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QUANTUM MECHANICAL ANTIPASTO

Critical introduction to some of the concepts, issues and most basic methods of non-relativistic quantum mechanics

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Introduction. Before you can cook you must collect your ingredients and light the fire. That is my present business. And a prosaic business it is, even in the kitchen of a master chef. Though my own modest establishment is listed in none of the gourmet guides, it does present a few exotic dishes on its menu— a *spécialité de la maison* or two—and, since we try to introduce a memorably uncommon note even to our more standard fare, all takes careful—if necessarily brisk—preparation.

I proceed in the presumption that my diners have already consumed the contents of a good introductory text, such as (say) Griffiths' *Introduction to Quantum Mechanics*(1994), and have at least tasted such of the fruit presented there that they have chosen to set aside. And that they are at least a passingly acquainted with other standard sources—that they are familiar enough with the differences in style and substance which distinguish Bohm from Schiff from Mertzbacher ...that they have been able to form some sense of which they individually find most congenial.

My readers will understand that it would be futile to try to produce a comprehensive compilation of the best to be found in those standard sources, that in a brief series of lectures I must be highly selective, that the most I can hope to accomplish is to cast useful light on a few topics recommended either by their acknowledged high importance or typical neglect. And that my own neglect of a topic should not be read as an indication that the topic is, in my view, "unimportant;" it means simply that I did not have time to treat the

topic in question, or that I found it to be a topic to which I had nothing fresh to contribute.

I intent in this introductory chapter will more to pose issues than to indicate how they might be resolved. And to assemble some of the tools we will need to undertake work of the latter sort.

Representations of configuration & state in classical & quantum physics. I have been reminded recently[1] that, in the opinion of Aristotle (384–322 B.C.), "To be ignorant of motion is to be ignorant of Nature." But that bald assertion does not take us very far. Motion of what? And with respect to what? "Theories of motion" and "theories of constitution" have been in interactive dialog throughout the long history of Natural Philosophy, developments in each serving to inspire progress in the other. Consider, for a moment, of the objects real or imagined

- celestial bodies
- "atoms" of Democritus
- earth, moon & planets (but not sun or stars)
- terrestrial projectiles
- "vortices" of Descartes
- "monads" of Leibniz
- "point particles" of Newton
- undulatory sound and light
- gas molecules
- electromagnetic fields
- æther
- nuclear atom
- warped spacetime
- ψ-field of Schrödinger
- elementary particles
- quantum fields
- supersymmetric strings
- hyperdimensional M-branes

which have been discovered/invented/transformed/abandoned/reinvented in the long history of physics, and of how various are the theories which have been successively devised to launch those objects into motion. What those theories—whether they involve celestial spheres or spin space, Riemannian geometry or Teichmüller space—have all in common is that, from Pythagorus (c582–c500 B.C.: "Number rules the universe") down to the present day, they have lived not so much in the world of appearances as in the mathematical mind. Yet *not just* in the mathematical mind: *connected*, by a train of associations however long and tenuous, to the world of direct perception. The imagination of the physicist is invited by the manifest complexity of Nature to spin, yet prevented by that thread from spinning free. It is that connective thread, that anchor line itself which at the moment interests me—that, and the variety of its attachment points to classical/quantum mechanics.

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[1] Dava Sobel, *Galileo's Daughter* (1999), p. 30.

To describe the motion of that thing relative to this ground on which we stand it is sufficient, in the simplest instance, and at the most naive level, simply to point (though it would be difficult by such means to describe the motion of the sea; easier to describe the motion of the gull). But such handwaving is not yet physics.[2]

Erect scaffolding on a secure foundation: physical scaffolding, from boards, screws and glue, with corners just and true, the whole in accordance with your best understanding of the (locally) Euclidean geometry of physical space. Construct also a clock, a physical device which ticks (in Newton's phrase, which would seem profoundly circular had he not held that he was referring to something external and absolute) "uniformly," and hang it on a scaffold peg, to which you have previously attached also an orthogonal triad of regularly ticked sticks. Equip yourself finally with an arrow, which—with its tail always in contact with some selected fiducial point (origin of the triad)—you will use to indicate the momentary position of the moving point-like object of interest.

You have, by such means, constructed a "digitized finger"—means and a procedure for representing the momentary placement of a physical point by a triple of real numbers, and the motion of such a point as a parameterized sequence of such triples. The real numbers which issue from physical theories become purported statements about the physical world through the agency of measurement devices, and all such devices are elaborations—(theory-laden) extensions—of the rudimentary scaffolding just described.

So are we placed in position to write $\boldsymbol{x}$ when we have in mind the position of a Newtonian "point mass," $\boldsymbol{x}(t)$ when we have in mind the motion of such an (idealized) object, $\{\boldsymbol{x}_1(t), \boldsymbol{x}_2(t), \ldots, \boldsymbol{x}_N(t)\}$ when we have in mind an N-particle system, $\{q^1, q^2, \ldots, q^n\}$ with $q^i = q^i(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)$ when we find it analytically convenient to abandon Cartesian coordinates and/or to represent the system by a point in some imagined hyperspace.[3]

Having penetrated the world of mathematics, we acquire freedom (provided we never snip the thread) to draw upon our mathematical imaginations to construct "representations of configuration" of ascending complexity. We might, for example, write $\{\boldsymbol{x}, \mathbb{R}\}$—with $\mathbb{R}$ a rotation matrix—to describe the placement and orientation of a rigid body (idealized assembly of Newtonian particles). Or, in the kinetic theory of gases, we might in place of $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_{\text{Avagodro}}\}$ find

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[2] One is reminded of Omar Khayyam's "moving finger," and of the fact that he was a mathematician. Omar Khayyam (c1050–1123), though he had much to say poetically concerning the nature of time, drew his inspiration not from physics but from the interplay between algebra and geometry, in a tradition which led directly to Descartes; see Chapter 13 in Carl Boyer's *A History of Mathematics* (2nd edition 1991).

[3] Notice that one cannot use planks and a pair of dividers to construct physical scaffolding in hyperspace! It is by a thread of associations that one lends physical meaning/interest to such a point in such a place.

it more convenient—and a more accurate reflection of the true state of our knowledge—to write

$$\rho(\boldsymbol{x}) \equiv \begin{cases} \text{course-grained density of molecules} \\ \text{in the neighborhood of the point } \boldsymbol{x} \end{cases}$$

which is to represent the instantaneous configuration of the molecular system by a "point in the space of such density functions."

It is when we turn from kinematics to dynamics—symbolized $m\ddot{\boldsymbol{x}} = \boldsymbol{\bar{F}}(\boldsymbol{x})$— that the physics begins to become more overtly theory-laden: we discover that we are forced to recognize a distinguished class of scaffolds; to distinguish "inertial frames" from frames-in-general. And we discover that specification of $\boldsymbol{x}(0)$ is insufficient to determine the subsequent trajectory $\boldsymbol{x}(t)$; that to specify the latter we must—because the dynamical equations are differential equations of second order—stipulate the initial values of both $\boldsymbol{x}$ and $\boldsymbol{v} \equiv \dot{\boldsymbol{x}}$. So we learn to distinguish

- *descriptors of configuration* (typified, in the simplest instance, by $\boldsymbol{x}$) from
- *descriptors of state* (typified by $\{\boldsymbol{x}, \boldsymbol{v}\}$).

The former serve collectively to identify a "point in configuration space," and the latter to identify a "point in (double-dimensioned) state space."

In the relatively more powerful setting afforded by Lagrangian mechanics we have

$$\{q^1, q^2, \ldots, q^n\} \quad : \quad \text{descriptor of configuration}$$
$$\{q^1, q^2, \ldots, q^n; \dot{q}^1, \dot{q}^2, \ldots, \dot{q}^n\} \quad : \quad \text{descriptor of state}$$

Passage to the Hamiltonian formalism leads to a theory in which a doubled population of variables

$$\xi \equiv \{q^1, q^2, \ldots, q^n; p_1, p_2, \ldots, p_n\} \quad : \quad \text{descriptor of state}$$
$$p_i \equiv \partial L / \partial \dot{q}^i$$

is subject to a coupled system of differential equations of only first order. In Hamiltonian mechanics the concept of "configuration" assumes subordinate status; "trajectories" live now not in configuration space but in state space ("phase space"), and through each $\xi(0)$ passes a single such trajectory $\xi(t)$.

Consider again, from this point of view, our former mole of gas molecules. To describe the instantaneous state of the gas we might mark a point in a phase space of $6N$ dimensions (here N is Avagodro's number). But—in the approximation that the weakly-interactive gas molecules are non-interactive— we could, alternatively, sprinkle a population of N points on a phase space of only 6 dimensions. It becomes then natural to introduce a

statistical distribution $\rho(\boldsymbol{x}, \boldsymbol{p})$ on phase space

to describe what we might actually know (or pretend we know) concerning the state of the gas. And to write something like

$$\dot{\rho} = \frac{\partial \rho}{\partial \boldsymbol{x}}\,\dot{\boldsymbol{x}} + \frac{\partial \rho}{\partial \boldsymbol{p}}\,\dot{\boldsymbol{p}} = \frac{\partial \rho}{\partial \boldsymbol{x}}\frac{\partial H}{\partial \boldsymbol{p}} - \frac{\partial \rho}{\partial \boldsymbol{p}}\frac{\partial H}{\partial \boldsymbol{x}} = \left[\rho, H\right] \tag{1}$$

to describe (as a "curve in the space of ρ-functions") the dynamical evolution of the state of the gas.

We have been brought thus to quite a congenial mathematical place, but the thread that connects us back to the rude scaffold which was our point of departure and must be our ultimate point of return ... has grown rather long.

Which brings me to the threshold of quantum mechanics.

By Dirac's interpretation of the theory created by Heisenberg/Schrödinger the state—not the configuration but the state—of a quantum mechanical system is to be represented by a complex vector, an element of a certain ∞-dimensional complex vector space. That is certainly not a place in which we can erect physical scaffolding. So we confront the question: How, in such a place, do we secure ground to stand on? To what do we tie the thread that anchors us in experienced reality?

Complex vector spaces and Dirac notation. Since the theory of complex vector spaces is patterned upon the more familiar theory of real vector spaces, we begin with a sketch of the essential elements of the later theory.

Objects $\big\{A, B, \dots\big\}$ are elements of a *real vector space* R_N if the set is *closed under real linear combination*:

$$c_1 A + c_2 B \in R_N \text{ for all } A, B \in R_N \text{ if } c_1 \text{ and } c_2 \text{ are real numbers}$$

If $\big\{K_1, K_2, \dots, K_N\big\}$ are *linearly independent*

$$c_1 K_1 + c_2 K_2 + \cdots + c_N K_N = 0 \text{ if and only if } c_1 = c_2 = \cdots = c_N = 0$$

and if every $A \in R_N$ can be developed

$$A = a^1 K_1 + a^2 K_2 + \cdots + a^N K_N \quad : \quad \text{written } a^i K_i$$

then the vectors $\big\{K_1, K_2, \dots, K_N\big\}$ comprise a basis in R_N, and $\big\{a^1, a^2, \dots, a^N\big\}$ are the *coordinates* of A with *respect to that basis*. Every basis has the same number of elements; that number N is the *dimension* of the vector space. The vector space R_N becomes an *inner product space* if there is defined on R_N a real number valued symmetric bilinear function (A, B)

$$(A, B) \text{ is a real number}$$
$$(A, B) = (B, A)$$
$$(A, c_1 B_1 + c_2 B_2) = c_1(A, B_2) + c_2(A, B_2)$$

with the added property that

$$|A| \equiv (A, A) \geqslant 0, \text{ with equality if and only if } A = 0$$

Specification of an inner product can be achieved by specification of the symmetric array of real numbers

$$g_{ij} \equiv (K_i, K_j)$$

and by imposing the requirement that $\mathbb{G} = \|g_{ij}\|$ be positive definite (i.e., that all eigenvalues of $\mathbb{G}$ be positive). We then have

$$(A, B) = (a^i K_i, b^j K_j) = a^i g_{ij} b^j = \begin{pmatrix} a^1 \\ a^2 \\ \vdots \\ a^N \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} g_{11} & g_{12} & \cdots & g_{1N} \\ g_{21} & g_{22} & \cdots & g_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ g_{N1} & g_{N2} & \cdots & g_{NN} \end{pmatrix} \begin{pmatrix} b^1 \\ b^2 \\ \vdots \\ b^N \end{pmatrix}$$

Given an inner product—thus defined—we are positioned to introduce a second "dual" basis $\left\{K^1, K^2, \ldots, K^N\right\}$ with elements defined

$$K^i = g^{ij} K_j \quad \text{with} \quad \|g^{ij}\| \equiv \|g_{ij}\|^{-1}$$

This we do so as to achieve

$$(K^i, K_j) = \delta^i{}_j$$

from which it follows that the $\left\{K_1, K_2, \ldots, K_N\right\}$-coordinates of an arbitrary vector A can be described

$$a^i = (K^i, A)$$

It is always possible (in infinitely many ways, and by any of several available strategies) to construct in R_N a basis $\left\{E_1, E_2, \ldots, E_N\right\}$ which is *orthonormal* in the sense that

$$(E_i, E_j) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Such bases are distinguished by the property that they are "self-dual:" the distinction between E^i and E_i has evaporated, and we have (for all A) the "Fourier expansion formula"

$$A = \sum_i E_i (E_i, A)$$

Similarly … objects $\left\{A, B, \ldots\right\}$ are elements of a *complex vector space* C_N if the set is *closed under complex linear combination* and if, moreover,

$$A \in C_N \implies A^* \in C_N$$

To say that $\left\{K_1, K_2, \ldots, K_N\right\}$ comprise a basis in C_N is to assert that every $A \in C_N$ can be developed

$$A = a^1 K_1 + a^2 K_2 + \cdots + a^N K_N$$

where the coordinates $\{a^1, a^2, \ldots, a^N\}$ are now allowed to be (and typically required to be) complex numbers. The vector space C_N becomes an *inner product space* if there is defined on C_N a complex number valued *symmetric function (A, B)

$$(A, B) \text{ is a complex number}$$
$$(A, B) = (B, A)^*$$

which is linear in the second argument but *linear in the first argument

$$(A, c_1 B_1 + c_2 B_2) = c_1(A, B_2) + c_2(A, B_2)$$
$$(c_1 A_1 + c_2 A_2, B) = c_1^*(A, B_2) + c_2^*(A, B_2)$$

Necessarily $|A| \equiv (A, A)$ is real; we impose, however, the stronger requirement that

$$|A| \equiv (A, A) \geqslant 0, \text{ with equality if and only if } A = 0$$

Specification of an inner product can be achieved by specification of the *symmetric array of complex numbers

$$h_{ij} \equiv (K_i, K_j) = h_{ji}^*$$

and by imposing the requirement that $\mathbb{H} = \|h_{ij}\|$ be positive definite (i.e., that all eigenvalues of $\mathbb{H}$—which will be shown presently to be necessarily real—be positive). We then have

$$(A, B) = (a^i K_i, b^j K_j) = a^{*i} h_{ij} b^j = \begin{pmatrix} a^1 \\ a^2 \\ \vdots \\ a^N \end{pmatrix}^\dagger \begin{pmatrix} h_{11} & h_{12} & \cdots & h_{1N} \\ h_{21} & h_{22} & \cdots & h_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ h_{N1} & h_{N2} & \cdots & h_{NN} \end{pmatrix} \begin{pmatrix} b^1 \\ b^2 \\ \vdots \\ b^N \end{pmatrix}$$

Given an inner product—thus defined—we proceed as before to introduce a second "dual" basis $\{K^1, K^2, \ldots, K^N\}$ with elements defined

$$K^i = h^{ij} K_j \quad \text{with} \quad \|h^{ij}\| \equiv \|h_{ij}\|^{-1}$$

We then have $(K^i, K_j) = \delta^i{}_j$ from which it follows that the coordinates of an arbitrary vector A can be described $a^i = (K^i, A)$. The familiar advantages of self-duality are achieved by bases $\{E_1, E_2, \ldots, E_N\}$ which is *orthonormal* in the familiar sense that

$$(E_i, E_j) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

With respect to such a basis every $A \in C_N$ can be developed

$$A = \sum_i E_i (E_i, A) \tag{2}$$

A *linear operator* L sends vector→vector in such a way as to conform to the linearity condition

$$\mathsf{L}(c_1 A_1 + c_2 A_2) = c_1(\mathsf{L} A_1) + c_2(\mathsf{L} A_2)$$

The implication is that if one knows how L acts on the elements of a basis then one knows how L acts on every vector A in the vector space. To describe the action of L on $\{K_1, K_2, \ldots, K_N\}$ we write

$$K_j \longrightarrow \mathsf{L} K_j = \sum_i K_i \underbrace{(K^i, \mathsf{L} K_j)}_{\equiv L^i{}_j, \text{ elements of } \mathbb{L}}$$

Then $A \to B = \mathsf{L} A$ acquires (with respect to the K-basis) the representation

$$a^i \longrightarrow b^i = L^i{}_j a^j$$

The *adjoint* M (usually denoted L^+) of a linear operator L is defined

$$(\mathsf{M} A, B) = (A, \mathsf{L} B) \quad : \quad \text{all } A, B \in C_N$$

It is a basis-independent notion, though clearly sensitive to specification of the metric. In K-representation we have

$$(M^k{}_i a^i)^* h_{kj} b^j = (a^i)^* h_{ik} L^k{}_j b^j$$

giving $\mathbb{M}^{*\mathsf{T}} \mathbb{H} = \mathbb{H} \mathbb{L}$, which by conjugated transposition becomes

$$\mathbb{M} = \mathbb{H}^{-1} \mathbb{L}^\dagger \mathbb{H}$$
$$\downarrow$$
$$= \mathbb{L}^\dagger \quad \text{if the basis is orthonormal: } \mathbb{H} = \mathbb{I}$$

In short: "adjunction" of a linear operator becomes "Hermitian conjugation" in every orthonormal representation. Clearly

$$(\mathsf{L}_1 \mathsf{L}_2)^+ = (\mathsf{L}_2)^+ (\mathsf{L}_1)^+ \quad \text{and} \quad (\mathsf{L}^+)^+ = \mathsf{L}$$

—the matrix counterparts of which are familiar.

It was Dirac's inspiration[4] to
- let the elements of C_N be notated $|\psi)$, and be called "ket vectors;"
- let the inner product of $|\phi)$ on $|\psi)$ be notated $(\phi|\psi)$, and be called a "bracket."

What Dirac called a "bra vector," and denoted $(\phi|$, is actually not an element of C_N but of C_N's "dual"—the vector space of complex-valued linear functionals $F[\bullet]$ whose arguments range on C_N and satisfy the linearity condition

$$F[c_1|\psi_1) + c_2|\psi_2)] = c_1 F[|\psi_1)] + c_2 F[|\psi_2)]$$

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[4] See §§5–9 in *The Principles of Quantum Mechanics* (4$^\text{th}$ edition 1958). Easier-to-read accounts of the formalism can be found in Griffiths' Chapter 3 and in virtually every quantum text. For more carefully detailed discussion see, for example, T. F. Jordan, *Linear Operators for Quantum Mechanics* (1969).

According to "Riesz' theorem"[5] there corresponds to every such $F[\bullet]$ a $|\phi) \in C_N$ such that, for every $|\psi) \in C_N$, $F[|\psi)] = (\phi|\psi)$. So $(\phi|$ might better be written $(\phi|\bullet)$. But in all applications one can proceed as though

$$(\psi| = |\psi)^* \quad \text{informally, as a manner of speaking}$$

and can on that basis recover

$$(\phi|\psi)^* = (\psi|\phi)$$

In any (orthonormal) representation all mystery disappears: the representative of $(\phi|$ is a row vector, the conjugate transpose of the column vector which represents $|\psi)$.

