, that is closest to the initial state $|\psi\rangle$.

It is easiest to express this for *maximal* i.e. *non-degenerate* quantities. Then: if the individual measurement yields the ith eigenvalue, $|\psi\rangle := \Sigma_i c_i|\psi_i\rangle$ collapses to the (unique: up to a phase) eigenstate $|\psi_i\rangle$; and of course (so as to vindicate the elementary Born rule!) does so with a probability $||c_i||^2$. (NB: idea of irreducible indeterminism!)

So the representation of the *non-selective* measurement ("keep all the bins/channels"; "don't look at the result!") is: the pure state $|\psi\rangle := \Sigma_i c_i|\psi_i\rangle$ transits to a (intuitive, 'ignorance-interpretable') mixture $\rho := \Sigma_i ||c_i||^2 |\psi_i\rangle\,\langle\psi_i|$. One might write:

$$\text{Pure state } |\psi\rangle := \Sigma_i\ c_i|\psi_i\rangle \quad \mapsto \quad \text{mixed state } \Sigma_i\ ||c_i||^2|\psi_i\rangle\,\langle\psi_i| \ . \tag{66}$$

But in the density matrix formalism, the pure state on the left is written $|\psi\rangle\,\langle\psi| \ \equiv\ \Sigma_{ij}\ c_i c_j^*|\psi_i\rangle\,\langle\psi_j|$. So: in the density matrix formalism, one should write:

$$|\psi\rangle\,\langle\psi| \ \equiv\ \Sigma_{ij}\ c_i c_j^*|\psi_i\rangle\,\langle\psi_j| \quad \mapsto \quad \Sigma_i\ ||c_i||^2|\psi_i\rangle\,\langle\psi_i| \ . \tag{67}$$

Taking convex combinations of initial pure states, the projection postulate should of course preserve the convex combination. (Think of a non-selective measurement, described by the projection postulate, made on a mixed beam, supplied by a ham-fisted lab assistant!) The density matrix transition, for this general situation—and now without assuming the measured quantity Q is maximal—turns out to be: with E^{q_a} being the spectral projector of the measured quantity Q for eigenvalue q_a:

$$\rho \quad \mapsto \quad \Sigma_a\ E^{q_a}\rho E^{q_a} \ . \tag{68}$$

(viii) Hence the idea (albeit not quite standard jargon!) that for any given pure state, and any given quantity Q—and so: expression of the pure state as a superposition of eigenstates of Q—there is a *corresponding mixture*. Namely: the mixture that, according, to the projection postulate, the state is thrown into by a *non-selective* measurement of Q.

Of course: for Q itself, any state and its corresponding mixture give the same probability distribution. In the above case of Q maximal: probability $||c_i||^2$ for the ith eigenvalue.

But of course: any state and its corresponding mixture, for any Q, will differ in their probability distributions for most quantities that do not commute with Q. Jargon: *interference terms*.

This is the mathematical, density matrix, expression of the fact learnt in elementary quantum mechanics: that we cannot think of a superposition as a mixture: i.e. an ignorance interpretable mixture: i.e. as representing that each individual case is in some definite eigenstate of the quantity Q concerned.

More generally: any pure state, and any mixture—in the quantum formalism: any vector-state and any density matrix—differ in their predicted statistics for some quantity or other. (Qualification: this is so provided the set of quantities is "rich" enough: in quantum theory, this is a matter of having no *superselection rules*.)

We will take up superselection, and develop the Comments (vi) and (vii) in Paragraph 6 below.

Beware! Composite systems give an (unintuitive!) 'not-ignorance-interpretable' idea of mixture, called 'improper mixture'—which is at the very heart of the measurement problem, and of Schrödinger's 'cat' paper of 1935, and the contemporaneous EPR paradox of 1935, and quantum non-locality ...

3: *A representation theorem for states: von Neumann's "no hidden variables" theorem of 1932*: Cf. von Neumann (1932, Chap. IV, Section 2). Let us assume that a *state* assigns to every bounded operator B a complex number ("expectation value") $\langle B\rangle$ subject to:

(i): If B is self-adjoint, then $\langle B\rangle \in \mathbb{R}$

(ii): If B is self-adjoint and positive, then $\langle B\rangle \geq 0$

(iii): $\forall c \in \mathbb{C} : \langle cB\rangle = c\langle B\rangle$

(iv): $\langle A+B\rangle = \langle A\rangle + \langle B\rangle$: *As discussed: this is suspicious!*

(v): $\langle \mathbb{1}\rangle = 1$

(vi): (cf item (d) in Paragraph 1, above): *countable additivity*: If the $\{E_k\}$ are mutually orthogonal , then: $\langle \Sigma_k\, E_k\rangle = \Sigma_k \langle\, E_k\rangle$.

