Remarks concerning the status & some ramifications of

EHRENFEST'S THEOREM

Nicholas Wheeler, Reed College Physics Department
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Introduction & motivation. Folklore alleges, and in some texts it is explicitly—if, as will emerge, not quite correctly—asserted, that "quantum mechanical expectation values obey Newton's second law." The pretty point here at issue was first remarked by Paul Ehrenfest (1880–1933), in a paper scarcely more than two pages long.[1] Concerning the substance and impact of that little gem, Max Jammer, at p. 363 in his *The Conceptual Development of Quantum Mechanics* (1966), has this to say:

> *"That for the harmonic oscillator wave mechanics agrees with ordinary mechanics had already been shown by Schrödinger...*[2] *A more general and direct line of connection between quantum mechanics and Newtonian mechanics was established in 1927 by Ehrenfest, who showed 'by a short elementary calculation without approximations' that the expectation value of the time derivative of the momentum is equal to the expectation value of the negative gradient of the potential energy function. Ehrenfest's affirmation of Newton's second law in the sense of averages taken over the wave packet had a great appeal to many physicists and did much to further the acceptance of the theory. For it made it possible to describe the particle by a localized wave packet which, though eventually spreading out in space, follows the trajectory of the classical motion. As emphasized in a different context elsewhere,*[3] *Ehrenfest's theorem*

[1] "Bemerkung über die angenäherte Gültigkeit der klassichen Machanik innerhalb der Quanatenmechanik," Z. Physik **45**, 455–457 (1927).

[2] Jammer alludes at this point to Schrödinger's "Der stetige Übergang von der Mikro- zur Makromechanik," Die Naturwissenschaften **28**, 664 (1926), which in English translation (under the title "The continuous transition from micro- to macro-mechanics") appears as Chapter 3 in the 3rd (augmented) English edition of Schrödinger's *Collected Papers on Wave Mechanics* (1982).

[3] See Jammer's *Concepts of Mass* (1961), p. 207.

> *and its generalizations by Ruark*[4]*... do not conceptually reduce quantum dynamics to Newtonian physics. They merely establish an analogy—though a remarkable one in view of the fact that, owing to the absence of a superposition principle in classical mechanics, quantum mechanics and classical dynamics are built on fundamentally different foundations."*

"Ehrenfest's theorem" is indexed in most quantum texts,[5] though the celebrated authors of some classic monographs[6] have (so far as I have been able to determine, and for reasons not clear to me) elected pass over the subject in silence. The authors of the texts just cited have been content simply to rehearse Ehrenfest's original argument, and to phrase their interpretive remarks so casually as to risk (or in several cases to invite) misunderstanding. Of more lively interest to me at present are the mathematically/interpretively more searching discussions which can be found in Chapter 6 of A. Messiah's *Quantum Mechanics* (1966) and Chapter 15 of L. E. Ballentine's *Quantum Mechanics* (1990). Also of interest will be the curious argument introduced by David Bohm in §9.26 of his *Quantum Theory* (1951): there Bohm uses Ehrenfest's theorem "backwards" to *infer the necessary structure of the Schrödinger equation.*

I am motivated to reexamine Ehrenfest's accomplishment by my hope (not yet ripe enough to be called an expectation) that it may serve to illuminate the puzzle which I may phrase this way:

> I look about me, in this allegedly "quantum mechanical world," and see objects moving classically along well-defined trajectories. How does this come to be so?

I have incidental interest also some mathematical ramifications of Ehrenfest's theorem in connection with which I am unable to cite references in the published literature. Some of those come instantly into focus when one looks to the general context within which Ehrenfest's argument is situated.

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[4] The allusion here is to A. E. Ruark, ". . . the force equation and the virial theorem in wave mechanics," Phys. Rev. **31**, 533 (1928).

[5] See E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (1937), p. 49; L. I. Schiff, *Quantum Mechanics* (3rd edition, 1968), p. 28; E. Mertzbacher, *Quantum Mechanics* (2nd edition, 1970), p. 41; J. L. Powell & B. Crassmann, *Quantum Mechanics* (1961), p. 98; D. J. Griffiths, *Introduction to Quantum Mechanics* (1995), pp. 17, 43, 71, 150, 162 & 175. Of the authors cited, only Griffiths draws recurrent attention to concrete *applications* of Ehrenfest's theorem.

[6] I have here in mind P. A. M. Dirac's *The Principles of Quantum Mechanics* (revised 4th edition, 1958) and L. D. Landau & E. M. Lifshitz' *Quantum Mechanics* (1958). W. Pauli's *Wellenmechanik* (1943) is a reprint of his famous Handbuch article, which appeared—incredibly—in 1926, which is to say: too early to contain any reference to Ehrenfest's accomplishment.