Dirac achieves enhanced formal elegance/simplicity by *excluding from consideration all non-orthonormal bases* (i.e., by excluding bases in which up/down index placement—for which his notation makes no provision—makes a difference). To express the orthonormality of a basis $\{|1), |2), \ldots, |N)\}$ he writes

$$\text{ORTHONORMALITY} \quad : \quad (m|n) = \delta_{mn} \tag{3}$$

Every $|\psi) \in C_N$ can, by (2), be developed

$$|\psi) = \sum_n |n)(n|\psi) \tag{4}$$

To indicate that the set $\{|n)\}$ is "complete" in the sense that is *spans* C_N, and permits *every* $|\psi) \in C_N$ to be developed in this way, Dirac writes

$$\text{COMPLETENESS} \quad : \quad \mathsf{I} = \sum_n |n)(n| \tag{5}$$

Notice that, while (bra)·(ket) is a complex number, (ket)·(ket) is a linear operator: $|\alpha)(\beta|$ applied to $|\psi)$ gives $(\beta|\psi)\cdot|\alpha)$. More particularly, the operators

$$\mathsf{p}_n \equiv |n)(n| \tag{6.1}$$

comprise a complete $(\sum_n \mathsf{p}_n = \mathsf{I})$ set of orthogonal $(\mathsf{p}_m \mathsf{p}_n = \mathbf{0}$ if $m \neq n)$ projection operators $(\mathsf{p}_n^2 = \mathsf{p}_n)$, and each p_n projects onto its associated basis element:

$$\mathsf{p}_n|n) = |n) \tag{6.2}$$

The expanded set of operators $|m)(n|$ permits one to develop *any* linear operator:

$$\mathsf{L} = \mathsf{I} \cdot \mathsf{L} \cdot \mathsf{I} = \sum_m \sum_n |m)(m|\mathsf{L}|n)(n| \tag{7}$$
$$= \sum_m \sum_n L_{mn}|m)(n| \quad \text{with} \quad L_{mn} \equiv (m|\mathsf{L}|n)$$

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[5] See p. 13 in Jordan or L. E. Ballentinie, *Quantum Mechanics* (1989), p. 3.

Looking back in this light to (5) we have, associated with every orthonormal basis, what is called a "resolution of the identity" into summed orthogonal projection operators.

To express, within the Dirac formalism, the condition which lends meaning to the statment $\mathbf{M} = \mathbf{L}^+$ one might write

$$(\phi|\overleftarrow{\mathbf{M}}|\psi) = (\phi|\overrightarrow{\mathbf{L}}|\psi) \quad \text{all } |\phi), |\psi) \in C_N \tag{8.1}$$

to indicate that $\mathbf{M}$ acting to the left yields always the same result as $\mathbf{L}$ acting to the right. This is frequently a useful point of view, but it would be notationally less cluttered to write

$$(\psi|\mathbf{M}|\phi) = [(\phi|\mathbf{L}|\psi)]^* \tag{8.2}$$

which when referred to the $\{|n)\}$ basis becomes (with $\sum_{m,n}$ understood)

$$(\psi|m)(m|\mathbf{M}|n)(n|\phi) = [(\phi|n)]^*[(n|\mathbf{L}|m)]^*[(m|\psi)]^*$$
$$= (\psi|m)[(n|\mathbf{L}|m)]^*(n|\phi)$$

giving back again $(m|\mathbf{M}|n) = [(n|\mathbf{L}|m)]^*$; i.e., $\mathbb{M} = \mathbb{L}^\dagger$.

The spectral properties of an operator $\mathbf{A}$ arise from writing

$$\mathbf{A}|a) = a|a)$$

Let $\mathbf{A}$ be self-adjoint. Then $[(a|\mathbf{A}|a)]^* = (a|\mathbf{A}^+|a) = (a|\mathbf{A}|a)$ is on the one hand assuredly real, but on the other equal to $a(a|a)$. Since $(a|a)$ is also known to be real, we may conclude that

> the eigenvalues $a_1, a_2, \ldots, a_N$ of any self-adjoint $\mathbf{A}$
> are necessarily *real* (though not necessarily distinct)

Next, let a_1 and a_2 be distinct eigenvalues of $\mathbf{A}$:

$$\mathbf{A}|a_1) = a_1|a_2) \quad \text{and} \quad \mathbf{A}|a_2) = a_2|a_2)$$

Then

$$(a_1|\mathbf{A}|a_2) = \begin{cases} a_2(a_1|a_2) & \text{if } \mathbf{A} \text{ looks right, but} \\ a_1(a_1|a_2) & \text{if } \mathbf{A} \text{ looks left} \end{cases}$$

Consistency with $a_1 \neq a_2$ entails $(a_1|a_2) = 0$:

> eigenvectors $|a_1)$ and $|a_2)$ associated with distinct eigenvalues
> of any self-adjoint $\mathbf{A}$ are necessarily orthogonal: $(a_1|a_2) = 0$

If the spectrum of $\mathbf{A}$ is non-degenerate, and if we assume the eigenvectors to have been normalized $(a_i|a_i) = 0$, then the population of eigenvectors $\{|a_i)\}$

supplies an orthonormal *basis* in C_N, and when $\mathbf{A}$ is developed in its own basis we obtain

$$\begin{aligned}
\mathbf{A} &= \sum_i \sum_j |a_i)(a_i|\mathbf{A}|a_j)(a_j| \\
&= \sum_i |a_i)a_i(a_i|
\end{aligned} \tag{9}$$

by $(a_i|\mathbf{A}|a_j) = (a_i|a_j)a_j = \delta_{ij}a_j$. We observe that the matrix representative of $\mathbf{A}$ in its own eigenbasis is *diagonal*

$$\mathbb{A} = \begin{pmatrix} a_1 & 0 & & 0 \\ 0 & a_2 & & 0 \\ & & \ddots & \\ 0 & 0 & & a_N \end{pmatrix}$$

The right side of (9) presents what is called the "spectral representation" of the self-adjoint operator $\mathbf{A}$.

We have finally to consider "linear isometries" in C_N. If a linear operator $\mathbf{U}$ preserves all inner products (brackets)

$$(\alpha|\mathbf{U}^+\mathbf{U}|\beta) = (\alpha|\beta) \quad : \quad \text{all } |\alpha), |\beta) \in C_N$$

then necessarily it preserves all norms

$$(\psi|\mathbf{U}^+\mathbf{U}|\psi) = (\psi|\psi) \quad : \quad \text{all } |\psi) \in C_N$$

But the latter condition can be expressed

$$(\psi|\mathbf{A}|\psi) = 0 \quad \text{where } \mathbf{A} \equiv \mathbf{U}^+\mathbf{U} - \mathbf{I} \text{ is self-adjoint}$$

which, if valid for all $|\psi)$, pretty clearly[6] requires $\mathbf{A} = \mathbf{0}$. We conclude that $|\psi) \rightarrow \mathbf{U}|\psi)$ will be isometric if and only if $\mathbf{U}$ is *unitary*:

$$\mathbf{U}^+\mathbf{U} = \mathbf{I} \tag{10}$$

In orthonormal representation we have $\mathbb{U}^\dagger\mathbb{U} = \mathbb{I}$, which is the complex analog of the stipulation $\mathbb{R}^\mathsf{T}\mathbb{R} = \mathbb{I}$ that $\mathbb{R}$ be a rotation matrix; i.e., that the associated linear operator $\mathbf{R}$ act isometrically upon R_N.

Quantum state, and rudiments of the quantum theory of measurement. Though a variety of other—equivalent or generalized—modes of representation will emerge, we can, for starters, assert that

$$\begin{array}{l} \text{the momentary } state \text{ of a quantum system } \mathfrak{S} \\ \text{can be represented by a unit vector } |\psi) \in C_N \end{array} \tag{11}$$

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[6] See Paul Halmos, *Finite-dimensional Vector Spaces* (2nd edition 1958), §73.

The specific identity of C_N is contingent ... upon general principles yet to be described, and upon the physical details of $\mathfrak{S}$.

Earlier we had occasion to ask: How, in such a place [as C_N] as do we secure ground to stand on? To what do we tie the thread that anchors us in experienced reality? The answers are provided by the theory of self-adjoint operators. Specifically, to every "classical observable"—i.e., to every real-valued function $A(x, p)$ defined on classical phase space—we associate a self-adjoint linear operator $\mathbf{A}$ which acts upon the elements of C_N. We then associate
- the possible meter-readings which can result from A-measurement with the (necessarily real) *eigenvalues* of $\mathbf{A}$;
- the possible quantum states immediately subsequent to such a measurement with the *eigenvectors* of $\mathbf{A}$.

Each observable contrives spectrally to erect its own individual "orthogonal scaffold $\{|a)\}$ in the space of states." How that abstract construction becomes tied to the scaffold which we have constructed from boards here in the laboratory hinges upon our answer to this fundamental question:

By what specific **rule of correspondence** is the association

$$A(x, p) \;\longleftrightarrow\; \mathbf{A} \tag{12}$$

to be established?

This is a question to which we will return. But for the moment...

Look more closely to the idealized measurement process to which I have alluded. System $\mathfrak{S}$, in unknown quantum state $|\psi)$, is presented to (meaning "brought into interaction with") the measurement device represented by the operator $\mathbf{A}$ (I will call such a device an "A-meter"). After the interaction is complete
- the device is in the state a reported by its read-out mechanism, and this is interpreted to mean that
- the system $\mathfrak{S}$ is in state $|a)$.

Quantum mechanically fundamental is the fact that *repetitions yield statistically scattered results*: we obtain

$$|\psi) \xrightarrow[\text{A-measurement}]{} \begin{cases} |a_1) \text{ with probability } P_1 = |(a_1|\psi)|^2 \\ |a_2) \text{ with probability } P_2 = |(a_2|\psi)|^2 \\ \vdots \\ |a_n) \text{ with probability } P_n = |(a_n|\psi)|^2 \\ \vdots \end{cases}$$

Quantum measurement is, by this scheme, a "state-preparation process," and measurement devices are, in effect, sieves: the input state $|\psi)$ is resolved

$$|\psi) = \sum_i |a_i)(a_i|\psi)$$

and the device acts (probabilistically) to
- to pass one of the eigen-components, and
- to annihilate all others.

We assert that a measurement has actually taken place on these grounds: if the output $|a_n)$ of a measurement which registered a_n is immediately re-presented to an A-meter we have

$$|a_n) \xrightarrow[\text{repeated } A\text{-measurement}]{} \begin{cases} |a_1) \text{ with probability } P_1 = |(a_1|a_n)|^2 = 0 \\ |a_2) \text{ with probability } P_2 = |(a_2|a_n)|^2 = 0 \\ \vdots \\ |a_n) \text{ with probability } P_n = |(a_n|a_n)|^2 = 1 \\ \vdots \end{cases}$$

which is to say: we recover (or "confirm") the previous result with certainty.

The expected average of many independent A-measurements (i.e., of the results obtained when many identical copies of $|\psi)$ are presented serially to an A-meter) can be described

$$\begin{aligned} \langle a \rangle_\psi &= \textstyle\sum_i a_i P_i \\ &= \textstyle\sum_i a_i |(a_i|\psi)|^2 \\ &= (\psi| \left\{ \textstyle\sum_i |a_i) a_i (a_i| \right\} |\psi \\ &= (\psi| \mathbf{A} |\psi) \end{aligned} \tag{13.1}$$

but alernative descriptions exist and are sometimes more useful. For example, let $\{|n)\}$ be some arbitrary orthonormal basis in the space of states. Drawing upon the completeness condition (5), we have

$$\begin{aligned} &= \textstyle\sum_n (\psi|n)(n|\mathbf{A}|\psi) \\ &= \textstyle\sum_n (n|\mathbf{A}|\psi)(\psi|n) \\ &= \textstyle\sum_n (n|\mathbf{A}\boldsymbol{\psi}|n) \quad \text{where } \boldsymbol{\psi} \equiv |\psi)(\psi| \text{ projects onto } |\psi) \\ &= \operatorname{tr} \mathbf{A}\boldsymbol{\psi} \end{aligned} \tag{13.2}$$

In $\boldsymbol{\psi}$ we have encountered the germ of what will grow up to become the "density matrix," which plays an indispensable role in a broad assortment of applications. The mth moment of the measured data can be described variously

$$\begin{aligned} \langle a^m \rangle_\psi &= \textstyle\sum_i (a_i)^m P_i \\ &= (\psi| \mathbf{A}^m |\psi) \\ &= \operatorname{tr} \mathbf{A}^m \boldsymbol{\psi} \end{aligned} \tag{13.3}$$

where use has been made of $\mathbf{A}^m = \sum_i |a_i) a_i^m (a_i|$. In the case $m = 0$ we have (for *any* observable)

$$\begin{aligned} \langle a^0 \rangle_\psi &= \textstyle\sum_i P_i = 1 &:& \quad \text{probabilities sum to unity} \\ &= (\psi|\psi) &:& \quad \text{state vector is normalized} \\ &= \operatorname{tr} \boldsymbol{\psi} \end{aligned} \tag{13.4}$$

Complex multiples $c|\alpha)$ of any $|\alpha) \in C_N$ are elements of a 1-dimensional subspace of C_N, the "ray" indicated by $|\alpha)$. State vectors $|\psi)$ live at the points where rays puncture the "unit ball" in C_N. We observe that

$|\psi)$ a state vector $\implies c|\psi)$ a state vector if and only if $c = e^{i(\text{phase})}$

and that the formulæ (13) which describe the physical output of quantum theory are phase-insensitive.

Superimposed (more generally: linearly combined) state vectors are, in general, *not state vectors until renormalized*, and linear combination followed by renormalization

$$c_1|\psi_1) + c_2|\psi_2) \longrightarrow |\psi) \equiv \frac{c_1|\psi_1) + c_2|\psi_2)}{\text{norm}}$$

$$\text{norm } |\varphi) \equiv \sqrt{(\varphi \,|\varphi)} \equiv \| \,|\varphi) \, \| \qquad (14)$$

is a non-linear process. In this fundamental respect quantum mechanics (wave mechanics) departs from the classical wave physics (acoustics, physical optics) which historically served as it model: superimposed sounds yield sound.[7]

We note in passing that

$$\|e^{i\alpha}|a) + e^{i\beta}|b)\|^2 = (a|a) + (b|b) + e^{i(\alpha-\beta)}(b|a) + e^{i(\beta-\alpha)}(a|b)$$

which shows the norm of linearly combined vectors to be invariant with respect to adjustment of the absolute phase (set $\alpha = \beta$), but sensitive to adjustment of the relative phase.

Turn the A-meter back on, and let $|a)$ be some designated one of its eigenstates. In operation, it stimulates the projective transition

$$|a) \longleftarrow |\psi) \quad \text{with probability } P = |(a|\psi)|^2 \qquad (15)$$

Let $\{|b)\}$ be any orthonormal basis (which may but for present purposes need not be thought of as eigenstates of an B-meter). Ditto $\{|c)\}$. Then

$$(a|\psi) = \sum_j (a|b_j)(b_j|\psi) \qquad (16.1)$$

It was, so far as I am aware, Richard Feynman[8] who first stressed the utility of considering $(a|b_j)(b_j|\psi)$ to describe (not the probability but) the "*probability*

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[7] At this point my reader might very usefully give close reading to Dirac's Chapter I (especially §4), which provides a very careful discussion of the formative role of the *principle of superposition* in quantum mechanics.

[8] "Space-time approach to non-relativistic quantum mechanics," Rev. Mod. Phys. **20**, 267 (1948); *The Feynman Lectures of Physics* (1965), Volume III, Chapter 3.

amplitude" that the transition $|a) \longleftarrow |\psi)$ proceeded *via* the intermediate state $|b_j)$. In this language

$$|a) \longleftarrow |b_1) \longleftarrow |\psi) \quad \text{proceeds with amplitude } (a|b_1)(b_1|\psi)$$
$$|a) \longleftarrow |b_2) \longleftarrow |\psi) \quad \text{proceeds with amplitude } (a|b_2)(b_2|\psi)$$
$$\vdots$$

But one could equally well write

$$(a|\psi) = \sum_j \sum_k (a|b_j)(b_j|c_k)(c_k|\psi) \tag{16.2}$$

and claim that (for example)

$$|a) \leftarrow |b_1) \leftarrow |c_5) \leftarrow |\psi) \quad \text{proceeds with amplitude } (a|b_2)(b_2|c_5)(c_5|\psi)$$

Evidently there is an element of "creative fiction" associated with any claim that $|a) \longleftarrow |\psi)$ proceeds *via* one or another of a population of independent channels or "paths," but every reason to suppose that Feynman's proposal that we (*i*) identify a population of paths which contribute independently to the process $|a) \longleftarrow |\psi)$; (*ii*) assign a probability amplitude to each such path, and (*iii*) write

$$\text{probability amplitude [process]} = \sum_{\text{paths}} \text{probability amplitude [path]} \tag{17}$$

will give correct results if properly managed. We are placed on notice, however, that—owing to the large element of arbitrariness built into the program—it would be a profound mistake (called by philosophers the "fallacy of misplaced concreteness") to suppose that (17) provides a physically literal/correct account of "how quantum processes proceed."[9] But (17) does serve to underscore how radically different from ordinary probability is the probabilistic view of the world presented by the quantum theory:
- in ordinary probability theory one adds the *probabilities* of independent events, while
- in quantum mechanics one adds *probability amplitudes*

and of course

$$\left| \sum \text{amplitudes} \right|^2 \neq \sum \left| \text{amplitudes} \right|^2$$

In a manner of speaking, we have

$$\text{quantum statistics} = \sqrt{\text{ordinary statistics}}$$

---

[9] The meaning I ascribe to a phrase introduced into philosophy in relatively recent times by Alfred North Whitehead may well depart from that intended by him. Virtually all of what physicists say about the structure of the world is susceptible in *some* degree to a charge of "misplaced concreteness," but some statements by some physicists are more blatantly defective than others.

Quantum kinematics/dynamics & the concept of "picture". Acts of quantum mechanical "measurement"—projective state-preparation—are, in all but the most refined accounts, assumed to take place instantaneously. The notion of a "path" $|a) \leftarrow |b_j) \leftarrow |c_k) \leftarrow |\psi)$, as evoked at (16), draws upon a concept of *temporal sequence* (before/after; first this, then that), but makes no use of "metrized time," no use of any concept of *temporal rate of change*. Introduction of the latter notion takes us from the "geometry of quantum mechanics" to quantum kinematics/dynamics.

"Wave mechanics" was designed to provide an account of interference effects which is directly imitative of the interference theory provided by classical acoustics and physical optics. The latter theories are *linear field theories* to which the *principle of superposition* is central: superimposed fields move by superposition of the motion of their component parts. We are led thus to contemplate a quantum kinematics in which—during the intervals between measurements—$|\psi)$ wanders around on the "unit ball," not just any old way, but by <u>*linear*</u> isometry:

$$|\psi)_0 \longrightarrow |\psi)_t = \mathsf{U}(t)|\psi)_0 \tag{18}$$

with $\mathsf{U}(t)$ unitary. Differentiation of (18) gives

$$\tfrac{d}{dt}|\psi)_t = \tfrac{d\mathsf{U}}{dt}\,\mathsf{U}^+|\psi)_t \tag{19}$$

But differentiation of the unitarity condition $\mathsf{U}\mathsf{U}^+ = \mathsf{I}$ gives

$$\tfrac{d\mathsf{U}}{dt}\,\mathsf{U}^+ = -\big\{\text{ditto}\big\}^+ \; : \; \tfrac{d\mathsf{U}}{dt}\,\mathsf{U}^+ \text{ is always and necessarily } \textit{antiself-adjoint}$$

and every antiself-adjoint linear operator A can be written $\mathsf{A} = -i\mathsf{S}$ with S self-adjoint.[10] The implication is that (19) can always be expressed

$$i\tfrac{d}{dt}|\psi)_t = \mathsf{S}|\psi)_t \tag{20.1}$$

and that the "propagator" $\mathsf{U}(t)$ always satisfies a first-order differential equation of the form

$$\tfrac{d}{dt}\mathsf{U} = -i\mathsf{S}\,\mathsf{U} \tag{20.2}$$

Here S can, in principle, be any self-adjoint linear operator with the physical dimension of reciprocal time: $[\mathsf{S}] = (\text{time})^{-1}$.