Theorem: Any state defined on all bounded operators Bin the above sense is represented by a unique density matrix ρ, in the sense that

$$\forall B,\ \langle B\rangle = \mathrm{Tr}(\rho B)\,. \tag{69}$$

Ideas of the proof. (1): Uniqueness: use straightforward algebra to get an arbitrary matrix element $(\phi, \rho\psi)$ of ρ fixed by letting each one-dimensional projector substtute for B.

(2): It is is straightforward that any such ρ is self-adjoint, positive and trace 1. So it is a density matrix.

(3): For $\mathcal{H}$ *finite*-dimensional, so that every operators is bounded: the vector space $Lin(\mathcal{H}) \equiv End(\mathcal{H},\mathcal{H})$ of linear operators on $\mathcal{H}$ has an inner product: $(A,B) := \mathrm{Tr}(A^\dagger B)$. Then properties (iii) and (iv) imply that $\langle\cdot\rangle$ is a linear functional on $Lin(\mathcal{H})$, and so (finite-dimensional version of Riesz representation theorem!) there is an operator ρ such that for all operators B:

$$\langle B\rangle = (\rho, B) \equiv \mathrm{Tr}(\rho^\dagger B)\ ; \tag{70}$$

And one then notes that by (1) and (2) above ρ is unique and is a density matrix.

(4): For $\mathcal{H}$ *infinite*-dimensional, $\mathrm{Tr}(A^\dagger B)$ does not converge for all bounded operators A, B.

4: *Probabilities, Uncertainty principle, Simultaneous measurability ...*:

(A): We briefly recall probability distributions, probability density functions and characteristic functions for quantities with continuous spectra, for *vector states*. For example, the joint distribution for two quantities A_1, A_2 that commute with each other:–

We write: $A_r = \int_{\mathbb{R}} x\, dE_x^{(r)}$, $r = 1, 2$. Then the expectation value in the state ψ of the bounded function $f(A_1, A_2)$ is

$$\langle f(A_1,A_2)\rangle_\psi = (\psi, f(A_1,A_2)\psi) = \int\int f(x,y) d_x d_y (\psi, E_x^{(1)} E_y^{(2)}\psi) = \int\int f(x,y) d_x d_y ||E_x^{(1)} E_y^{(2)}\psi||^2\,. \tag{71}$$

And so the probability that the value of $A_1 \leq x$ and the value of $A_2 \leq y$ is:

$$||E_x^{(1)} E_y^{(2)}\psi||^2 = (\psi, E_x^{(1)} E_y^{(2)}\psi) = \langle E_x^{(1)} E_y^{(2)}\rangle_\psi \tag{72}$$

Similarly for probabilities of joint outcomes/values of complete sets of commuting operators.

(B): We set aside the *uncertainty principle*. But we sketch the argument that if two quantities A_1, A_2 with continuous spectra are jointly measurable with arbitrary precision, then they are represented by self-adjoint operators that commute.

We again write the two quantities as: $A_r = \int_{\mathbb{R}} x\, dE_x^{(r)}$, $r = 1, 2$. We take *joint measurability with arbitrary precision* to mean that for any two real numbers x, y (no matter how close!), measurements can determine which if the following possibilities holds: that the two values are, respectively:

$$\leq x \text{ and } \leq y \; ; \leq x \text{ and } > y \; ; > x \text{ and } \leq y \; ; > x \text{ and } > y \tag{73}$$

We can associate a 4-valued quantity with these four outcomes, assigning eigenvalues, say 1, 2, 3, 4, to the four possibilities, respectively; and spectral projectors F_1, F_2, F_3, F_4—again respectively. Then one argues that $E_x^{(1)} E_y^{(2)} = F_1 = E_y^{(2)} E_x^{(1)}$, so that $[E_x^{(1)}, E_y^{(2)}] = 0$. So the two quantities A_1, A_2 commute.

5: *A representation theorem for states: Gleason's theorem of 1957*:
Probabilities of projectors are sufficient to determine a state of the orthodox kind, i.e. a density matrix. This is the content of Gleason's theorem. It improves on von Neumann by dispensing with the assumption of linearity for an arbitrary (and so maybe non-commuting) pair of operators. Its only material assumptions are:

(a) that the dimension of the Hilbert space is greater than 2 (there is an elegant geometric reason for this!); and is separable;

(b) countable additivity on orthogonal projectors (which was assumption (vi) in von Neumann's theorem, above).