1. Quantum motion of moments: general principles. Let $|\psi)$ signify the state of a quantum system with Hamiltonian H, and let A refer to some time-independent observable.[7] The expected mean of a series of A-measurements can, by standard quantum theory, be described

$$\langle \mathsf{A}\rangle = (\psi|\mathsf{A}|\psi)$$

and the time-derivative of $\langle \mathsf{A}\rangle$—whether one works in the Schrödinger picture,[8] the Heisenberg picture,[9] or any intermediate picture—is given therefore by

$$\tfrac{d}{dt}\langle \mathsf{A}\rangle = \tfrac{1}{i\hbar}\langle \mathsf{AH}-\mathsf{HA}\rangle \tag{1}$$

Ehrenfest himself looked to one-dimensional systems of type

$$\mathsf{H} \equiv \tfrac{1}{2m}\mathsf{p}^2 - \mathsf{V} \quad \text{with} \quad \mathsf{V} \equiv V(\mathsf{x})$$

and confined himself to a single instance of (1):

$$\begin{aligned}\tfrac{d}{dt}\langle \mathsf{p}\rangle &= \tfrac{1}{i\hbar}\langle \mathsf{pH}-\mathsf{Hp}\rangle\\ &= \tfrac{1}{i\hbar}\langle \mathsf{pV}-\mathsf{Vp}\rangle\end{aligned}$$

Familiarly

$$[\mathsf{x},\mathsf{p}] = i\hbar\mathbf{1} \quad\Longrightarrow\quad [\mathsf{x}^n,\mathsf{p}] = i\hbar\cdot n\mathsf{x}^{n-1} \quad \text{whence} \quad [V(\mathsf{x}),\mathsf{p}] = i\hbar\cdot V^{'}(\mathsf{x})$$

so with Ehrenfest we have

$$\tfrac{d}{dt}\langle \mathsf{p}\rangle = -\langle V^{'}(\mathsf{x})\rangle \tag{2.1}$$

A similar argument supplies

$$\tfrac{d}{dt}\langle \mathsf{x}\rangle = \tfrac{1}{m}\langle \mathsf{p}\rangle \tag{2.2}$$

though Ehrenfest did not draw explicit attention to this fact.

Equation (2.1) is *notationally reminiscent* of Newton's 2$^{\text{nd}}$ law

$$\dot p = -V^{'}(x) \quad \text{with} \quad p \equiv m\dot x$$

and equations (2) are jointly reminiscent of the first-order "canonical equations of motion"

$$\left.\begin{aligned}\dot x &= \tfrac{1}{m}p\\ \dot p &= -V^{'}(x)\end{aligned}\right\} \tag{3}$$

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[7] I will be using **sans serif boldface** type to distinguish operators (q-numbers) from real/complex numbers (c-numbers).

[8] A is constant, but $|\psi)$ moves: $\frac{d}{dt}|\psi) = \frac{1}{i\hbar}\mathsf{H}|\psi)$.

[9] $|\psi)$ is constant, but A moves: $\frac{d}{dt}\mathsf{A} = \frac{1}{i\hbar}[\mathsf{A},\mathsf{H}]$.

that associate classically with systems of type $H(x,p) = \frac{1}{2m}p^2 + V(x)$. But except under special circumstances which favor the replacement

$$\langle V'(\mathsf{x})\rangle \quad \longmapsto \quad V'(\langle\mathsf{x}\rangle) \tag{3}$$

the systems (2) and (3) pose profoundly different mathematical and interpretive problems. Whence Jammer's careful use of the word "analogy," and of the careful writing (and, in its absence, of the risk of confusion) in some of the texts to which I have referred.

The simplest way to achieve (3) comes into view when one looks to the case of a harmonic oscillator. Then $V'(x) = m\omega^2 x$ is *linear* in x, (3) reduces to a triviality, and from (2) one obtains

$$\left.\begin{aligned} \tfrac{d}{dt}\langle\mathsf{p}\rangle &= -m\omega^2\langle\mathsf{x}\rangle \\ \tfrac{d}{dt}\langle\mathsf{x}\rangle &= \tfrac{1}{m}\langle\mathsf{p}\rangle \end{aligned}\right\} \tag{4}$$

For harmonic oscillators it is true in every case (i.e., without the imposition of restrictions upon $|\psi)$) that the expectation values $\langle\mathsf{x}\rangle$ and $\langle\mathsf{p}\rangle$ move classically.