If S is itself t-independent then (20.2) entails

$$\mathsf{U}(t) = e^{-i\mathsf{S}t}\mathsf{U}(0) \tag{21.1}$$
$$\mathsf{U}(0) = \mathsf{I} \text{ was stipulated at (18)}$$

which when introduced into (18) gives

$$|\psi)_t = e^{-i\mathsf{S}t}|\psi)_0 \tag{21.2}$$

---

[10] The minus sign has been introduced to achieve agreement with established convention.

The unitarity of $\mathbf{U}(t)$ is by itself sufficient to insure that one can in *all* cases write

$$\mathbf{U}(t) = e^{-i\,\mathbf{W}(t)} \quad \text{with } \mathbf{W}(t) \text{ self-adjoint}$$

but only exceptionally[11] does $\mathbf{W}(t)$ admit of simple description.

The differential equation (20.1) can also be expressed

$$|\psi)_t = |\psi)_0 - i\int_0^t \mathbf{S}(\tau)|\psi)_\tau \, d\tau \tag{22}$$

The advantages of doing so are that (i) initial date is built into the design of (22), while at (20.1) it must be carried as a side-condition, and that (ii) invites solution by iteration

$$|\psi)_t = \left\{ \mathbf{I} - i\int_0^t \mathbf{S}(\tau)\,d\tau + (-i)^2 \int_0^t\!\!\int_0^\tau \mathbf{S}(\tau)\mathbf{S}(\sigma)\,d\sigma d\tau + \cdots \right\}|\psi)_0 \tag{23}$$

which in some contexts proves very useful.

Quantum kinematics goes over into quantum dynamics when, as an instance of (12), one posits an association of the form

$$H(x,p) \;\longleftrightarrow\; \mathbf{H} \quad : \quad \text{introduction of the } \textit{Hamiltonian operator} \tag{24}$$

and to $\mathbf{S}$ assigns the specific interpretation $\mathbf{S} = \frac{1}{\hbar}\mathbf{H}$. Equation (20.1) then becomes the time-dependent Schrödinger equation

$$\mathbf{H}|\psi) = i\hbar\tfrac{d}{dt}|\psi) \tag{25}$$

In an important class of cases $\frac{d\mathbf{H}}{dt} = \mathbf{0}$; in such cases one has

$$|\psi)_t = \mathbf{U}(t)|\psi)_0 \quad \text{with} \quad \mathbf{U}(t) = e^{-(i/\hbar)\,\mathbf{H}\,t} \tag{26}$$

If, in such a case, one adopts as an *ansatz* the proposition that

$$|\psi)_t = f(t)\cdot|\Psi)$$

—if one, in other words, assumes "time separation"— then (25) reads

$$f\cdot\mathbf{H}|\Psi) = i\hbar\tfrac{df}{dt}\cdot|\Psi)$$

Assume additionally (and without loss of generality) that $(\Psi|\Psi) = 1$. Then

$$(\Psi|\mathbf{H}|\Psi) = i\hbar\tfrac{df}{dt}\big/f = \text{separation constant } E$$

and we obtain

$$|\psi)_t = e^{-(i/\hbar)E\,t}\cdot|\Psi) \quad \text{with} \quad \mathbf{H}|\Psi) = E\,|\Psi) \tag{27}$$
$$\underset{\text{time-independent Schrödinger equation}}{\uparrow\!\rule{0pt}{0pt}}$$

---

[11] For example: if $\frac{d\mathbf{S}}{dt} = \mathbf{0}$, when—as we have seen—$\mathbf{W}(t) = \mathbf{S}t$.

Exponientated operators are usually (and for many purposes most simply) developed as formal power series—for example

$$\mathsf{U}(t) = \sum_{k=0}^{\infty} \tfrac{1}{k!} \big[-(i/\hbar)\mathsf{H}t \big]^k \tag{28}$$

—but other descriptions are available, and frequently more useful. For example: let $\{|n)\}$ refer to the orthonormal basis which H erects in C_N

$$\mathsf{H}|n) = E_n|n) \tag{29}$$

and assume the spectrum of H to be non-degenerate. Then as an instance of (9) we have

$$\mathsf{H} = \sum_n |n) E_n (n| \tag{30}$$

Orthonormality entails $|m)(m|\cdot|n)(n| = \delta_{mn}|n)(n|$ whence $\mathsf{H}^k = \sum_n |n) E_n^k (n|$ which introduced back into (28) gives

$$\mathsf{U}(t) = \sum_n |n) e^{-(i/\hbar)E_n t} (n| \tag{31}$$

Equation (30) provides the "spectral representation of the Hamiltonian," and (31) the spectral representation of the associated propagator. Application to $|\psi)_0$ yields

$$|\psi)_t = \sum_n |n) e^{-(i/\hbar)E_n t} (n|\psi)_0 \tag{32}$$

which can be interpreted this way: $|n)(n|$ projects out the $|n)$-component which was present in $|\psi)_0$, which the $e^{-(i/\hbar)E_n t}$ factor sets buzzing, with angular frequency $\omega_n = E_n/\hbar$. The motion of $|\psi)_t$ is results from the superposition of those independent (and generally asynchronous) buzzings.

All of which is imagined to proceed *only so long as we don't look*! An A-measurement, if performed at time τ, would yield the (eigen)value a_i with probability $|(a_i|\psi)_\tau|^2$; assuming that the measurement in fact yielded the value a_8 then the subsequent state (up until the time of the next measurement) would be described

$$|\psi)_t = \sum_n |n) e^{-(i/\hbar)E_n(t-\tau)} (n|a_8)_0 \quad : \quad t \geqslant \tau$$

Measurement is projective, and entails (not only the extraction of but also—unavoidably) a *loss of latent information*; from $|\psi)_{t>\tau}$ it is *not possible to retrodict*, not possible to recover properties of $|\psi)_t$ prior to the time of most recent measurement.

Look now to the time-dependence of the expectation value $\langle \mathsf{A} \rangle$. We will make the simplifying assumption (consistent with the facts in most cases) that the operating characteristics of the A-meter are held constant. Then (25) entails

$$\begin{aligned} \tfrac{d}{dt}\langle \mathsf{A} \rangle_t &= \tfrac{1}{i\hbar} \big\{ {}_t(\psi|\mathsf{A}\mathsf{H}|\psi)_t - {}_t(\psi|\mathsf{H}\mathsf{A}|\psi)_t \big\} \\ &= -\tfrac{1}{i\hbar}(\psi|[\mathsf{H},\mathsf{A}]|\psi) \end{aligned} \tag{33}$$

where $[\mathbf{H}, \mathbf{A}] \equiv \mathbf{HA} - \mathbf{AH}$ is the *commutator* of $\mathbf{H}$ with $\mathbf{A}$, and where as henceforth the pedantic $_t$ has been/will be dropped except where its absence might cause confusion. The procedural meaning of $\frac{d}{dt}\langle \mathbf{A} \rangle_t$ is clear, if a little contrived:

- With system $\mathfrak{S}$ in the prepared state $|\psi)_0$, wait a time t, then perform an A-measurement;
- Do this many times, and compute the average of your results. $\langle \mathbf{A} \rangle_t$ is the theoretical estimator of the number thus produced.
- Proceed similarly to obtain the number estimated by $\langle \mathbf{A} \rangle_{t+\delta t}$.
- Construct the datum estimated by $\{\langle \mathbf{A} \rangle_{t+\delta t} - \langle \mathbf{A} \rangle_t\}/\delta t$.

We were led to (33) on the assumption that $\langle \mathbf{A} \rangle_t$ inherits its t-dependence from $|\psi)$, which moves while $\mathbf{A}$ just sits there. That is the "Schrödinger picture" of events. But $\langle \mathbf{A} \rangle = (\psi|\mathbf{A}|\psi)$ is a duplex construct, and we are free to reapportion responsibility for its time-dependence amongst its parts . . . which is to say: we might, for example, consider (33) be result from the proposition that *observables move* by the law

$$\tfrac{d}{dt}\mathbf{A} = -\tfrac{1}{i\hbar}[\mathbf{H}, \mathbf{A}] \tag{34}$$

while the state vector $|\psi)$ just sits there. This is the "Heisenberg picture" of events. To phrase the distinction another way, we have

$$\left. \begin{array}{l} |\psi)_0 \longrightarrow |\psi)_t = \mathbf{U}(t)|\psi)_0 \\ \mathbf{A}_0 \longrightarrow \ \ \mathbf{A}_t = \mathbf{A}_0 \end{array} \right\} \ : \ \text{SCHRÖDINGER PICTURE} \tag{35.1}$$

$$\left. \begin{array}{l} |\psi)_0 \longrightarrow |\psi)_t = |\psi)_0 \\ \mathbf{A}_0 \longrightarrow \ \ \mathbf{A}_t = \mathbf{U}^+(t)\mathbf{A}_0\mathbf{U}(t) \end{array} \right\} \ : \ \text{HEISENBERG PICTURE} \tag{35.2}$$

and in either case obtain

$$(\psi|\mathbf{A}|\psi) \longrightarrow (\psi|\mathbf{U}^+(t)\,\mathbf{A}\,\mathbf{U}(t)|\psi)$$

An infinitude of alternative/intermediate pictures become available when one writes

$$\begin{array}{l} |\psi)_0 \longrightarrow |\psi)_t = \mathbf{W}(t)|\psi)_0 \\ \mathbf{A}_0 \longrightarrow \ \ \mathbf{A}_t = \mathbf{V}^+(t)\mathbf{A}_0\mathbf{V}(t) \end{array}$$

and requires that $\mathbf{V}(t)$ and $\mathbf{W}(t)$ (unitary) satisfy $\mathbf{V}(t)\mathbf{W}(t) = \mathbf{U}(t)$; at least one of those—the so-called "interaction picture," introduced by Dirac in 1926—is of major importance.[12]

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[12] The interaction picture comes into play in situations where $\mathbf{H}$ has the perturbed form $\mathbf{H} = \mathbf{H}_0 + \lambda \mathbf{H}_1$. One lets $\mathbf{H}_0$ govern the motion of operators, and $\mathbf{H}_1$ govern the motion of states. See S. S. Schweber *An Introduction to Relativistic Quantum Field Theory* (1961) §11c; K. Huang, *Quantum Field Theory: From Operators to Path Integrals* (1998) §8.2 or J. Jauch & F. Rohrlich, *The Theory of Photons & Electrons* (1955) §4–3 for details.

Though little mystery attaches to the i which appears on the right side of (34), I mention in passing that its presence can be understood as follows: if $\mathbf{A}(t)$ is self-adjoint then so, necessarily, is its derivative. On the other hand

$$[(\text{self-adjoint}), (\text{self-adjoint})] = \text{antiself-adjoint}$$
$$= i\,(\text{self-adjoint}) \tag{36}$$

And the $\hbar$ is required for dimensional reasons, since $[\mathbf{H}] = (\text{energy})$.

The motion (in the Schrödinger picture) of the density matrix $\boldsymbol{\psi} \equiv |\psi)(\psi|$ can by (25) be described

$$\tfrac{d}{dt}\boldsymbol{\psi} = +\tfrac{1}{i\hbar}[\mathbf{H},\boldsymbol{\psi}] \tag{37.1}$$

or again

$$\boldsymbol{\psi}_0 \longrightarrow \boldsymbol{\psi}_t = \mathbf{U}(t)\,\boldsymbol{\psi}_0 \mathbf{U}^+(t) \tag{37.2}$$

Equation (37.1) resembles (34) except for the sign; similarly, (37.2) resembles (35.2) except for the reversed placement of the $^+$ marks. The origin of those critical distinctions can be understood as follows:

$$\langle \mathbf{A} \rangle_0 = \text{tr}\,\mathbf{A}\boldsymbol{\psi} \longrightarrow \langle \mathbf{A} \rangle_t = \underset{\text{Schrödinger}}{\text{tr}\,\mathbf{A} \cdot \mathbf{U}\boldsymbol{\psi}\mathbf{U}^+} = \underset{\text{Heisenberg}}{\text{tr}\,\mathbf{U}^+\mathbf{A}\mathbf{U} \cdot \boldsymbol{\psi}} \tag{38}$$

where we have made use of a fundamental property of the trace: $\text{tr}\mathbb{A}\mathbb{B} = \text{tr}\mathbb{B}\mathbb{A}$.

In the Heisenberg picture operators, generally speaking, move. But it is an immediate implication of (34) that if $\mathbf{A}$ *commutes* with $\mathbf{H}$ then $\mathbf{A}$ does *not* move but just sits there—a constant of the motion:

$$\text{if } [\mathbf{H}, \mathbf{A}] = \mathbf{0} \text{ then } \mathbf{A}_t = \mathbf{A}_0 \text{ (all } t) \tag{39}$$

The motion of *expectation values* is picture-independent (and therefore of deeper intrinsic interest); evidently

$$\langle \mathbf{A} \rangle_\psi \text{ is, for all } |\psi), \text{ a constant of the motion iff } [\mathbf{H}, \mathbf{A}] = \mathbf{0} \tag{40}$$

The "picture" concept is latent (if seldom exploited) already in classical mechanics. If $\rho(\xi; 0)$ describes some initial distribution of state points on phase space, and if $A(\xi)$ is some observable,[13] then

$$\langle A \rangle_0 = \int A(\xi)\rho(\xi, 0)\,d\xi$$

describes the average of the values assumed by A at those state points. By solution of (1) we obtain $\rho(\xi, t)$, and in the "classical Schrödinger picture" would at subsequent times write

$$\langle A \rangle_t = \int A(\xi)\rho(\xi, t)\,d\xi$$

---

[13] I again use ξ to stand for the entire set $\{q^1, q^2, \ldots, q^n;\ p_1, p_2, \ldots, p_n\}$ of phase space coordinates, and understand $d\xi$ to mean $dq^1 \cdots dq^n dp_1 \cdots dp_n$.

But $\langle A \rangle$ is a "duplex construct;" we could, if we wished, transfer some or all of the time-dependence from the distribution ρ to the observable A, writing (in the latter instance)

$$\langle A \rangle_t = \int A(\xi, t) \rho(\xi) \, d\xi$$

We would have arrived then in the "classical Heisenberg picture."

Poisson brackets & commutators. Hamilton's canonical equations of motion can be written

$$\left. \begin{array}{l} \frac{d}{dt} q^i = -[H, q^i] = +\partial H/\partial p_i \\[2mm] \frac{d}{dt} p_i = -[H, p_i] = -\partial H/\partial q^i \end{array} \right\} \tag{41}$$

where the Poisson bracket is defined

$$[A, B] \equiv \sum_k \left\{ \frac{\partial A}{\partial q^k} \frac{\partial B}{\partial p_k} - \frac{\partial B}{\partial q^k} \frac{\partial A}{\partial p_k} \right\} \tag{42}$$

The rate of variation of $A(q, p)$, induced by the dynamical variation of its arguments, can therefore be described

$$\frac{d}{dt} A = -[H, A] \tag{43}$$

from which (41) can be recovered as particular instances. Equations (43) and (34) present similar marks on the page, but mean quite different things. Yet—as will ultimately emerge—not so different as might at first appear.

What follows is a list of *general properties of the Poisson bracket*.[14]

$$\begin{array}{rll} \text{ANTISYMMETRY} : & [A, B] + [B, A] = 0 & (44.1) \\[2mm] \text{BILINEARITY} : & [A, \beta_1 B_1 + \beta_2 B_2] = \beta_1[A, B_1] + \beta_2[A, B_2] & (44.2) \\[2mm] \text{PRODUCT RULE} : & [A, BC] = [A, B]C + B[A, C] & (44.3) \\[2mm] \text{JACOBI IDENTITY} : & [A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 & (44.4) \end{array}$$

The product rule stems from the circumstance that

$$\mathcal{D}_A \equiv [A, \bullet] \equiv \sum_k \left\{ \frac{\partial A}{\partial q^k} \frac{\partial}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial}{\partial q^k} \right\} \tag{45}$$

is a kind of glorified differentiation operator; note, however, the placement of the factors (C comes *after* the $[A, B]$ bracket, and B before the $[A, C]$ bracket), which makes no difference at present, but will after A, B and C have been transmuted into non-commutative operators A, B and C. Note also that the Jacobi identity, rewritten $[A, [B, \bullet]] - [B, [A, \bullet]] = [[A, B], \bullet]$, entails

$$\mathcal{D}_A \mathcal{D}_B - \mathcal{D}_B \mathcal{D}_A = \mathcal{D}_{[A,B]} \tag{46}$$

---

[14] For more detailed discussion and references see CLASSICAL MECHANICS (1983), pp. 258 *et seq*.

which is sometimes useful.

Remarkably, the list (44) is precisely mimiced by the following list of *general properties of the commutator*:

$$\text{ANTISYMMETRY} : \quad [\mathbf{A}, \mathbf{B}] + [\mathbf{B}, \mathbf{A}] = \mathbf{0} \tag{47.1}$$

$$\text{BILINEARITY} : \quad [\mathbf{A}, \beta_1 \mathbf{B}_1 + \beta_2 \mathbf{B}_2] = \beta_1 [\mathbf{A}, \mathbf{B}_1] + \beta_2 [\mathbf{A}, \mathbf{B}_2] \tag{47.2}$$

$$\text{PRODUCT RULE} : \quad [\mathbf{A}, \mathbf{B}\,\mathbf{C}] = [\mathbf{A}, \mathbf{B}]\mathbf{C} + \mathbf{B}[\mathbf{A}, \mathbf{C}] \tag{47.3}$$

$$\text{JACOBI IDENTITY} : \quad [\mathbf{A}, [\mathbf{B}, \mathbf{C}]] + [\mathbf{B}, [\mathbf{C}, \mathbf{A}]] + [\mathbf{C}, [\mathbf{A}, \mathbf{B}]] = \mathbf{0} \tag{47.4}$$

In (47.3) the placement of the $\mathbf{B}$ and $\mathbf{C}$ factors has now become critical.