Thus we have:

Theorem: If $\mathcal{H}$ is separable, and $\dim(\mathcal{H})$ is greater than 2, and to each projector E is assigned $\langle E \rangle \in \mathbb{R}$, subject to: $\langle E \rangle \geq 0$, $\langle \mathbb{1} \rangle = 1$, and countable additivity on mutually orthogonal projectors, i.e. $\langle \Sigma_k E_k \rangle = \Sigma_k \langle E_k \rangle$:
then there is a unique density matrix ρ, such that

$$\forall E, \; \langle E \rangle = \mathrm{Tr}(\rho E) \, . \tag{74}$$

From a mathematical viewpoint, this theorem's content is elegant. As we said in (d) of Paragraph 1, countable additivity on mutually orthogonal projectors amounts to a natural generalisation, to the non-Boolean lattice $\mathcal{L}$ of projectors of a Hilbert space, of the countable additivity of classical measure theory on *Boolean* algebras. It is remarkable that the delicate interlacing of the various Boolean sublattices of $\mathcal{L}$—if the dimension is greater than 2!—forces this generalised measure to be given by a density matrix.

But from a philosophical viewpoint, we must recall Bell's 1966 lesson. (Recall the last part, viz. (iii), of the Philosophical Remarks in Paragraph 9 of Section 3: about Bell's 1966 paper.) Namely: countable additivity implies constraints on the probability assignments to *non*-commuting quantities, even though its explicit topic is the mutually orthogonal (and so commuting) E_k.

6: *Superselection*:—
The idea is that not every self-adjoint operator represents a measurable quantity: very plausible! A bounded operator that commutes with every operator represent a measurable quantity (but is not itself a multiple of the identity) is called a *superselection operator*.

Superselection means that the density operator representing a state need not be unique. But there is an analogue of von Neumann's theorem; as follows:— Theorem: Consider the von Neumann algebra generated by the self-adjoint operators that represent measurable quantity. If to

every B in this algebra, a finite expectation value $\langle B\rangle$ is assigned subject to the conditions (i) to (vi) as in von Neumann's theorem, then: there is a density operator ρ representing this assignment, i.e, such that: $\langle B\rangle = \mathrm{Tr}(\rho B)$.

Suppose there is a complete set $\{A_k\}$ of commuting self-adjoint operators representing measurable quantities. Then every superselection operator S commutes with all the A_k and so is a function of them. So all the superselection operators $S, S', ...$ commute with each other. We assume they can be simultaneously diagonalized with a discrete decomposition. That is: there is a complete orthogonal family $\{E_k\}$ of projectors with $\Sigma_k\, E_k = \mathbb{1}$ such that:

(i) every S has the form $\Sigma_k\, c_k E_k$; :

(ii) if $k \neq k'$, then there is a superselection operator $S = \Sigma_j\, c_j E_j$ with $c_k \neq c_{k'}$.

This is the usual structure of superselection.

Assuming this structure of superselection, one readily proves: Theorem: Let $\mathcal{A}$ be the von Neumann algebra generated by the self-adjoint operators representing measurable quantities. Then a bounded operator B commutes with all the E_k iff $B \in \mathcal{A}$.

We can now develop the Comments (vii) and (viii) at the end of Paragraph 2 above. If ρ is a density matrix, so is $\Sigma_k\, E_k \rho E_k$. If B commutes with all the E_k, then since (using cyclicity of trace and the $\{E_k\}$ being complete)

$$\mathrm{Tr}(\rho B) = \mathrm{Tr}(\Sigma_k\, (E_k \rho B E_k)) = \mathrm{Tr}(\Sigma_k\, (E_k \rho E_k))B \tag{75}$$

we infer that ρ and $\Sigma_k\, E_k \rho E_k$ represent the same state (in our orthodox sense, of assignments of probability distributions, in particular expectation values, to operators representing measurable quantities ...).

Thus a state is represented equally well by: :

(i) as usual: a vector ψ, with $||\psi|| = 1$: now think of it as skew to the various subspaces that are the ranges of the E_k; and :

(ii) the corresponding density matrix that Comment (viii) at the end of Paragraph 2:

$$\Sigma_k\, (E_k|\psi\rangle\langle\psi|E_k) \tag{76}$$

To sum up: No wonder people have argued that a solution to the measurement problem—i.e. the desired transition from a pure state to the corresponding mixture defined by a suitable choice of quantity (or quantities)—can be obtained by justifying suitable limitations on what is measurable, so as to give superselection rules.

Nowadays, the main programme of this type appeals to *decoherence*: which amounts to—and is sometimes called—*environmentally induced superselection.*