Reverting for a moment from commutators to Poisson brackets: Let $A(q, p)$ and $B(q, p)$ be present as sums/products of their arguments. Then with the aid of (44) the bracket $[A(q, p), B(q, p)]$ can be reduced to the form

$$[A, B] = \sum \text{terms of the form } (\text{stuff}) \cdot [q^i, p_j] \cdot (\text{stuff})$$

so that if one possessed descriptions of the "primitive brackets" $[q^i, p_j]$ one would be in position to evaluate $[A, B]$ without doing any differentiation. And if fact we do possess descriptions of the primitive brackets; we have

$$\left. \begin{array}{c} [q^i, q^j] = [p_i, p_j] = 0 \qquad (\text{all } i \text{ and } j) \\[2mm] [q^i, p_j] = \delta^i{}_j \end{array} \right\} \tag{48}$$

EXAMPLE: Let $\boldsymbol{x} \equiv \{x_1, x_2, x_3\}$ refer to a Cartesian coordinate system, and look to the triple of observables (components of angular momentum) defined

$$L_1(x, p) \equiv x_2 p_3 - x_3 p_2$$
$$L_2(x, p) \equiv x_3 p_1 - x_1 p_3$$
$$L_3(x, p) \equiv x_1 p_2 - x_2 p_1$$

Then

$$[L_1, L_2] = [x_2 p_3, x_3 p_1] - [x_2 p_3, x_1 p_3] - [x_3 p_2, x_3 p_1] + [x_3 p_2, x_1 p_3]$$

But $[x_i p_j, x_k p_l] = [x_i, x_k]p_j p_l + x_k[x_i, p_l]p_j + x_i[p_j, x_k]p_l + x_i x_k[p_j, p_l]$ so we have

$$\begin{aligned} [L_1, L_2] =& + [x_2, x_3]p_3 p_1 + x_3[x_2, p_1]p_3 + x_2[p_3, x_3]p_1 + x_2 x_3[p_3, p_1] \\ & - [x_2, x_1]p_3 p_3 - x_1[x_2, p_3]p_3 - x_2[p_3, x_1]p_3 - x_2 x_1[p_3, p_3] \\ & - [x_3, x_3]p_2 p_1 - x_3[x_3, p_1]p_2 - x_3[p_2, x_3]p_1 - x_3 x_3[p_2, p_1] \\ & + [x_3, x_1]p_2 p_3 + x_1[x_3, p_3]p_2 + x_3[p_2, x_1]p_3 + x_3 x_1[p_2, p_3] \\ =& -x_2 p_1 + x_1 p_2 + \text{fourteen 0's} \\ =& \ L_3 \end{aligned}$$

Similarly $[L_2, L_3] = L_1$ and $[L_3, L_1] = L_2$. Moreover

$$
\begin{aligned}
[L_1, L^2] =\ & [L_1, L_1]L_1 + L_1[L_1, L_1] \\
& + [L_1, L_2]L_2 + L_2[L_1, L_2] \\
& + [L_1, L_3]L_3 + L_3[L_1, L_3] \\
=\ & L_3 L_2 + L_2 L_3 - L_2 L_3 - L_3 L_2 \\
=\ & 0
\end{aligned}
$$

and by the same argument $[L_2, L^2] = [L_3, L^2] = 0$. I don't claim "bracket evaluation by atomization" (i.e, by reduction to primitive brackets) is a notably efficient procedure, only that it works (though it is in fact much more efficient than the pedantic detail of the example might suggest; in practice one would omit all obvious steps, and find the procedure to be actually quite efficient).

The point is that the procedure just described would work also quantum mechanically if one possessed descriptions of the primitive commutators. Those were supplied by Dirac, who postulated that quantization sends the statements (48) over into

$$
\left.
\begin{aligned}
[\mathbf{q}^i, \mathbf{q}^j] = [\mathbf{p}_i, \mathbf{p}_j] = \mathbf{0} \quad \text{(all } i \text{ and } j) \\
[\mathbf{q}^i, \mathbf{p}_j] = i\hbar \delta^i{}_j \mathbf{I}
\end{aligned}
\right\}
\tag{49}
$$

The rationale for the introduction of the $i\hbar$ factor has already been explained in another connection: the $\hbar$ is dimensionally forced, and the i is needed to make the right expression on the right conform to the antiself-adjointness of the expression on the left.

Drawing upon (49), our recent example can be used without change to supply

$$
[\mathbf{L}_1, \mathbf{L}_2] = i\hbar \mathbf{L}_3, \quad \text{etc.} \tag{50.1}
$$

and

$$
[\mathbf{L}_1, \mathbf{L}^2] = \mathbf{0}, \quad \text{etc., with} \quad \mathbf{L}^2 \equiv (\mathbf{L}_1)^2 + (\mathbf{L}_2)^2 + (\mathbf{L}_3)^2 \tag{50.2}
$$

For an alternative (and, in my view, even more tedious) derivation of these classic formulæ see §4.3 in Griffiths.

In quantum mechanics the phase coordinates q^i and p_j are replaced by self-adjoint linear operators $\mathbf{q}^j$ and $\mathbf{p}_k$ which *fail to commute, but only weakly*, in the sense that (according to (49)) they *commute with their commutators*:[15]

$$
[\mathbf{q}^i, [\mathbf{q}^j, \mathbf{p}_k]] = [\mathbf{p}_i, [\mathbf{q}^j, \mathbf{p}_k]] = \mathbf{0} \quad \text{(all } i, j \text{ and } k) \tag{51}
$$

"Weak non-commutativity" is, however, the ultimate source of much that is most distinctive about the quantum theory.

---

[15] The argument can be turned around: one can show that if $\mathbf{q}^i$ and $\mathbf{p}_j$ satisfy (49) and if $[\mathbf{q}^i, \mathbf{M}] = [\mathbf{p}_i, \mathbf{M}] = \mathbf{0}$ then necessarily $\mathbf{M}$ is a multiple of $\mathbf{I}$. See Appendices A & B in Ballentine[5] or §19 in Jordan[4] for details.

Why is quantum state space necessarily infinite-dimensional? The simple answer is implicit in the thread that ties formalism to observation. If we propose to associate position-measuring metersticks with linear operators $\mathbf{x}$, if we propose more particularly to associate the results x of position measurement with the eigenvalues of $\mathbf{x}$, and if the conceivable results of such measurement are to be associated with (which is to say: as numerous as) points on the real line, then the *spectrum of* $\mathbf{x}$ *must be continuous*, and no finite-dimensional matrix $\mathbb{X}$ can claim that distinction. (The argument would, however, fail if physical space were in fact discrete and finite, and we can only advance good but imperfect observational evidence in defense of the proposition that it isn't.)

Actually, we lost the prospect of a "finite-dimensional quantum mechanics" when at (49) we postulated a commutation relation of the form

$$[\mathbf{x}, \mathbf{p}] = i\hbar\, \mathbf{I} \tag{52}$$

for in $N \times N$ matrix representation

$$\mathbb{X}\,\mathbb{P} - \mathbb{P}\,\mathbb{X} = i\hbar\,\mathbb{I} \tag{53}$$

it would follow upon formation of the trace that $0 = i\hbar N$, which is absurd: finite-dimensional matrices $\mathbb{X}$ and $\mathbb{P}$ which satisfy (53)—whether hermitian or not—*cannot exist*. It is not immediately evident how the force of that simple argument fails in the limit $N \to \infty$, but examples (of which we will encounter many) serve to clarify the point; the following example has been borrowed from the quantum theory of oscillators.[16] Let

$$\mathbb{X}_6 \equiv \sqrt{\hbar/2}\begin{pmatrix} 0 & +\sqrt{1} & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & +\sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & +\sqrt{3} & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & +\sqrt{4} & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 & +\sqrt{5} \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \end{pmatrix}$$

$$\mathbb{P}_6 \equiv i\sqrt{\hbar/2}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 & -\sqrt{5} \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \end{pmatrix}$$

Then (ask *Mathematica*)

$$\mathbb{X}_6\mathbb{P}_6 - \mathbb{P}_6\mathbb{X}_6 = i\hbar\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -5 \end{pmatrix}$$

---

[16] See pp. 48, 34 & 80 in Chapter 2 of QUANTUM MECHANICS (1967).

which make obvious how one should define $\mathbb{X}_N$ and $\mathbb{P}_N$, and that

$$\mathbb{X}_N\mathbb{P}_N - \mathbb{P}_N\mathbb{X}_N = i\hbar \underbrace{\begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & (1-N) \end{pmatrix}}$$

traceless ... funny entry gets pushed off page as $N\to\infty$

So every matrix representation of the fundamental commutation relation $[\mathbf{x}, \mathbf{p}] = i\hbar\,\mathbf{I}$ is necessarily ∞-dimensional, ∞-dimensional representations do in fact exist, and it can be shown, moreover, that distinct representations $\{\mathbb{X}, \mathbb{P}\}$ and $\{\mathbb{X}', \mathbb{P}'\}$ are always unitarily equivalent. Finite-dimensional models of quantum mechanics are impossible, but *models of those aspects of quantum theory which are independent of* $[\mathbf{x}, \mathbf{p}] = i\hbar\,\mathbf{I}$ *are possible, and are often quite informative.*

In full-blown quantum theory all previous references to C_N should be replaced by references to C_∞. Which is quite a different place. Does

$$C_N \longrightarrow C_\infty$$

make a difference? Certainly. Infinite-dimensionality means that finite sums become infinite sums, and one must introduce sufficient structure to insure convergence, and attend to other delicate matters; one must, in short, invent "Hilbert space." [17]

Well-bred physicists are often quick to genuflect toward Hilbert space, and some physicists (typically those with nothing more physical to do) seem actually to enjoy visits to that arid land, from which they tend to return fired with the zeal of missionaries, muttering obscurely. But most work-a-day physicists give thought to the established religion only in moments of peril, when their work has gone off-track ... or threatens to. They are content—as I am content—to proceed with sometimes reckless informality, confident that Nature will forgive and correct their errors. What was good enough for Dirac is—if not good enough for von Neumann, who wrote in reaction to Dirac—good enough for us.

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[17] See sources like Griffiths, p. 100; Ballentine §1–4 or Jordan §3 for short introductions. And monographs (of which there are many) like P. Halmos, *Introduction to Hilbert Space* (1951), F. Riesz & B. Sz.-Nagy, *Functional Analysis* (1955) or J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (1927/1932, English translation 1955) for the gory details. Hilbert's work was done in connection with the theory of integral equations, during the first decade of the century; its special appropriateness to quantum mechanics was first emphasized by the 23-year-old von Neumann (1903–1957). Historical details can be found in §6.3 in Max Jammer's indispensable (but currently out of print) *Conceptual Development of Quantum Mechanics* (1966).

On the assumption that **A** has a (non-degenerate) *discrete* spectrum, we have in the past written

$$\mathbf{A}|a_i) = a_i|a_i)$$

with

$$\sum_i |a_i)(a_i| = \mathbf{I} \quad \text{and} \quad (a_i|a_j) = \delta_{ij}$$

With $N \to \infty$ we are forced to recognize the possibility that the spectrum of **A** may be continuous, and find it natural in such cases to write

$$\mathbf{A}|a) = a|a) \tag{54}$$

with

$$\int |a)\,da(a| = \mathbf{I} \quad \text{and} \quad (a|b) = \delta(a-b) \tag{55}$$

and (with Dirac) to impute such properties to the "δ-function" (continuous analog of the Kronecker delta) as are sufficient to insure

$$\int |a)\,da(a|b) = \int |a)\,\delta(a-b)\,da = |b)$$

We will frequently find it convenient to retain that continuity-adapted notation even in cases where the spectrum is discrete (or mixed discrete/continuous, like the energy spectrum of the hydrogen atom).

The position operator **X** (which in a 3-dimensional world would be written $\mathbf{X}^1$ joined also by $\mathbf{X}^2$ and $\mathbf{X}^3$) provides just such an occasion: we write

$$\mathbf{X}|x) = x|x) \tag{56}$$

and claim

$$\int |x)\,dx(x| = \mathbf{I} \quad \text{and} \quad (x|y) = \delta(x-y) \tag{57}$$

Then

$$\begin{aligned}|\psi) &= \int |x)\,dx(x|\psi) \\ &= \int |x)\,\underbrace{\psi(x)}\,dx \end{aligned} \tag{58}$$

"wavefunction" $\equiv$ coordinates $(x|\psi)$ of $|\psi)$ in the x-representation

It was in x-representation—as a theory about $\psi(x)$—that Schrödinger's version of quantum mechanics was first presented to the world, but it appears to have evident from the outset to both Dirac and Jordan[18] that the abstract essence of the situation was much simpler and more elegant than Schrödinger initially represented it to be.

[18] Ernst Pascual Jordan (1902–1980) became associated with Courant, Born, Debye and others soon after he arrived as an undergraduate in Göttingen, where

The abstract Schrödinger equation (25) can, in x-representation, be written

$$\int (x|\mathbf{H}|y)\psi(y,t)\,dy = i\hbar\tfrac{\partial}{\partial t}\psi(x,t) \tag{59}$$

which in integrated form (26) becomes

$$\psi(x,t) = \int (x|\mathbf{U}(t)|y)\,\psi(y,0)\,dy$$

$$= \int G(x,t;y,0)\,\psi(y,0)\,dy \quad \text{with} \quad G(x,t;y,0) \equiv (x|\mathbf{U}(t)|y) \tag{60}$$

The *propagator* $\mathbf{U}(t)$ has in representation become the *Green's function*. If the Hamiltonian is time-independent then we have (31), which becomes

$$G(x,t;y,0) = \sum_n (x|n)e^{-(i/\hbar)E_n t}(n|y) \tag{61.1}$$

$$= \sum_n e^{-(i/\hbar)E_n t}\,\Psi_n(x)\Psi_n^*(y) \tag{61.2}$$

where the energy eigenfunctions (no longer called eigen*vectors*) arise from (29):

$$\int (x|\mathbf{H}|y)\Psi(y)\,dy = E_n\Psi(x) \tag{62}$$

(continued from the preceding page) he assisted in the editorial work on the first volume of Courant & Hilbert (1924) and became Born's assistant (successor to Heisenberg and Pauli). He received his doctorate in 1924 at the age of twenty-two, for work which engaged the interest of Einstein. For a period of less than a decade he contributed brilliantly to the development of quantum mechanics—M. Born & P. Jordan, "Zur Quantenmechanik. I" Z. Physik **34**, 858 (1925), which provided elaborate commentary on Heisenberg's quantum theory and presented the first clear indication of the central importance of $[\mathbf{x},\mathbf{p}] = i\hbar\,\mathbf{I}$, appeared only two months after that theory was announced, and a companion paper (co-authored by Heisenberg: Z. Physik **35**, 557 (1925)) laid the foundations of what was to become quantum field theory; in 1926 he and Dirac (independently) created the synthesis of then-prevailing variants of quantum mechanics which became known as "statistical transformation theory" —but by the mid-1930's his work had shifted to "quantum biology." His Nazi sympathies (he appears to have been something of a political opportunist) complicated his post-war professional life, though he served 1957–1961 as a member of the German Bundestag under Adenauer, and was active in the creation of law relating to the peaceful uses of atomic energy. His early work was very highly regarded by his peers (Pauli *et al*), and was often marked by deft mathematical finesse. See Volume 17, Supplement II of the *Dictionary of Scientific Biography* for more detail relating to the life and accomplishment of this strange man, this neglected founding father of quantum mechanics.

Spectral discreteness (such as the discreteness of the energy spectrum assumed in the last few equations) arises—here as in the theory of musical strings—from physically-motivated stipulations that $(x|\psi)$ must conform to certain *side conditions*, which invariably include

- single-valuedness
- normalizability

and, more contingently, may include

- boundary conditions
- periodicity conditions
- symmetry conditions.

Notice that some of these are difficult to formulate *except* in the language afforded by a representation (though their physical significance must, in the end—as all things must—be representation independent).

Expectation values can in x-representation be described by formulæ of the form

$$\langle \mathbf{A} \rangle = \iint \psi^*(y)(y|\mathbf{A}|x)\psi(x)\,dydx \tag{63}$$

which is a special case becomes

$$\begin{aligned}
\langle \mathbf{X} \rangle &= \iint \psi^*(y)(y|\mathbf{X}|x)\psi(x)\,dydx \\
&= \iint \psi^*(y)\,x\,\delta(y-x)\psi(x)\,dydx \\
&= \int \psi^*(x)\,x\,\psi(x)\,dx
\end{aligned} \tag{64}$$

It is from this result that we acquire the familiar statement

$$\begin{aligned}
P(x) \equiv \text{probability density in } x\text{-space} &= |\psi(x,t)|^2 \tag{65} \\
&= (\psi|\boldsymbol{x}|\psi) \text{ with } \boldsymbol{x} \equiv |x)(x| \\
&= (x|\boldsymbol{\psi}|x) \text{ with } \boldsymbol{\psi} \equiv |\psi)(\psi|
\end{aligned}$$

from which it follows that[19]

$$\tfrac{\partial}{\partial t}P + \tfrac{1}{i\hbar}(\psi|[\mathbf{H},\boldsymbol{x}]|\psi) = 0 \tag{66}$$

This equation describes the "local conservation of probability," and will later be brought to more familiar form.

When at (59) we drew upon the "abstract Schrödinger equation" (25) we lapsed tacitly into the Schrödinger picture. Results of rather different appearance (which are in some contexts more useful) are obtained if one elects instead to work in the Heisenberg picture ... where observables move (unless

---

[19] Be careful not to confuse the projection operator $\boldsymbol{x} \equiv |x)(x|$ with the position operator $\mathbf{x} = \int |x)x\,dx(x|$.

they happen to commute with the Hamiltonian), and carry their eigenvectors with them. In the Heisenberg picture we would, in place of (56), write

$$\mathbf{X}(t)|x,t) = x|x,t) \tag{67}$$

with[20] $\mathbf{X}(t) = \mathbf{U}^{-1}(t)\,\mathbf{X}\,\mathbf{U}(t)$ and

$$|x,t) \equiv \mathbf{U}^{-1}(t)|x) \quad \text{whence} \quad (x,t| = (x|\,\mathbf{U}(t) \tag{68}$$

and in place of (57) write (at all times t)

$$\int |x,t)\,dx\,(x,t| = \mathbf{I} \quad \text{and} \quad (x,t|y,t) = \delta(x-y) \tag{69}$$

The state ket $|\psi)$ does now not move, but its *coordinates with respect to the moving basis* do; we have (compare (58): I write $|\psi)_{\text{fixed}}$ in place of $|\psi)$ for emphasis, but will immediately abandon that device)

$$|\psi)_{\text{fixed}} = \int |x,t)\,dx\,(x,t|\psi)_{\text{fixed}}$$

which lends a new interpretation to $\psi(x,t)$:

$$\psi(x,t) = \begin{cases} (x|\psi)_t & \text{in the Schrödinger picture} \\ (x|\,\mathbf{U}(t)|\psi) & \\ (x,t|\psi) & \text{in the Heisenberg picture} \end{cases} \tag{70}$$

The Green's function acquires the description

$$G(x,t;y,0) = (x,t|y,0) = \begin{cases} \text{inner products of evolved eigenbasis} \\ \text{with respect to original eigenbasis} \end{cases} \tag{71}$$

which marks the starting point of some important work by Julian Schwinger that we will have occasion to examine.[21]

I have now to agree with the attentive reader who has remarked that, as it stands, (59) does not look much like the Schrödinger equation

$$\left\{ \tfrac{1}{2m}\left(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\right)^2 + V(x) \right\}\psi(x,t) = i\hbar\tfrac{\partial}{\partial t}\psi(x,t)$$

of the textbooks, and that (66) does not much resemble the familiar continuity equation

$$\tfrac{\partial}{\partial t}P + \tfrac{\partial}{\partial x}\left[\tfrac{\hbar}{2im}\left(\psi^*\tfrac{\partial}{\partial x}\psi - \psi\tfrac{\partial}{\partial x}\psi^*\right) \right] = 0$$

---

[20] Since $\mathbf{U}$ is unitary we can write $\mathbf{U}^+$ and $\mathbf{U}^{-1}$ interchangeably; I find it convenient here to use the latter notation.

[21] In the meantime, see Chapter 3 in Schwinger's *Quantum Kinematics & Dynamics* (1970). It is typical of Schwinger that he neglects to *mention* that he works in the Heisenberg picture.

To get from here to there we must digress to acquire sharper tools for the management of non-commutative objects (linear operators, matrices), and more particularly for developing the implications of $[\mathbf{x}, \mathbf{p}] = i\hbar\,\mathbf{I}$.

Rudiments of Campbell-Baker-Hausdorff theory. The theory to which I allude was, for the most part, ready-made by the time quantum physicists discovered they had need of it, having been developed $\sim$1900 by mathematicians who (it is my understanding) drew their inspiration from problems posed by the classical theory of Lie groups/algebras. Founding fathers of the field were J. E. Campbell (1898), H. F. Baker (1902/3/4) and F. Hausdorff (1906).[22] It is, if still relatively little known, a seductive subject of broad applicability; I will try to confine my remarks here to the most characteristic methods and most immediately useful results.

Let $\mathbf{A}$ and $\mathbf{B}$ be any objects which can be added and multiplied. They may be linear operators, or matrices ... but for present purposes need carry no such specific interpretation. Multiplication is assumed to be associative but need not be commutative; indeed, it is *management of non-commutativity* that sparks the whole enterprise. We agree to manipulate infinite series formally, writing things like

$$e^{\mathbf{A}} = \mathbf{I} + \mathbf{A} + \tfrac{1}{2!}\mathbf{A}^2 + \cdots$$

$$(\mathbf{I} - \mathbf{A})^{-1} = \mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \cdots$$

without regard to questions of convergence (which we would be powerless to address anyway, so simply have we equipped ourselves).

We begin with the demonstration that

$$e^{\mathbf{A}}\,\mathbf{B}\,e^{-\mathbf{A}} = \mathbf{B} + [\mathbf{A}, \mathbf{B}] + \tfrac{1}{2!}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \cdots \tag{72.1}$$

To that end we—characteristic trick—*introduce a parameter*, writing

$$\mathbf{F}(u) \equiv e^{u\mathbf{A}}\,\mathbf{B}\,e^{-u\mathbf{A}}$$

Then

$$\tfrac{d}{du}\mathbf{F}(u) = e^{u\mathbf{A}}[\mathbf{A}, \mathbf{B}]e^{-u\mathbf{A}}$$

$$\left(\tfrac{d}{du}\right)^2 \mathbf{F}(u) = e^{u\mathbf{A}}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]]e^{-u\mathbf{A}}$$

$$\vdots$$

$$\left(\tfrac{d}{du}\right)^n \mathbf{F}(u) = e^{u\mathbf{A}}\underbrace{[\mathbf{A}, \ldots [\mathbf{A}, [\mathbf{A}, \mathbf{B}]]\ldots]}_{n\text{-fold ``nested commutator''}}e^{-u\mathbf{A}}$$

and by formal Taylor expansion about $u = 0$ we have

$$e^{u\mathbf{A}}\,\mathbf{B}\,e^{-u\mathbf{A}} = \mathbf{B} + [\mathbf{A}, \mathbf{B}]u + \tfrac{1}{2!}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]]u^2 + \cdots$$

---

[22] A splendid review of the field, with many references, has been published by R. M. Wilcox: "Exponential operators and parameter differentiation in quantum physics," J. Math. Phys. **8**, 962 (1967).

which at $u = 1$ gives the identity we sought to establish.

The occurance of "nested commutators"[23]—which some authors[24] call "Lie brackets"—is, by the way, a characteristic feature of Campbell-Baker-Hausdorff theory. It often proves convenient to write

$$\{\mathbf{A}^n, \mathbf{B}\} \equiv \begin{cases} \mathbf{B} & : \quad n = 0 \\ [\mathbf{A}, \dots, [\mathbf{A}, [\mathbf{A}, \mathbf{B}]] \dots] & : \quad n = 1, 2, \dots \end{cases}$$

in which notation (72.1) becomes

$$e^{\mathbf{A}} \mathbf{B} e^{-\mathbf{A}} = \{e^{\mathbf{A}}, \mathbf{B}\}$$

If $f(\cdot)$ refers to any formal power series, then it is elementary that

$$e^{\mathbf{A}} f(\mathbf{B}) e^{-\mathbf{A}} = f(e^{\mathbf{A}} \mathbf{B} e^{-\mathbf{A}})$$

which in the case $f(\cdot) = \exp(\cdot)$ becomes

$$e^{\mathbf{A}} e^{\mathbf{B}} e^{-\mathbf{A}} = \exp\{e^{\mathbf{A}} \mathbf{B} e^{-\mathbf{A}}\} = e^{\mathbf{B} + [\mathbf{A}, \mathbf{B}] + \frac{1}{2}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \cdots} \tag{72.2}$$

Suppose it were the case that

SPECIAL CIRCUMSTANCE : $\mathbf{A}$ and $\mathbf{B}$ <u>commute</u> with $[\mathbf{A}, \mathbf{B}]$ $\qquad (\star)$

The infinite series then truncates; we have $e^{\mathbf{A}} e^{\mathbf{B}} e^{-\mathbf{A}} = e^{\mathbf{B} + [\mathbf{A}, \mathbf{B}]} = e^{[\mathbf{A}, \mathbf{B}]} \cdot e^{\mathbf{B}}$ giving[25]

$$e^{\mathbf{A}} e^{\mathbf{B}} = e^{[\mathbf{A}, \mathbf{B}]} \cdot e^{\mathbf{B}} e^{\mathbf{A}} \tag{$\star$72.3}$$

Let $(\star)$ be expressed

$$[\mathbf{A}, \mathbf{C}] = [\mathbf{B}, \mathbf{C}] = \mathbf{0} \quad \text{with} \quad \mathbf{C} \equiv [\mathbf{A}, \mathbf{B}] \tag{$\star\star$}$$

and note that the left side of $(\star72.3)$ is "$\mathbf{AB}$-ordered:" all $\mathbf{A}$'s stand to the left of all $\mathbf{B}$'s. Equation $(\star72.3)$ describes the result of using

$$\mathbf{A}\,\mathbf{B} = \mathbf{B}\,\mathbf{A} + \mathbf{C} \tag{73.4}$$

and $(\star\star)$ to pull all $\mathbf{A}$'s through to the right, so as to achieve the reversed "$\mathbf{BA}$-ordering." Reordering can be tedious business, and the design of rational procedures for accomplishing such an objective is a problem area central to the present theory.

---

[23] Commutators of commutators ... are "nested" if and only if all ['s stand to the left of all]'s: $[\bullet[\bullet[\bullet[\bullet, \bullet]]]]$ is nested, but $[[\bullet[\bullet, \bullet]], [\bullet, \bullet]]$ isn't.

[24] See W. Magnus, "On the exponential solution of differential equations for a linear operator," Comm. Pure & Appl. Math. **7**, 649 (1954)

[25] I will use $\star$ to flag equations in which $[\mathbf{A}, [\mathbf{A}, \mathbf{B}]] = [\mathbf{B}, [\mathbf{A}, \mathbf{B}]] = \mathbf{0}$ are presumed.

Expansion of $e^{\mathbf{A}+\mathbf{B}}$ presents $\mathbf{A}$'s and $\mathbf{B}$'s in all orders:

$$
\begin{aligned}
e^{\mathbf{A}+\mathbf{B}} = \ &\mathbf{I} + (\mathbf{A}+\mathbf{B}) \\
&+ \tfrac{1}{2!}(\mathbf{A}\,\mathbf{A} + \mathbf{A}\,\mathbf{B} + \mathbf{B}\,\mathbf{A} + \mathbf{B}\,\mathbf{B}) \\
&+ \tfrac{1}{3!}(\mathbf{A}\,\mathbf{A}\,\mathbf{A} + \mathbf{A}\,\mathbf{A}\,\mathbf{B} + \mathbf{A}\,\mathbf{B}\,\mathbf{A} + \mathbf{B}\,\mathbf{A}\,\mathbf{A} \\
&\qquad\ + \mathbf{B}\,\mathbf{B}\,\mathbf{A} + \mathbf{B}\,\mathbf{A}\,\mathbf{B} + \mathbf{A}\,\mathbf{B}\,\mathbf{B} + \mathbf{B}\,\mathbf{B}\,\mathbf{B}) + \cdots
\end{aligned}
$$

What can one say—in general, and in the special case $(\star)$—about the $\mathbf{AB}$-ordered (else $\mathbf{BA}$-ordered) form of the expression on the right? Zassenhaus, in unpublished work first reported by Magnus, obtained

$$
e^{\mathbf{A}+\mathbf{B}} = e^{\mathbf{A}} e^{\mathbf{B}} e^{\mathbf{C}_2} e^{\mathbf{C}_3} \cdots \tag{73.5}
$$

with

$$
\begin{aligned}
&\mathbf{C}_2 = -\tfrac{1}{2}[\mathbf{A},\mathbf{B}] \\
&\mathbf{C}_3 = \tfrac{1}{6}[\mathbf{A},[\mathbf{A},\mathbf{B}]] + \tfrac{1}{3}[\mathbf{B},[\mathbf{A},\mathbf{B}]] \\
&\quad\vdots \\
&\mathbf{C}_n = \text{recursively-determined linear combination of nested commutators}
\end{aligned}
$$

In the special case $(\star)$ the $\mathbf{C}_n$ with $n > 2$ all vanish, leaving

$$
e^{\mathbf{A}+\mathbf{B}} = \begin{cases} e^{-\frac{1}{2}\mathbf{C}} \cdot e^{\mathbf{A}} e^{\mathbf{B}} & : \quad \mathbf{AB}\text{-ordered} \\[2ex] e^{+\frac{1}{2}\mathbf{C}} \cdot e^{\mathbf{B}} e^{\mathbf{A}} & : \quad \mathbf{BA}\text{-ordered} \end{cases} \tag{$\star$73.6}
$$

which were first obtained by W. O. Kermack & W. H. McCrea.[26] This result will assume such importance that I give now a direct derivation, along lines devised by N. H. McCoy.[27]

Let us agree to write

$$
{}_{\mathbf{A}}\big[f(A,B)\big]_{\mathbf{B}} = \text{result of } \mathbf{AB}\text{-ordered substitution into } f(A,B) \tag{73.7}
$$

Thus

$$
{}_{\mathbf{A}}\big[e^{A+B}\big]_{\mathbf{B}} = e^{\mathbf{A}} e^{\mathbf{B}} \qquad \text{but} \qquad {}_{\mathbf{B}}\big[e^{A+B}\big]_{\mathbf{A}} = e^{\mathbf{B}} e^{\mathbf{A}}
$$

The idea, now, is to look for a $f(A,B)$ such that

$$
\mathbf{F} \equiv e^{\mathbf{A}+\mathbf{B}} = {}_{\mathbf{A}}\big[f(A,B)\big]_{\mathbf{B}}
$$

Clearly $\frac{\partial}{\partial \mathbf{A}}\mathbf{F} = \frac{\partial}{\partial \mathbf{B}}\mathbf{F} = \mathbf{F}$ so it must be the case that $\frac{\partial}{\partial A}f = \frac{\partial}{\partial B}f = f$. The most general such $f(A,B)$ is

$$
f(A,B) = K e^{A+B}
$$

---

[26] "On Professor Whittaker's solution of differential equations by definite integrals," Proc. Edingurgh Math. Soc. (Second Series) **2**, 205 (1931).

[27] "Certain expansions in the algebra of quantum mechanics," *loc cit* **3**, 118 (1932).

Our problem, therefore, is to discover the K for which $e^{\mathbf{A}+\mathbf{B}} = K e^{\mathbf{A}} e^{\mathbf{B}}$ is a valid identity, where K is interpreted now to mean "an object which commutes with both $\mathbf{A}$ and $\mathbf{B}$," and might better be written $\mathbf{K}$. We resort again to the "parameter trick" to get analytical leverage on the problem, writing

$$K(u) = e^{u(\mathbf{A}+\mathbf{B})} e^{-u\mathbf{B}} e^{-u\mathbf{A}}$$

Then

$$\frac{d}{du}K = e^{u(\mathbf{A}+\mathbf{B})}(\mathbf{A}+\mathbf{B})e^{-u\mathbf{B}}e^{-u\mathbf{A}}$$
$$- e^{u(\mathbf{A}+\mathbf{B})}\mathbf{B}e^{-u\mathbf{B}}e^{-u\mathbf{A}} - e^{u(\mathbf{A}+\mathbf{B})}e^{-u\mathbf{B}}\mathbf{A}e^{-u\mathbf{A}}$$
$$= e^{u(\mathbf{A}+\mathbf{B})}[\mathbf{A}, e^{-u\mathbf{B}}]e^{-u\mathbf{A}} \quad \text{after simplification}$$

$$[\mathbf{A}, e^{-u\mathbf{B}}] = -u\mathbf{C}e^{-u\mathbf{B}} \quad \text{as will be shown in a moment}$$

$$= -u\mathbf{C}K$$

implies

$$K(u) = K(0)e^{-\frac{1}{2}u^2\mathbf{C}}$$
$$= e^{-\frac{1}{2}u^2\mathbf{C}} \quad \text{since clearly } K(0) = 1$$

So we have $e^{u(\mathbf{A}+\mathbf{B})} = e^{-\frac{1}{2}u^2\mathbf{C}}e^{u\mathbf{A}}e^{u\mathbf{B}}$, which gives back $(\star73.6)$ at $u = 1$. It remains only to take care of a detail, as promised:

Drawing upon (44.3) we have $[\mathbf{A}, \mathbf{B}^2] = [\mathbf{A}, \mathbf{B}]\mathbf{B} + \mathbf{B}[\mathbf{A}, \mathbf{B}]$ which in the presence of $(\star)$ becomes $[\mathbf{A}, \mathbf{B}^2] = 2[\mathbf{A}, \mathbf{B}]\mathbf{B}$ and by easy extension (induction) gives $[\mathbf{A}, \mathbf{B}^n] = n[\mathbf{A}, \mathbf{B}]\mathbf{B}^{n-1}$ whence

$$[\mathbf{A}, e^{\mathbf{B}}] = +\mathbf{C}e^{\mathbf{B}} \qquad (\star73.8)$$

which readily gives the result used above. "Dualization" (interchange $\mathbf{A} \rightleftharpoons \mathbf{B}$ and reverse the sign of the commutator: $\mathbf{C} \to -\mathbf{C}$) supplies

$$[\mathbf{B}, e^{\mathbf{A}}] = -\mathbf{C}e^{\mathbf{A}}$$

in this instance, and is often useful: given an identity, it permits one to obtain a second (usually different, and sometimes more interesting) identity for free. The identity $(\star73.8)$ can be written as a "shift rule"

$$e^{-\mathbf{B}}\mathbf{A}e^{\mathbf{B}} = \mathbf{A} + \mathbf{C} \qquad (\star73.9)$$

from which it follows readily that $e^{-\mathbf{B}}\mathbf{A}^n e^{\mathbf{B}} = (\mathbf{A}+\mathbf{C})^n$ whence

$$e^{-\mathbf{B}}f(\mathbf{A})e^{\mathbf{B}} = f(\mathbf{A}+\mathbf{C})$$

We have barely scratched the surface of a subject which over the years has seduced more than its share of mathematicians and physicists,[28] and which we

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[28] For Richard Feynman's contribution to the subject see "An operator calculus having applications to quantum electrodynamics," Phys. Rev. **84**, 108 (1951).

may have occasion to revisit. Here I present only one further result, of which we will have physical need, and which serves to illustrate the remarkable power of McCoy's method:

$$e^{(\alpha_1 \mathsf{A} + \beta_1 \mathsf{B})(\alpha_2 \mathsf{A} + \beta_2 \mathsf{B})} = K e^{\frac{1}{2} P \mathsf{A}^2} e^{Q \mathsf{A} : \mathsf{B}} e^{\frac{1}{2} R \mathsf{B}^2} \tag{$\star$73.10}$$

where

$$P = \frac{1 - e^{-D\mathsf{C}}}{\mathsf{C}(\alpha_1\beta_2 - \alpha_2\beta_1 e^{-2D\mathsf{C}})} \cdot \alpha_1\alpha_2(1 + e^{-D\mathsf{C}})$$

$$Q = \underline{\quad\quad} \text{ditto} \underline{\quad\quad} \cdot (\alpha_1\beta_2 + \alpha_2\beta_1 e^{-D\mathsf{C}})$$

$$R = \underline{\quad\quad} \text{ditto} \underline{\quad\quad} \cdot \beta_1\beta_2(1 + e^{-D\mathsf{C}})$$

$$K = \sqrt{\frac{D}{\alpha_1\beta_2 - \alpha_2\beta_1 e^{-2D\mathsf{C}}}}$$

with $D \equiv \alpha_1\beta_2 - \alpha_2\beta_1$, and where

$$e^{Q\mathsf{A}:\mathsf{B}} \equiv {}_\mathsf{A}\big[e^{QAB}\big]_\mathsf{B}$$

Amazingly, this complicated-looking result[29] says very sharp things about the quantum physics of oscillators, and its utility in a variety of special cases has been pointed out by Schwinger.[30,31]

Momentum representation. The fundamental commutation relation (52) can be expressed

$$[\mathsf{x}, \tfrac{1}{i\hbar}\xi\mathsf{p}] = \xi\mathsf{I}$$

where ξ is a parameter to which we may assign the dimension $[\xi] = $ length (thus to render $\frac{1}{i\hbar}\xi\mathsf{p}$ dimensionless). As an instance of the "shift rule" ($\star$73.9) we therefore have

$$\mathsf{x}\,\mathsf{T}(\xi) = \mathsf{T}(\xi)(\mathsf{x} + \xi\mathsf{I}) \quad \text{with} \quad \mathsf{T}(\xi) \equiv e^{-\frac{i}{\hbar}\xi\mathsf{p}} \text{ unitary} \tag{74}$$

Application to $|x)$ gives

$$\mathsf{x}\,\mathsf{T}(\xi)|x) = (x + \xi)\,\mathsf{T}(\xi)|x) \tag{75}$$

from which we infer

$$\mathsf{T}(\xi)|x) = |x + \xi) \;:\; \mathsf{T}(\xi) \text{ "translates" along the } \mathsf{x}\text{-spectrum} \tag{76}$$

---

[29] A detailed derivation can be found in "An operator ordering technique with quantum mechanical applications," Notes for a Reed College Physics Seminar presented 12 October 1966.

[30] "On Angular Momentum," US Atomic Energy Commission publication NY0–3071 (1952), Appendix A. The complexity of ($\star$73.10) tends to evaporate in the interesting special cases.

[31] Further discussion of Campbell-Baker-Hausdorff theory can be found in CLASSICAL DYNAMICS (1964), Chapter 1, pp. 22–35; CLASSICAL MECHANICS (1983), pp. 282–287.

Notice now that we can, on the one hand, write

$$\mathsf{T}(\xi)|\psi) = \iint |x)\,dx\,(x|e^{-\frac{i}{\hbar}\xi\,\mathsf{p}}|y)\psi(y)\,dy$$

while on the other hand (assuming whatever may be necessary to make the argument work)

$$
\begin{aligned}
\mathsf{T}(\xi)|\psi) &= \int \mathsf{T}(\xi)|y)\,dy\,(y\,|\psi) \\
&= \int |y+\xi)\,dy\,\psi(y) \\
&= \int |x)\,dx\,\psi(x-\xi) \quad \text{by change of variables} \\
&= \int |x)\,dx\,e^{-\xi\frac{\partial}{\partial x}}\,\psi(x) \quad \text{by Taylor's theorem} \\
&= \iint |x)\,dy\,\delta(y-x)e^{-\xi\frac{\partial}{\partial y}}\psi(y)\,dy
\end{aligned}
$$

We possess now two descriptions of the same thing, which upon comparison (equating similar powers of ξ) give

$$(x|\mathsf{p}^k|y) = \delta(y-x)\left(\tfrac{\hbar}{i}\tfrac{\partial}{\partial y}\right)^k \tag{77}$$

From this result it follows in particular that

$$
\begin{aligned}
(\varphi|\mathsf{p}|\psi) &= \iint (\varphi|x)\,dx\,(x|\mathsf{p}|y)\,dy\,(y\,|\psi) \\
&= \iint \varphi^*(x)\,dx\,\delta(y-x)\left(\tfrac{\hbar}{i}\tfrac{\partial}{\partial y}\right)\psi(y)\,dy \\
&= \int \varphi^*(x)\left(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\right)\psi(x)\,dx \tag{78}
\end{aligned}
$$

Now introduce the momentum eigenbasis, writing

$$\mathsf{p}|p) = p|p) \quad \text{with} \quad \int |p)\,dp\,(p| = \mathsf{I} \quad \text{and} \quad (p|q) = \delta(p-q) \tag{79}$$

Side conditions—imposed upon $(x|\psi)$ whence upon $(x|p)$—may force the momentum spectrum to be discrete (think of the particle-in-a-box), of at least to have a discrete component; in such cases one might write

$$\sum |p)(p| = \mathsf{I} \quad \text{or even} \quad \sum\!\!\!\!\!\int |p)(p| = \mathsf{I} \quad \text{and} \quad (p|q) = \delta_{pq}$$

but we will assign such elastic meanings to $\int$ and δ as to make those notational

distractions unnecessary, except on rare occasions when special emphasis seems in order. Evidently

$$(x|\mathbf{p}|p) = p(x|p)$$

On the other hand, (77) supplies

$$(x|\mathbf{p}|p) = \int (x|\mathbf{p}|y)\,dy\,(y|p) = \tfrac{\hbar}{i}\tfrac{\partial}{\partial x}(x|p)$$

So $(x|p)$, looked upon as a p-indexed function of x, satisfies $\frac{d}{dx}(x|p) = \frac{i}{\hbar}p(x|p)$, and has therefore the form

$$(x|p) = g(p)\cdot e^{\frac{i}{\hbar}px}$$

Therefore

$$(p|q) = \int (p|x)\,dx\,(x|q) = g^*(p)g(q)\cdot\int e^{-\frac{i}{\hbar}(p-q)x}\,dx$$

But the *Fourier integral formula* $f(t) = \frac{1}{2\pi}\int dk \int f(s)e^{-ik(t-s)}ds$ can (on the presumption that integration in reversed order is formally allowed) be expressed

$$\delta(s-t) = \tfrac{1}{2\pi}\int e^{-i(s-t)k}dk$$

so we have

$$(p|q) = g^*(p)g(q)\cdot h\delta(p-q)$$
$$= \delta(p-q) \quad\text{if we set } g(p) = \tfrac{1}{\sqrt{h}}e^{i\,\phi(p)}$$

Without loss of generality we set the phase factor $\phi(p)\to 0$ and obtain

$$(x|p) = \tfrac{1}{\sqrt{h}}e^{\frac{i}{\hbar}px} \tag{80}$$

We now have

$$\left.\begin{aligned}
|p) &= \int |x)\,dx\,(x|p) = \tfrac{1}{\sqrt{h}}\int e^{+\frac{i}{\hbar}px}|x)\,dx\\[2mm]
|x) &= \oint |p)\,dp\,(p|x) = \tfrac{1}{\sqrt{h}}\oint e^{-\frac{i}{\hbar}px}|p)\,dp
\end{aligned}\right\} \tag{81}$$

in description of the relationship between the $\{|x)\}$-basis and the $\{|p)\}$-basis, giving

$$\left.\begin{aligned}
\Psi(p) &\equiv (p|\psi) = \tfrac{1}{\sqrt{h}}\int e^{-\frac{i}{\hbar}px}\,\psi(x)\,dx \quad\text{with}\quad \psi(x)\equiv (x|\psi)\\[2mm]
\psi(x) &\equiv (x|\psi) = \tfrac{1}{\sqrt{h}}\oint e^{+\frac{i}{\hbar}px}\,\Psi(p)\,dp \quad\text{with}\quad \Psi(x)\equiv (p|\psi)
\end{aligned}\right\} \tag{82}$$

We have at this point established that the familiar association

$$(x|\psi) \xleftarrow[\text{Fourier transformation}]{\hspace{4cm}} (p|\psi)$$

was *forced upon us by the fundamental commutator* $[\mathbf{x}, \mathbf{p}] = i\hbar\mathbf{I}$.

Or, to be more precise, forced <u>modulo some refined slip and slide</u> ... which I now digress to describe. It is clearly the case that

i) $\mathbf{P} \equiv \mathbf{p} + \phi'(\mathbf{x})$ will be self-adjoint if $\phi(\cdot)$ is real-valued, and satisfies the same commutation relation as $\mathbf{p}$:

$$[\mathbf{x}, \mathbf{p}] = i\hbar\mathbf{I} \quad \Longleftrightarrow \quad [\mathbf{x}, \mathbf{P}] = i\hbar\mathbf{I}$$

ii) If $\{|x)\}$ comprises an orthonormal eigenbasis of $\mathbf{x}$ then so also does $\{e^{-\frac{i}{\hbar}\phi(x)}|x)\}$, provided $\phi(\cdot)$ is real.

What we show is that those two remarks are complementary aspects of the *same* remark. Let $\mathbf{D}$ and $\mathbf{x}$ be the operators defined

$$\begin{aligned}
\mathbf{D} : &\quad f(x) \longrightarrow \mathbf{D}f(x) \equiv f'(x) &:&\quad \text{differentiation}\\
\mathbf{x} : &\quad f(x) \longrightarrow \mathbf{x}f(x) \equiv x \cdot f(x) &:&\quad \text{multiplication by } x
\end{aligned}$$

From $\mathbf{D}\mathbf{x}f = \mathbf{x}\mathbf{D}f + f$ (all f) we have $[\mathbf{D}, \mathbf{x}] = \mathbf{I}$, and can argue either from this algebraic fact or from $\mathbf{D}e^{\phi(\mathbf{x})}f = e^{\phi(\mathbf{x})}\{\mathbf{D}f + \phi'(\mathbf{x})f\}$ to the "generalized shift rule"

$$e^{-\phi(\mathbf{x})}\mathbf{D}e^{\phi(\mathbf{x})} = \mathbf{D} + \phi'(\mathbf{x})$$

which (compare ($\star$73.9)) holds as an operator identity, and entails[32]

$$e^{-\frac{i}{\hbar}\phi(\mathbf{x})}\mathbf{p}\,e^{\frac{i}{\hbar}\phi(\mathbf{x})} = \mathbf{p} + \phi'(\mathbf{x})$$

The operator $\mathbf{W} \equiv e^{-\frac{i}{\hbar}\phi(\mathbf{x})}$ is manifestly unitary (any real $\phi(\cdot)$), and permits us to write

$$\left.\begin{aligned}
\mathbf{X} &= \mathbf{W}\mathbf{x}\mathbf{W}^{-1} = \mathbf{x}\\
\mathbf{P} &= \mathbf{W}\mathbf{P}\mathbf{W}^{-1} = \mathbf{p} + \phi'(\mathbf{x})
\end{aligned}\right\} \tag{83}$$

Moreover, if $\mathbf{x}|x) = x|x)$ and $|X) \equiv \mathbf{W}|x)$ then $\mathbf{X}|X) = x|X)$. These simple conclusions illustrate the *general* proposition that

> *all* realizations of the fundamental commutation relations $[\mathbf{x}, \mathbf{p}] = i\hbar\mathbf{I}$ are *unitarily equivalent*.

They anticipate the idea central to gauge field theory, and will acquire importance also when we look to the problem of "quantization in curvilinear coordinates."

---

[32] Multiply by $\frac{\hbar}{i}$ and notice that $[\frac{\hbar}{i}\mathbf{D}, \mathbf{x}] = [\mathbf{p}, \mathbf{x}]$.

We are in position now to cast some of the results in hand into more familiar form. For example: Whatever may be the resolution of the "correspondence problem" $A(x,p) \longleftrightarrow \mathbf{A}$ posed at (12), we certainly expect—and on physical grounds require—that it will send

$$H(x,p) = \tfrac{1}{2m}p^2 + U(x) \quad \longleftrightarrow \quad \mathbf{H} = \tfrac{1}{2m}\mathbf{p}^2 + U(\mathbf{x}) \tag{84}$$

Drawing upon (77) we have

$$(x|\mathbf{H}|y) = \delta(y-x)\Big\{ \tfrac{1}{2m}\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial y}\big)^2 + U(x) \Big\} \tag{85}$$

which when introduced into (59) gives the equation

$$\Big\{ \tfrac{1}{2m}\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial y}\big)^2 + U(x) \Big\}\psi(x,t) = i\hbar\tfrac{\partial}{\partial t}\psi(x,t) \tag{86}$$

which marked Schrödinger's *point of departure*.

Or look back again to (66), where we encounter the expression

$$(\psi|[\mathbf{H},\boldsymbol{x}]|\psi) = (\psi|\mathbf{H}|x)\psi(x,t) - \psi^*(x,t)(x|\mathbf{H}|\psi)$$
$$= -\Big\{ \psi^*(x,t)(x|\mathbf{H}|\psi) - \text{complex conjugate} \Big\}$$

Using (85) in

$$(x|\mathbf{H}|\psi) = \int (x|\mathbf{H}|y)\psi(y,t)\,dy$$

we have

$$= \Big\{ \tfrac{1}{2m}\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\big)^2 + U(x) \Big\}\psi(x,t)$$

and with this information (66) is readily brought to the form

$$\tfrac{\partial}{\partial t}P + \boldsymbol{\nabla}\cdot\boldsymbol{J} = 0 \tag{87}$$
$$\boldsymbol{J} \equiv \tfrac{\hbar}{im}\big\{ \psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^* \big\}$$

in which "conservation of probability" is more commonly expressed.

The "mixed representation trick". Suppose we were in position to write

$$A(x,p)$$
$$\downarrow$$
$$\mathbf{A} = {}_{\mathbf{x}}\big[A_{xp}(x,p)\big]_{\mathbf{p}} \tag{88}$$

For the same reason that—with $\mathbf{x}$ acting to the left and $\mathbf{p}$ acting to the right—$(x|\mathbf{x}\,\mathbf{p}|p) = xp(x|p)$, we would then have

$$(x|\mathbf{A}|p) = A_{xp}(x,p)\cdot(x|p) = \tfrac{1}{\sqrt{h}}A_{xp}(x,p)\,e^{\frac{i}{\hbar}px} \tag{89}$$

and find ourselves in position to write (for example)

$$(x|\mathbf{A}|y) = \int (x|\mathbf{A}|p)\, dp\,(p\,|\,y)$$

$$= \tfrac{1}{h}\int A_{xp}(x,p)\, e^{\frac{i}{\hbar}p(x-y)}\, dp \tag{90.1}$$

$$(q|\mathbf{A}|p) = \int (q\,|\,x)\, dx\,(x|\mathbf{A}|p)$$

$$= \tfrac{1}{h}\int A_{xp}(x,p)\, e^{\frac{i}{\hbar}(p-q)x}\, dx \tag{90.2}$$

$$\langle\mathbf{A}\rangle = (\psi|\mathbf{A}|\psi) = \int (\psi|x)\, dx\,(x|\mathbf{A}|p)\, dp\,(p\,|\,\psi)$$

$$= \tfrac{1}{h}\iint \psi^*(x)A_{xp}(x,p)\, e^{\frac{i}{\hbar}px}\,\Psi(p)\, dxdp \tag{90.3}$$

Though such formulæ are infrequently encountered in the literature—for, I suppose, the reason that they presume solution of the **operator ordering problem** —they are, in my experience, often very useful, and will enter repeatedly future discussion.

Look to the FREE PARTICLE Green's function; i.e., to (see again (60))

$$G(x,t;y,0) = (x|\mathbf{U}(t)|y) \quad \text{with} \quad \mathbf{U}(t) = e^{-\frac{i}{\hbar}\frac{1}{2m}\mathbf{p}^2 t} \tag{91.1}$$

The ordering problem is in this case trivial

$$\mathbf{U}(t) = {}_{\mathsf{x}}\Big[e^{-\frac{i}{\hbar}\frac{1}{2m}p^2 t}\Big]_{\mathbf{p}} \tag{91.2}$$

so as an instance of (90.1) we have

$$G(x,t;y,0) = \tfrac{1}{h}\int e^{-\frac{i}{\hbar}\frac{1}{2m}p^2 t}\, e^{\frac{i}{\hbar}p(x-y)}\, dp \tag{91.3}$$

$$= \tfrac{1}{h}\int e^{-(ap^2+2bp)}\, dp \quad \text{with} \quad a = (i/\hbar)\tfrac{t}{2m},\ b = -(i/\hbar)\tfrac{x-y}{2}$$

$$= \tfrac{1}{h}\sqrt{\tfrac{\pi}{a}}\, e^{b^2/a} \quad \text{provided} \quad \Re[a] > 0$$

To achieve compliance with the side condition we
- require $t > 0$ (*quantum dynamics is predictive, not retrodictive*) and[33]
- place $\hbar$ on the upper half of the "complex $\hbar$ plane," so as to have

$$\frac{i}{\hbar} = \lim_{\epsilon\downarrow 0}\left\{\frac{i}{\hbar+i\epsilon} = \frac{\epsilon}{\hbar^2+\epsilon^2} + i\,\frac{\hbar}{\hbar^2+\epsilon^2}\right\} \tag{91.4}$$

---

[33] This is one of Feynman's many tricks: see......Variants of the idea—the general effect of which is to *associate physical functions with the boundary values of analytic functions*—have become commonplace in a great variety of contexts.

We then obtain

$$G_{\text{free}}(x,t;y,0) = \sqrt{\tfrac{m}{iht}}\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-y)^2}{t}\right\} \tag{91.5}$$

This result will become progressively prettier (and acquire ever greater importance) as we proceed, and can be obtained by a variety of simpler means— we might, for example, write

$$G_{\text{free}}(x,t;y,0) = \iint (x|p)\,dp\,(p|e^{-\frac{i}{\hbar}\frac{1}{2m}\mathbf{p}^2 t}|q)\,dq\,(q|y)$$

$$= \iint (x|p)\,dp\,e^{-\frac{i}{\hbar}\frac{1}{2m}q^2 t}\delta(p-q)\,dq\,(q|y)$$

which returns us to (91.3) without allusion to the "ordering problem"—but the success of the method which led us to (91.5) is no fluke, as I demonstrate with a second example:[34]

Look to the HARMONIC OSCILLATOR Hamiltonian

$$\mathbf{H} = \tfrac{1}{2m}(\mathbf{p}^2 + m^2\omega^2\mathbf{x}^2) \tag{92.1}$$

and notice that McCoy's theorem ($\star$73.10) supplies

$$e^{\mathbf{A}^2+\mathbf{B}^2} = \sqrt{\sec 2\mathbf{C}}\,\exp\left\{\tfrac{\tan 2\mathbf{C}}{2\mathbf{C}}\mathbf{A}^2\right\}\exp\left\{\tfrac{1-\sec 2\mathbf{C}}{\mathbf{C}}\mathbf{A}{:}\mathbf{B}\right\}\exp\left\{\tfrac{\tan 2\mathbf{C}}{2\mathbf{C}}\mathbf{B}^2\right\}$$

We therefore have

$$\mathbf{U}(t) = e^{-\frac{i}{\hbar}\frac{1}{2m}(\mathbf{p}^2+m^2\omega^2\mathbf{x}^2)t}$$

$$= \sqrt{\sec\omega t}\,e^{-\frac{i}{\hbar}\frac{m\omega}{2}\tan\omega t\cdot\mathbf{x}^2}\,e^{-\frac{i}{\hbar}(1-\sec\omega t)\cdot\mathbf{x}{:}\mathbf{p}}\,e^{-\frac{i}{\hbar}\frac{1}{2m\omega}\tan\omega t\cdot\mathbf{p}^2} \tag{92.2}$$

So were are led again to a Gaussian integral, which after some manipulation gives

$$G_{\text{osc}}(x,t;y,0) = \sqrt{\tfrac{m\omega}{ih\sin\omega t}}\,\exp\left\{\frac{i}{\hbar}m\omega\left[\frac{(x^2+y^2)\cos\omega t - 2xy}{2\sin\omega t}\right]\right\} \tag{92.3}$$

from which we recover (91.5) in the limit $\omega \downarrow 0$. As is well known, the oscillator Hamiltonian (92.1) can also be written in "displaced factored form"

$$\mathbf{H} = = \hbar\omega(\mathbf{a}^+\mathbf{a} + \tfrac{1}{2}\mathbf{I}) \quad \text{with} \quad \mathbf{a} \equiv \sqrt{m\omega/2\hbar}\,(\mathbf{x} + i\tfrac{1}{m\omega}\mathbf{p}) \tag{92.4}$$

$$\mathbf{a}^+ = \sqrt{m\omega/2\hbar}\,(\mathbf{x} - i\tfrac{1}{m\omega}\mathbf{p})$$

---

[34] Omitted details can be found in some seminar notes previously cited.[29] The method is due to Schwinger; as Bernoulli remarked on reading some of Newton's unsigned work, "One can recognize the lion by his paw."

where $[\mathbf{x}, \mathbf{p}] = i\hbar\, \mathbf{I}$ entails $[\mathbf{a}, \mathbf{a}^+] = \mathbf{I}$ and where we notice that the factors $\mathbf{a}$ and $\mathbf{a}^+$ are *not self-adjoint*. It follows again from McCoy's theorem that

$$e^{u\,\mathbf{A}\mathbf{B}} = \exp\left\{\frac{1 - e^{u\,\mathbf{C}}}{\mathbf{C}}\,\mathbf{A}\!:\!\mathbf{B}\right\}$$

so we have

$$\begin{aligned}
\mathbf{U}(t) = e^{-i\omega(\mathbf{a}^+\mathbf{a} + \frac{1}{2}\mathbf{I})t} &= e^{-i\frac{1}{2}\omega t}e^{-i\omega t\,\mathbf{a}^+\mathbf{a}}\\
&= e^{-i\frac{1}{2}\omega t}\exp\left\{(e^{-i\omega t} - 1)\mathbf{a}^+\!:\!\mathbf{a}\right\}\\
&= \sum_n e^{-\frac{i}{\hbar}(n+\frac{1}{2})\hbar\omega t}\frac{1}{\sqrt{n!}}(\mathbf{a}^+)^n e^{-\mathbf{a}^+:\mathbf{a}}\frac{1}{\sqrt{n!}}(\mathbf{a})^n \quad (92.5)
\end{aligned}$$

Comparison with (31)

$$\mathbf{U}(t) = \sum_n e^{-\frac{i}{\hbar}E_n t}|n)(n|$$

gives

$$\begin{aligned}
E_n = (n + \tfrac{1}{2})\hbar\omega \quad\text{and}\quad |n)(n| &= \tfrac{1}{\sqrt{n!}}(\mathbf{a}^+)^n e^{-\mathbf{a}^+:\mathbf{a}}\tfrac{1}{\sqrt{n!}}(\mathbf{a})^n \quad (92.6)\\
&= \tfrac{1}{\sqrt{n!}}(\mathbf{a}^+)^n\,|0)(0|\,\tfrac{1}{\sqrt{n!}}(\mathbf{a})^n
\end{aligned}$$

$$|0)(0| = e^{-\mathbf{a}^+:\mathbf{a}}$$

$$\downarrow$$

$$|n) = \tfrac{1}{\sqrt{n!}}(\mathbf{a}^+)^n\,|0) \quad (92.7)$$

It is not difficult to show that

$$\mathbf{B}\,e^{u\,\mathbf{A}:\mathbf{B}} = (1 - u\mathbf{C})\,e^{u\,\mathbf{A}:\mathbf{B}}\,\mathbf{B}$$

and with the aid of this information we have

$$\mathbf{a}\,|0)(0| = \mathbf{a}\,e^{-\mathbf{a}^+:\mathbf{a}} = (1-1)e^{-\mathbf{a}^+:\mathbf{a}}\,\mathbf{a} = \mathbf{0}$$

which shows that $\mathbf{a}$ *annihilates the ground state*:

$$\mathbf{a}\,|0) = 0 \quad (92.8)$$

It is now a relatively straightforward matter[35] to construct the familiar oscillator eigenfunctions

$$\psi_n(x) = (x|n) \quad (92.9)$$

which permit one to write

$$G_{\mathrm{osc}}(x, t; y, 0) = \sum_n e^{-\frac{i}{\hbar}(n+\frac{1}{2})\hbar\omega t}\,\psi_n(x)\,\psi^*(y) \quad (92.10)$$

But valuable information can be obtained in a representation-independent way,

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[35] See Griffiths, §2.3.1.

as I now illustrate: it follows immediately from (92.7) that

$$\mathbf{a}^+ |n) = \sqrt{n+1}\,|n+1)\qquad\qquad(92.11a)$$

while $\mathbf{a}\,|n) = \mathbf{a}\,\frac{1}{\sqrt{n!}}(\mathbf{a}^+)^n\,|0) = \frac{1}{\sqrt{n!}}(\mathbf{a}^+)^n\,\mathbf{a}|0) + \frac{n}{\sqrt{n}}\frac{1}{\sqrt{(n-1)!}}(\mathbf{a}^+)^{(n-1)}\,|0)$ gives

$$\mathbf{a}\,|n) = \sqrt{n}\,|n-1)\qquad\qquad(92.11b)$$

and it is in view of these facts that one calls $\mathbf{a}^+$ and $\mathbf{a}$ "ladder operators" ("step-up" and "step-down" operators, respectively). The self-adjoint operator $\mathbf{N} \equiv \mathbf{a}^+\mathbf{a}$ and its nameless companion $\mathbf{a}\,\mathbf{a}^+$ have the properties

$$\left.\begin{array}{rl} \mathbf{N}|n) = & n|n) \\ \mathbf{a}\,\mathbf{a}^+|n) = & (n-1)|n) \end{array}\right\}\qquad\qquad(93)$$

for which reason $\mathbf{N}$ is called the "number operator."

Some commentary is in order: (92.10) is an instance of (31), and is as old as quantum mechanics itself. That $G_{\mathrm{osc}}(x,t;y,0)$ admits of the alternative description (92.3) is a fact which—though it had been previously remarked by an occasional physicist (and was known to mathematicians as "Mehler's theorem" already in the 19th Century)—was first emphasized by Feynman, for reasons which I will later discuss in detail. For the moment I must be content to introduce this evidence that (92.3) is not so obscurely bizarre, and its introduction not nearly so pointless . . . as might at first appear. The function

$$x(t) = \left[\frac{x_0\sin\omega t_1 - x_1\sin\omega t_0}{\sin\omega(t_1-t_0)}\right]\cos\omega t - \left[\frac{x_0\cos\omega t_1 - x_1\cos\omega t_0}{\sin\omega(t_1-t_0)}\right]\sin\omega t$$

satisfies $\ddot{x} + \omega^2 x = 0$, $x(t_0) = x_0$ and $x(t_1) = x_1$, so describes the *dynamical path*

$$(x_1,t_1)\longleftarrow\!\!\!\!\!\!\underset{x(t)}{\rule{2cm}{0pt}}\!\!\!\!\!\!(x_0,t_0)$$

of an harmonic oscillator. Dropping that $x(t)$ and the associated $\dot{x}(t)$ into

$$S(x_1,t_1;x_0,t_0) = \int_{t_0}^{t_1}\left\{\tfrac{1}{2}m\dot{x}^2(t) - \tfrac{1}{2}m\omega^2 x^2(t)\right\}dt$$

we obtain the *dynamical action* associated with that path, and find it to be given by

$$S(x_1,t_1;x_0,t_0) = m\omega\left[\frac{(x_1^2+x_0^2)\cos\omega(t_1-t_0) - 2x_1x_0}{2\sin\omega(t_1-t_0)}\right]\right\}\qquad(94.1)$$

which after notational adjustments ($t_0 \mapsto 0,\ t_1 \mapsto t,\ x_0 \mapsto y,\ x_1 \mapsto x$) yields an expression presented in the exponent of (92.3). Moreover

$$\frac{\partial^2 S(x_1,t_1;x_0,t_0)}{\partial x_1\partial x_0} = -\frac{m\omega}{\sin\omega(t_1-t_0)}\qquad\qquad(94.2)$$

yields (after those same adjustments) a factor which appears under the radical. So (92.3) can be written in a form

$$G(x_1, t_1; x_0, t_0) = \sqrt{\frac{i}{h} \frac{\partial^2 S(x_1, t_1; x_0, t_0)}{\partial x_1 \partial x_0}} \, \exp\left\{\tfrac{i}{\hbar} S(x_1, t_1; x_0, t_0)\right\} \qquad (95)$$

which has the "look of generality" about it … and raises this issue: *What can such an expression—assembled, as it is, from classical objects—have to do with the spectral representation of the quantum propagator?*

The methods applied above to the oscillator can be used to construct a similarly complete account of the quantum mechanics of FREE FALL

$$\mathsf{H} = \tfrac{1}{2m}\mathsf{p}^2 + mg\,\mathsf{x} \qquad (96)$$

but I postpone discussion of the interesting details.

Suppose, given $H(x, p) \longrightarrow \mathsf{H}$, we were in position to write

$$e^{\mathsf{H}} = {}_\mathsf{x}\!\left[e^{\mathcal{H}(x,p)}\right]_\mathsf{p} \qquad (97.1)$$

In straightforward generalization of (91.3) we would then have

$$G(x, t; y, 0) = \tfrac{1}{h}\int \exp\left\{\frac{i}{\hbar}\left[p\,\frac{x-y}{t} - \mathcal{H}(x, p)\right] t\right\} dp \qquad (97.2)$$

and if one "squints" the expression [etc.] resembles the expression on the right side of

$$L(x, \dot{x}) = p\,\dot{x} - H(x, p)$$

which, in collaboration with $\dot{x} = \partial H/\partial p$, serves in classical mechanics to achieve

$$H(x, p) \xrightarrow[\text{Legendre transformation}]{} L(x, \dot{x})$$

It will be awhile before this green fruit becomes ripe enough to pick … but will be worth the wait.

Gaussian representation of the delta function and its derivatives. When Dirac allowed himself to write[36]

$$\int_{-\infty}^{+\infty} \delta(x)\,dx = 1$$

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

—which he did in order to achieve

$$\int_{-\infty}^{+\infty} f(x)\delta(x - a)\,dx = f(a)$$

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[36] *Principles of Quantum Mechanics*, §15 in both the 3${}^{\text{rd}}$ and 4${}^{\text{th}}$ editions.

—he was perfectly well aware (and explicitly stated) that no such "function" $\delta(x)$ can exist, except as the idealized limit of such perfectly nice functions as the familiar Gaussian[37]

$$g(x - a; \epsilon) \equiv \tfrac{1}{\epsilon\sqrt{2\pi}} \exp\left\{ -\tfrac{1}{2}\left[\tfrac{x-a}{\epsilon}\right]^2 \right\} \tag{98}$$

In probabilistic contexts one would say that $g(x - a; \epsilon)$ describes a normal distribution—a "bell-shaped curve" which is centered at $x = a$ and becomes more sharply localized as ϵ decreases. One has

$$\int_{-\infty}^{+\infty} g(x - a; \epsilon)\, dx = 1 \quad : \quad \text{all } \epsilon > 0$$

$$\lim_{\epsilon \downarrow 0} g(x - a; \epsilon) = 0 \quad \text{for} \quad x \neq 0$$

and expects therefore to have

$$\lim_{\epsilon \downarrow 0} \int_{-\infty}^{+\infty} f(x) g(x - a; \epsilon)\, dx = f(a)$$

for all reasonable functions $f(x)$. These equations provide a concrete realization of Dirac's elementary idea, and show that the term "δ-function" refers not to a "function" but to a *program*: $\delta(x)$ lives always in the shade of a real or implied $\int$ because it's intent is to *assign value to the limit of an ϵ-parameterized sequence of integrals*. His notational objective was simply to remove the prolixity from a situation which seemed to him pretty obvious (but which got von Neumann all steamed up).

Evidently

$$\int_{\infty}^{x} \delta(y - a)\, dy = \theta(x - a) \equiv \begin{cases} 0 & : \quad x < a \\ 1 & : \quad x > a \end{cases}$$

so that formally

$$\delta(x - a) = \tfrac{d}{dx}\theta(x - a)$$

The "step function" $\theta(x - a)$ is in some respects a more elementary object than $\delta(x - a)$, and I have argued elsewhere[38] that it is from properties of the former

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[37] Alternatives such as

$$g_1(x - a; \epsilon) \equiv \tfrac{1}{2\epsilon} \operatorname{sech}^2\left[\tfrac{x-a}{\epsilon}\right]$$

$$g_2(x - a; \epsilon) \equiv \frac{\sin[(x - a)/\epsilon]}{\pi(x - a)}$$

are available in infinite variety, and sometimes lend themselves more naturally to particular applications, but it serves my present purposes to look only to implications of the "Gaussian representation of the δ-function."

[38]   "Simplified production of Dirac delta function identities," (1997).

that properties of the latter are most easily extracted. What I had there in mind were formal statements such as appear in the following list:

$$\delta(-x) = \delta(x)$$
$$x\delta(x) = 0$$
$$\delta(ax) = a^{-1}\delta(x) \qquad\qquad : \ a > 0$$
$$\delta(x^2 - a^2) = \tfrac{1}{2}a^{-1}\{\delta(x-a) + \delta(x+a)\} \ : \ a > 0$$
$$\int \delta(a-x)\,dx\,\delta(x-b) = \delta(a-b)$$
$$f(x)\delta(x-a) = f(a)\delta(x-a)$$

At present, however, I have interest in (because need of) certain *derivative* properties of the delta function.

What can one mean by the "derivative" of an object so singular as $\delta(x)$? Formal integration-by-parts supplies

$$\int f(x)\delta'(x-a)\,dx = -\int f'(x)\delta(x-a)\,dx$$
$$= -f'(a)$$
$$\int f(x)\delta''(x-a)\,dx = (-)^2 f''(a)$$
$$\vdots$$

And if we work in Gaussian representation (or any other similarly differentiable representation) it becomes entirely natural to write

$$\delta^{(n)}(x-a) = \lim_{\epsilon\downarrow 0} \left(\tfrac{d}{dx}\right)^n g(x-a;\epsilon)$$

where it is understood that $\lim_{\epsilon\downarrow 0}$ is to be taken only after the $\int$-process has been completed. It is at this point that the special merit of the Gaussian representation come first into view:

The (monic) Hermite polynomials $He_n(x)$ can be defined[39]

$$He_n(x) \equiv (-)^n e^{\frac{1}{2}x^2} \left(\tfrac{d}{dx}\right)^n e^{-\frac{1}{2}x^2} \tag{99}$$

so we have

$$\left(-\tfrac{d}{dx}\right)^n e^{-\frac{1}{2}x^2} = He_n(x)\cdot e^{-\frac{1}{2}x^2} \quad \text{with} \quad \begin{cases} He_0(x) = 1 \\ He_1(x) = x \\ He_2(x) = x^2 - 1 \\ \quad\vdots \end{cases}$$

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[39] Beware the alternative definition $H_n(x) \equiv e^{x^2}\left(\tfrac{d}{dx}\right)^n e^{-x^2}$ which is very frequently encountered (Griffiths, p. 41; Spanier & Oldham, *Atlas of Functions*, Chapter 24), and sometimes more useful. The polynomials $He_n(x)$ are treated on pp. 80–82 of Magnus & Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics*.

which after a few elementary adjustments gives

$$\left(-\tfrac{d}{dx}\right)^n g(x-a;\epsilon) = \tfrac{1}{\sqrt{2\pi}}\left(\tfrac{1}{\epsilon}\right)^{n+1} He_n\left(\tfrac{x-a}{\epsilon}\right)\exp\left\{-\tfrac{1}{2}\left[\tfrac{x-a}{\epsilon}\right]^2\right\}$$

Pulling this information together, we have

$$
\begin{aligned}
f^{(n)}(a) &= \int f(x)\left[(-)^n\delta^{(n)}(x-a)\right]dx \\[2mm]
&= \tfrac{1}{\sqrt{2\pi}}\cdot\lim_{\epsilon\downarrow 0}\left(\tfrac{1}{\epsilon}\right)^{n+1}\int f(x)He_n\left(\tfrac{x-a}{\epsilon}\right)\exp\left\{-\tfrac{1}{2}\left[\tfrac{x-a}{\epsilon}\right]^2\right\}dx \quad\quad (100)\\[1mm]
&\downarrow
\end{aligned}
$$

$$f(a) = \tfrac{1}{\sqrt{2\pi}}\cdot\lim_{\epsilon\downarrow 0}\left(\tfrac{1}{\epsilon}\right)^1\int f(x)\exp\left\{-\tfrac{1}{2}\left[\tfrac{x-a}{\epsilon}\right]^2\right\}dx$$

$$f'(a) = \tfrac{1}{\sqrt{2\pi}}\cdot\lim_{\epsilon\downarrow 0}\left(\tfrac{1}{\epsilon}\right)^2\int f(x)\cdot\left(\tfrac{x-a}{\epsilon}\right)\cdot\exp\left\{-\tfrac{1}{2}\left[\tfrac{x-a}{\epsilon}\right]^2\right\}dx$$

$$f''(a) = \tfrac{1}{\sqrt{2\pi}}\cdot\lim_{\epsilon\downarrow 0}\left(\tfrac{1}{\epsilon}\right)^3\int f(x)\cdot\left[\left(\tfrac{x-a}{\epsilon}\right)^2-1\right]\cdot\exp\left\{-\tfrac{1}{2}\left[\tfrac{x-a}{\epsilon}\right]^2\right\}dx$$

$$\vdots$$

which will be of use to people who, in the course of their mathematical wanderings, encounter (as we are destined to encounter) expressions such as appear on the right sides of the preceding equations—expressions to which they can now assign simple names and interpretations.[40]

The equations obtained above refer to what can in general terms be called the *asymptotic evaluation of integrals*—a subject pioneered by Laplace more than a century before Dirac appeared on the scene. Laplace was motivated to write

$$I(\lambda) = \int_{x_0}^{x_1} f(x)e^{\lambda g(x)}\,dx$$

and, on the assumption that $g(x)$ is bounded on $[x_0, x_1]$ and maximal at the interior point $x = a$, to ask "What can one say about $I(\lambda)$ as λ becomes large?" Expanding about a (where, by assumption, $g'(x)$ vanishes) he wrote

$$I(\lambda) = \int_{x_0}^{x_1} f(x)e^{\lambda\left\{g(a)+\frac{1}{2}g''(a)(x-a)^2+\cdots\right\}}\,dx$$

with $g''(a) < 0$ and argued that when λ is large the predominant contribution to the integral must arise in the immediate neighborhood of $x = a$. So he had

$$I(\lambda) \sim \int_{a-\epsilon}^{a+\epsilon} f(a)e^{\lambda g(a)}e^{-\frac{1}{2}\lambda|g''(a)|(x-a)^2}\,dx$$

$$\sim f(a)e^{\lambda g(a)}\int_{-\infty}^{+\infty} e^{-\frac{1}{2}\lambda|g''(a)|(x-a)^2}\,dx$$

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[40] For more detailed discussion of the material sketched above, see QUANTUM MECHANICS (1967), Chapter 1, pp. 70–74. The Hermite polynomials can be given natural (non-polynomial) meaning even when n is not an integer; in "Laplacian operators of eccentric order" (1998) I use this fact to construct a novel approach to the fractional calculus.

on which basis he (as a founding father of probability theory, and possibly the first person to know that $\int_{-\infty}^{+\infty} e^{-x^2}\,dx = \sqrt{\pi}$) was placed in position to write

$$\lim_{\lambda \to \infty} \int_{x_0}^{x_1} f(x) e^{\lambda\,g(x)}\,dx \sim \left[-\frac{2\pi}{\lambda g''(a)} \right]^{\frac{1}{2}} f(a) e^{\lambda\,g(a)} \qquad (101.1)$$

which is known as "Laplace' asymptotic expansion formula," and pretty clearly captures the germ of Dirac's idea.

LAPLACE' METHOD has been extended—often by physicists (Stokes, Kelvin, Debye, others) working on a variety of physical problems (geometrical limit of physical optics as frequency becomes large, thermodynamics limit of statistical mechanics as the number of particles becomes large, classical limit of quantum mechanics as $1/\hbar$ becomes large)—in several directions, by arguments which differ in their details, but which lead to results which are remarkably similar. Kelvin's METHOD OF STATIONARY PHASE leads, for example, to the conclusion that if $g(x)$ has a solitary stationary point at $x = a$ (i.e., if $g'(a) = 0$ and $g''(a) \neq 0$) then (taking the upper or lower sign according as $g''(a) \gtrless 0$)

$$\lim_{\lambda \to \infty} \int_{x_0}^{x_1} f(x) e^{i\,\lambda\,g(x)}\,dx \sim \left[\frac{2\pi}{\lambda g''(a)} \right]^{\frac{1}{2}} f(a) e^{i[\lambda\,g(a) \pm \frac{\pi}{4}]} \qquad (101.2)$$

. . . the argument now being that the integrand in

$$\int_{-\infty}^{+\infty} e^{i\frac{1}{2}\lambda g''(a)(x-a)^2}\,dx \quad \text{"buzzes to extinction" at points away from } x = a$$

The subject rapidly becomes technically demanding when pursued in rigorous detail, but we will need to draw (informally) upon only its simplest elements.[41]

Classical Legendre transformations from quantum Fourier transformations. We say already at (82) that—in consequence ultimately of $[\mathbf{x}, \mathbf{p}] = i\hbar\,\mathbf{I}$—the "wave functions" $\psi(x) \equiv (x|\psi)$ and $\Psi(p) \equiv (p|\psi)$ are Fourier transforms of one another. That

$$(\psi|\psi) = \int (\psi|x)\,dx\,(x|\psi) = \int (\psi|p)\,dp\,(p|\psi) = 1 \qquad (102)$$

is in Dirac notation almost trivial, though in Fourier transform theory the central equality is attributed to "Parseval's theorem," which can be argued to be the well-spring of the entire subject.[42]

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[41] For a good brief account of the essentials see Chapter 2 in A. Erdélyi, *Asymptotic Expansions* (1956), which is the Dover publication of some brief lecture notes. Elaborately detailed accounts of the theory can be found in Chapter 6 of C. Bender & S. Orszag's *Advanced Mathematical Methods for Scientists and Engineers* (1978) and in Chapters 3 & 4 of F. Olver, *Asymptotics and Special Functions* (1997).

[42] See P. M. Morse & H. Feshbach, *Methods of Theoretical Physics* (1953), pp. 456–462.

Let $(x|\psi)$ and $(p|\psi)$ be displayed in polar form

$$(x|\psi) = R(x)\, e^{\frac{i}{\hbar} S(x)} \quad \text{and} \quad (p|\psi) = A(p)\, e^{\frac{i}{\hbar} B(p)} \tag{103}$$

in which notation (82) reads

$$A(p)\, e^{\frac{i}{\hbar} B(p)} = \tfrac{1}{\sqrt{h}} \int R(y)\, e^{\frac{i}{\hbar}[S(y) - py]}\, dy$$

Let x be defined by the condition $\frac{\partial}{\partial y}[S(y) - py] = 0$; i.e., let x be the solution (assumed here to be unique) of $p = S'(x)$. By functional inversion we have

$$p = S'(x)$$
$$\downarrow$$
$$x = x(p)$$

and, drawing upon (101.2), find that we can, in the "classical limit" $1/\hbar \to \infty$, write

$$A(p)\, e^{\frac{i}{\hbar} B(p)} \sim \left[\frac{1}{S''(x)}\right]^{\frac{1}{2}} R(x)\, e^{\frac{i}{\hbar}[S(x) - px \pm \frac{1}{8}h]} \quad \text{with} \quad x \to x(p) \tag{104.1}$$

where the $\pm$ hinges on $S''(x) \gtrless 0$. Evidently $B(p)$ results from eliminating x between the two equations

$$B(p) = S(x) - px \pm \tfrac{1}{8}h$$
$$\updownarrow \tag{104.2}$$
$$p = \tfrac{d}{dx} S(x)$$

and so is—if we may be allowed to abandon the dangling $\pm \frac{1}{8}h$, which arose from writing $i\frac{\pi}{4} = \frac{i}{\hbar}\frac{2\pi\hbar}{8}$—precisely the *Legendre transform* of $S(x)$.

Had we worked from the inverse Fourier transform (i.e., from the other half of (82)) we would by the same argument have obtained

$$R(x)\, e^{\frac{i}{\hbar} S(x)} \sim \left[\frac{1}{B''(p)}\right]^{\frac{1}{2}} A(p)\, e^{\frac{i}{\hbar}[B(p) + px \mp \frac{1}{8}h]} \quad \text{with} \quad p \to p(x) \tag{105.1}$$

whence

$$S(x) = B(p) + xp \mp \tfrac{1}{8}h$$
$$\updownarrow \tag{105.2}$$
$$x = -\tfrac{d}{dp} B(p)$$

where the sign-reversal will be explained in a moment. The minus sign which famously distinguishes a Fourier transform from its inverse is seen here to be reflected in the sign which distinguishes a Legendre transform from its inverse.

Compare (105.1) with this simple rewrite of (104.1):

$$R(x)\, e^{\frac{i}{\hbar} S(x)} \sim \left[\frac{1}{S''(x)} \right]^{-\frac{1}{2}} A(p)\, e^{\frac{i}{\hbar}[B(p)+p\,x \mp \frac{1}{8}h]}$$

We would at the same time account for the sign-reversal (in the exponent) and establish consistency with (105.1) if we could show that $S''(x)B''(p) = -1$. But this follows immediately from

$$S'' = \frac{dp}{dx} \qquad \text{and} \qquad B'' = -\frac{dx}{dp}$$

One can, on the basis of the preceding discussion (and with high informality), assert that

$$\text{Fourier transformation} \sim e^{\frac{i}{\hbar}(\text{Legendre transformation})} \tag{106}$$

Classical/short-time asymptotics of Green's function. Look back in this light to the description (97.2) of the Green's function $G(x,t;y,0)$. In the classical limit $\hbar \downarrow 0$ that "quantum mechanics becomes classical" (whatever that might mean) we might plausibly expect (and this expectation will later be borne out) to have $\mathcal{H}(x,p) \to H(x,p)$, and in that approximation to be able to write

$$G(x,t;y,0) \sim \frac{1}{h} \int \exp\left\{ \frac{i}{\hbar}\left[p\,\frac{x-y}{t} - H(x,p) \right] t \right\} dp$$

Let t be small, and to emphasize the velocity-like meaning which $(x-y)/\tau$ then assumes write $v \equiv (x-y)/\tau$. Then

$$G(x,\tau;y,0) \sim \frac{1}{h} \int \exp\left\{ \frac{i}{\hbar}\left[p\,v - H(x,p) \right] \tau \right\} dp \tag{107}$$

The idea now is to use (101.2)—the "method of stationary phase"—to obtain an asymptotic approximation to the integral. By way of preparation we solve $\frac{\partial}{\partial p}[p\,v - H(x,p)] = v - \frac{\partial H}{\partial p} = 0$ (which on $v \mapsto \dot{x}$ would become one of Hamilton's equations!) to obtain $p = p(x,v)$, whence

$$G(x,\tau;y,0) \sim \left[\frac{1}{-hH''(x,p)} \right]^{\frac{1}{2}} e^{\frac{i}{\hbar}[\{pv-H(x,p)\}\tau \pm \frac{1}{8}h]} \quad \text{with} \quad p = p(x,v)$$

where H'' means $\partial^2 H/\partial p \partial p$. For systems of "standard type"

$$H = \frac{1}{2m}p^2 + U(x)$$

we have $H'' = \frac{1}{m} > 0$, and can write

$$G(x,\tau;y,0) \sim \left[\frac{m}{ih\tau} \right]^{\frac{1}{2}} e^{\frac{i}{\hbar}\{pv-H(x,p)\}\tau} \quad \text{with} \quad p = mv \tag{108}$$

But

$$L(x,v) = pv - H(x,p)$$
$$\updownarrow$$
$$v = \tfrac{\partial}{\partial p}H(x,p)$$

$$(109.1)$$

is precisely the Legendre transformation which in classical mechanics *leads from the Hamiltonian to the Lagrangian*, and for systems of standard type supplies

$$= \tfrac{1}{2}mv^2 - U(x)$$
$$= \tfrac{m}{2}[(x-y)/\tau]^2 - U(x)$$

$$(109.2)$$

whence

$$G(x,\tau\,;y,0) \sim \left[\tfrac{m}{i\hbar\tau}\right]^{\frac{1}{2}} \tfrac{1}{\sqrt{2\pi}}\, e^{-\frac{1}{2}\frac{m}{i\hbar\tau}(x-y)^2} \cdot e^{-\frac{i}{\hbar}U(x)\tau}$$

$$(110)$$

which merits several kinds of comment:

- If we identify $\left[\tfrac{i\hbar\tau}{m}\right]^{\frac{1}{2}}$ with the ϵ in (98) then the factor up front becomes just the Gaussian representative of $\delta(x-y)$, for reasons traceable in part to the circumstance that p enters *squared* into $H(x,p)$.

- $\hbar$ and τ enter into that factor as an $\hbar\tau$-package: the "classical" (small $\hbar$) and "short-time" (small τ) asymptotes have come into alignment. Also a part of the enlarged package is m: we could as well speak of a "large mass" asymptote.

Let (110) be written

$$G(x,\tau\,;y,0) \sim \left[\tfrac{m}{2\pi i\hbar\tau}\right]^{\frac{1}{2}} \cdot e^{\frac{i}{\hbar}S_0(x,\tau\,;y,0)}$$

with $S_0(x,\tau\,;y,0) \equiv L\tau = \tfrac{1}{2}m(x-y)^2/\tau - U(x)$.   Then $\partial^2 S_0/\partial x\partial y = -m/\tau$ puts one in position to write

$$G(x,\tau\,;y,0) \sim \left[\tfrac{i}{\hbar}\tfrac{\partial^2 S_0}{\partial x\partial y}\right]^{\frac{1}{2}} \cdot e^{\frac{i}{\hbar}S_0(x,\tau\,;y,0)}$$

which is of a form encountered already at (95). What kind of an action-like thing is S_0? If m is to move from y to x in vanishingly brief time τ then it must move briskly. In the limit we expect the motion to be, in the approximation that kinetic energy $\gg$ potential energy, essentially free

$$x(t) = y + [(x-y)/\tau]t + \tau \cdot (\text{correction terms})$$

In that approximation the *dynamical* action becomes

$$S(x,\tau\,;y,0) = \int_0^\tau L\,dt = \tfrac{m}{2\tau}(x-y)^2 - \int_0^\tau U\big(y + [(x-y)/\tau]t\big)\,dt$$

which in the oscillatory case $U(x) = \tfrac{1}{2}m\omega^2 x^2$ yields

$$S_{\text{osc}}(x,\tau\,;y,0) = \tfrac{m}{2\tau}(x-y)^2 - \tfrac{1}{6}m\omega^2(x^2 + xy + y^2)\cdot\tau + \cdots$$

—in precise agreement with the short-time expansion of the exact $S_{\text{osc}}(x,t;y,0)$, as it was described at (94.1).

Notice finally that in the case $U(x) = 0$ of a free particle the right side of (110) assumes a form which at (91.5) was seen to be exactly correct even at non-infinitesimal times t.

Expanded conception of quantum state: density matrices. Given a quantum system $\mathfrak{S}$, we *might* know it to be in state $|\psi)$—as heretofore we have been casually content to assume[43]—but more typically we know of $\mathfrak{S}$ only that it is

in state $|\psi_1)$ with probability p_1,

in state $|\psi_2)$ with probability p_2,

$\vdots \qquad\qquad\qquad \vdots$

in state $|\psi_n)$ with probability p_n,

$\vdots \qquad\qquad\qquad \vdots$

where the p_n are (not "probability amplitudes" but) *ordinary probabilities*: non-negative real numbers, subject to the constraint that $\sum p_n = 1$. Such a state of affairs might have come about because

• We did our recent state-preparation with an *A-meter of imperfect resolution*. If the sources of instrumental error are numerous and independent, then (by the central limit theorem) we may expect those errors to be normally distributed: a meter reading a_0 means[44] that the system was projected into

state $|a)$ with probability $p(a) = \frac{1}{\epsilon\sqrt{2\pi}}\exp\left\{-\frac{1}{2}\left[\frac{a-a_0}{\epsilon}\right]^2\right\}$

• We drew $\mathfrak{S}$ from a *thermalized population* of systems. We then expect $\mathfrak{S}$ to be

in energy eigenstate $|n)$ with probability $p_n = \frac{1}{Z}e^{-E_n/kT}$

where the "partition function" $Z(T) \equiv \sum_n e^{-E_n/kT}$.

In such cases we say that the system is in a "mixed" state, and otherwise (as heretofore) in a "pure state." The distinction is due to von Neumann (1927).[45]

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[43] But *how* would we actually know such a thing? Only by a recent act of precise state-preparation (measurement). In textbook situations we are usually engaging in innocent-seeming fantasy, playing "Suppose it were the case that we knew; then ..." We tend—most of us, most of the time—to speak as though it made sense to suppose that "$\mathfrak{S}$ is in some quantum state, whether or not we happen to know it." But does hazard lurk in such naive realism?

[44] See again (98).

[45] See §9.1 in Jammer's *Conceptual Development of Quantum Mechanics* (1966).

We plan to spend the afternoon doing A-measurements on identically prepared copies of $\mathfrak{S}$. The theoretical estimators of the expected statistical properties of our data invoke "probability" in now two distinct ways:

- once in reference to the ineffable/irreducible randomness of the mirco world, as written into the $|\psi)$ concept, and
- once again in reference to the statistical properties of the state mixture, as written into the distribution function p_ψ.

The expected mean of our data can be described as a "mean of means"

$$\langle \mathbf{A} \rangle = \sum_\psi p_\psi \cdot (\psi|\mathbf{A}|\psi)$$

$$= \sum_i p_i(\psi_i|\mathbf{A}|\psi_i) \quad \text{in a more explicit notation}$$

the expected second moment as an "averaged second moment"

$$\langle \mathbf{A}^2 \rangle = \sum_\psi p_\psi \cdot (\psi|\mathbf{A}^2|\psi)$$

and so on. Enlarging upon an idea introduced at (13.2), we can write

$$\langle \mathbf{A} \rangle = \sum_i \sum_n p_i(\psi_i|n)(n|\mathbf{A}|\psi_i)$$

$$= \sum_n \sum_i (n|\mathbf{A}|\psi_i)p_i(\psi_i|n)$$

$$= \text{tr}\,\mathbf{A}\boldsymbol{\rho} \tag{111}$$

$$\boldsymbol{\rho} \equiv \sum_i |\psi_i)p_i(\psi_i| = \sum_i p_i\boldsymbol{\psi}_i \quad \text{defines the "density matrix"}$$

The "density matrix" is, in reality, not a "matrix" at all, but a *linear operator* ... if a linear operator with some very special properties (and which admits, of course, of matrix *representation*, as every linear operator does). Evidently $\boldsymbol{\rho}$ is the p_i-weighted sum of *projection operators* $\boldsymbol{\psi}_i \equiv |\psi_i)(\psi_i|$. The operators $\boldsymbol{\psi}_i$ project onto the states imagined to be present in the mixture.[46] The $\sum_i$ is a "sum over states"—states which are under no constraint to be orthogonal, or even linearly independent.

Relative to an orthonormal basis $\{|n)\}$ the density matrix acquires the representation $(m|\boldsymbol{\rho}|n)$. Interpreting $\text{tr}\boldsymbol{\rho}$ to mean $\sum_n(n|\boldsymbol{\rho}|n)$, we have

$$\text{tr}\boldsymbol{\rho} = \sum_n \sum_i (n|\psi_i)p_i(\psi_i|n) = \sum_i p_i(\psi_i|\psi_i) = \sum_i p_i = 1 \tag{112}$$

in all cases. Because $0 \leqslant p_i \leqslant 1$ (all i) one has

$$p_i^2 \leqslant p_i \quad \text{with equality only if } p_i = 0 \text{ or } p_i = 1$$

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[46] The point of that "imagined to be," and my use later of words like "purported," will be explained on the next page.

and the latter equality can hold in (at most) only a single instance, forcing all the other p_i to vanish. So we have

$$\sum_i p_i^2 \leqslant 1 \text{ with equality if and only if } \boldsymbol{\rho} \text{ refers to a pure state}$$

If the $|\psi_i)$ happen, in particular, to be orthogonal then

$$\boldsymbol{\rho}^2 = \sum_i \sum_j |\psi_i) p_i (\psi_i|\psi_j) p_j (\psi_j| = \sum_i |\psi_i) p_i^2 (\psi_i|$$

and we obtain

$$\text{tr} \boldsymbol{\rho}^2 = \sum_i p_i^2 \leqslant \sum_i p_i = 1 = \text{tr} \boldsymbol{\rho} \tag{113}$$

with equality only for unmixed pure states.[47]

Notice that $\boldsymbol{\rho} = \sum |\psi_k) p_k (\psi_k|$ is *insensitive to the relative phases* of the admixed states; i.e., that it is invariant under $|\psi_k) \longrightarrow e^{i\phi_k} |\psi_k)$.

Let $\boldsymbol{\rho} = \sum |\psi_i) p_i (\psi_i|$ refer to some purported mixture of *non-orthogonal* states. The operator $\boldsymbol{\rho}$ is manifestly self-adjoint—therefore assuredly possesses real eigenvalues ρ_n and orthogonal eigenvectors $|n)$, and can in terms of those be described $\sum |n) \rho_n (n|$. But in

$$\begin{aligned}
\boldsymbol{\rho} &= \textstyle\sum_i |\psi_i) p_i (\psi_i| &:& \quad p\text{-weighted mixture of } |\psi)\text{-states} \\
&= \textstyle\sum_n |n) \rho_n (n| &:& \quad \rho\text{-weighted mixture of } |n)\text{-states}
\end{aligned}$$

we have displayed the <u>same mixture in two distinct ways</u> ... and, in so doing, denied "objective reality" to either. In this respect a "mixture of quantum states" is a strange kind of mixture: it makes objective good sense to say that "this box contains a mixture of apples and oranges," but in quantum mechanics we confront a situation in which that statement might continue "... but you may, if you wish, consider it to contain a mixture of watermelons and kumquats, or alternatively, a mixture of ..." It would be of interest to

> Describe the *population of equivalent*
> *mixtures* to which $\boldsymbol{\rho}$ evidently refers.

This is an issue to which I will return.

It is important not to confuse "*mixture* of states" with "*superposition* of states." We might write

$$|\psi) = \tfrac{1}{\sqrt{2(1 + r\cos\theta)}} \Big\{ |\psi_1) + |\psi_2) \Big\} \quad \text{with} \quad (\psi_1|\psi_2) = r e^{i\theta} \tag{114.0}$$

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[47] Some authors allow themselves to write $\boldsymbol{\rho}^2 \leqslant \boldsymbol{\rho}$ to express this idea.

to describe the pure state obtained by equi-weighted superposition of states $|\psi_1)$ and $|\psi_2)$, and would then write

$$\boldsymbol{\rho} = |\psi)(\psi|$$
$$= \tfrac{1}{2(1+r\cos\theta)}\Big\{|\psi_1)(\psi_1| + |\psi_1)(\psi_2| + |\psi_2)(\psi_1| + |\psi_2)(\psi_2|\Big\} \quad (114.1)$$

to describe the associated density matrix. Equi-weighted mixture would, on the other hand, give

$$\boldsymbol{\rho} = \tfrac{1}{2}\Big\{|\psi_1)(\psi_1| + |\psi_2)(\psi_2|\Big\} \tag{114.2}$$

Suppose $|\psi_1)$ and $|\psi_2)$ were known to be orthogonal $((\psi_1|\psi_2) = 0 \Rightarrow r = 0)$ but that their relative phase were unknown; then (114.0) becomes

$$|\psi) = \tfrac{1}{\sqrt{2}}\Big\{|\psi_1) + e^{i\alpha}|\psi_2)\Big\}$$

and in place of (114.1) we obtain

$$\boldsymbol{\rho}(\alpha) = \tfrac{1}{2}\Big\{|\psi_1)(\psi_1| + |\psi_1)(\psi_2|e^{-i\alpha} + e^{+i\alpha}|\psi_2)(\psi_1| + |\psi_2)(\psi_2|\Big\}$$

If we express our phase-ignorance by "phase-averaging"

$$\boldsymbol{\rho} \equiv \tfrac{1}{2\pi}\int_0^{2\pi} \boldsymbol{\rho}(\alpha)\,d\alpha$$

then, pretty clearly, we *recover precisely the result* (114.2) *of simple mixing*.

We may conclude that $\boldsymbol{\rho}$ conveys a concept of "state" which is fairer to the observational (and perhaps also to the philosophical) facts of quantum experience than that conveyed by $|\psi)$; that $|\psi)$ is an abstraction which becomes accidentally available only in degenerate cases[48]

$$|\psi) = \sqrt{\boldsymbol{\rho}} \quad : \quad \text{possible only if } \boldsymbol{\rho}^2 = \boldsymbol{\rho}$$

... but is none the less useful for that!

Classical/quantum master equations. I look briefly to this topic to consider what it might have to contribute to our understanding of the concept of "state," and about the distinctive placement of quantum mechanics.

Abandon quantum mechanics for the moment. Think of a stochastic classical system which at time t is in state n with probability p_n, and by time

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[48] The following statement is intended to be more memorably picturesque than literally meaningful.

$t + \tau$ can be expected to hop to state m with "transition probability" $\tau W_{m \leftarrow n}$. We expect then to have

$$p_m(t + \tau) = p_m(t) + \tau \Big\{ \sum_n W_{m \leftarrow n} p_n(t) - p_m(t) \sum_n W_{n \leftarrow m} \Big\}$$

giving

$$\tfrac{d}{dt} p_m(t) = \sum_n \Big\{ W_{m \leftarrow n} p_n(t) - W_{n \leftarrow m} p_m(t) \Big\} \qquad (115)$$

Built into the design of this so-called "master equation" are the assumptions that (i) the "propensity to hop" depends on where the system is, not where it was (the system is "memoryless"), and (ii) the transition probabilities are time -independent. These are defining characteristics of what are called "Markoff processes." Further conditions are sometimes assumed; for example, one might in some applications have reason to assume

$$\text{DETAILED BALANCE} \quad : \quad W_{n \leftarrow m} = W_{m \leftarrow n}$$

The Schrödinger equation can be written in a way

$$\tfrac{d}{dt}(m|\psi) = \sum_n W_{m \leftarrow n}(n|\psi) \quad \text{with} \quad W_{m \leftarrow n} = \tfrac{1}{i\hbar}(m|\mathsf{H}|n)$$

which shares many of the features of (115), though it speaks of the complex hopping of "probability amplitudes." If one looks to the implied motion of the associated probabilities $p_m \equiv (\psi|m)(m|\psi)$ one obtains

$$\tfrac{d}{dt} p_m = \tfrac{1}{i\hbar} \sum_n \Big\{ (\psi|m)(m|\mathsf{H}|n)(n|\psi) - (\psi|n)(n|\mathsf{H}|m)(m|\psi) \Big\} \qquad (116)$$

which (except in the trivial case $(m|\mathsf{H}|n) = E_n \delta_{mn}$) presents not probabilities but amplitudes on its right side. Which brings us to a problem—first considered by Pauli in 1928—which I must be content merely to state:[49] Under what weakest possible and physically most natural conditions can it be arranged for the amplitudes on the right side of (116) either to disappear or to assemble themselves into p_n's ... so that (116) becomes a statement about (irreversibly) evolving probabilities? Solutions of the problem typically involve some form of the *random phase approximation* (phase-averaging).

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[49] For discussion and good references see N. G. van Kampen, "Fundamental problems in statistical mechanics of irreversible processes," in E. G. D. Cohen, *Fundamental Problems in Statistical Mechanics* (1962) and Amnon Aharony, "Microscopic Irreversibility, Unitarity & the H-theorem" in B. Gal-Or, *Modern Developments in Thermodynamics* (1974).