The failure of (3) can, in the general case (i.e., when $V(x)$ is not quadratic), be attributed to the circumstance that for most distributions $\langle x^n\rangle \neq \langle x\rangle^n$. It becomes in this light natural to ask: What conditions on the distribution function $P(x) \equiv \psi^*(x)\psi(x)$ are necessary and sufficient to insure that $\langle x^n\rangle$ and $\langle x\rangle^n$ are (for all n) equal? Introducing the so-called "characteristic function" (or "moment generating function")

$$\varPhi(k) \equiv \sum_{n=0}^{\infty}\frac{1}{n!}(ik)^n\langle x^n\rangle = \int e^{ikx}P(x)\,dx$$

we observe that if $\langle x^n\rangle = \langle x\rangle^n$ (all n) then $\varPhi(k) = e^{ik\langle x\rangle}$, and therefore that

$$P(x) = \tfrac{1}{2\pi}\int e^{-ik[x-\langle x\rangle]}\,dk = \delta(x - \langle x\rangle)$$

It was this elementary fact which led Ehrenfest to his central point, which (assuming $V(x)$ to be now arbitrary) can be phrased as follows: If and to the extent that $P(x)$ is δ-function-like (refers, that is to say, to a narrowly confined wave packet), to that extent the exact equations (2) can be approximated

$$\left.\begin{aligned} \tfrac{d}{dt}\langle\mathsf{p}\rangle &= -V'(\langle\mathsf{x}\rangle) \\ \tfrac{d}{dt}\langle\mathsf{x}\rangle &= \tfrac{1}{m}\langle\mathsf{p}\rangle \end{aligned}\right\} \tag{5}$$

and *in that approximation* the means $\langle\mathsf{x}\rangle$ and $\langle\mathsf{p}\rangle$ move classically.

But while $P(x) = \delta(x - \langle x\rangle)$ may hold initially (as it is often assumed to do), such an equation cannot, according to orthodox quantum mechanics, persist, for functions of the form $\sqrt{\delta(x - x_{\text{classical}}(t))}e^{i\alpha(x,t)}$ cannot be made to satisfy the Schrödinger equation.

2. Example: the free particle. To gain insight into the rate at which $P(x)$ loses its youthfully slender figure—the rate, that is to say, at which the equations $\langle x^n\rangle = \langle x\rangle^n$ lose their presumed initial validity—one looks naturally to the time-derivatives of the "centered moments" $\langle(\mathsf{x} - \langle\mathsf{x}\rangle)^n\rangle$, and more particularly to the leading (and most tractable) case $n = 2$. From $\langle(\mathsf{x} - \langle\mathsf{x}\rangle)^2\rangle = \langle\mathsf{x}^2\rangle - \langle\mathsf{x}\rangle^2$ it follows that

$$\tfrac{d}{dt}\langle(\mathsf{x} - \langle\mathsf{x}\rangle)^2\rangle = \tfrac{d}{dt}\langle\mathsf{x}^2\rangle - 2\langle\mathsf{x}\rangle\tfrac{d}{dt}\langle\mathsf{x}\rangle \tag{6}$$

To illustrate the pattern of the implied calculation we look initially to the case of a free particle: $\mathsf{H} = \frac{1}{2m}\mathsf{p}^2$. From (2) we learn that

$$\begin{aligned} &\tfrac{d}{dt}\langle\mathsf{p}\rangle = 0 \quad \text{so } \langle\mathsf{p}\rangle \text{ is a constant; call it } p \equiv mv \\ &\tfrac{d}{dt}\langle\mathsf{x}\rangle = v \\ &\qquad\Downarrow \\ &\langle\mathsf{x}\rangle = x_0 + vt \quad \text{where } x_0 \equiv \langle\mathsf{x}\rangle_{\text{initial}} \text{ is a constant of integration} \end{aligned} \tag{7}$$

Looking now to the leading term on the right side of (6), we by (1) have

$$\tfrac{d}{dt}\langle\mathsf{x}^2\rangle = \tfrac{1}{2i\hbar m}\langle[\mathsf{x}^2, \mathsf{p}^2]\rangle$$

The fundamental commutation rule $[\mathsf{AB}, \mathsf{C}] = \mathsf{A}[\mathsf{B}, \mathsf{C}] + [\mathsf{A}, \mathsf{C}]\mathsf{B}$ implies (and can be recovered as a special consequence of) the identity

$$[\mathsf{AB}, \mathsf{CD}] = \mathsf{AC}[\mathsf{B}, \mathsf{D}] + \mathsf{A}[\mathsf{B}, \mathsf{C}]\mathsf{D} + \mathsf{C}[\mathsf{A}, \mathsf{D}]\mathsf{B} + [\mathsf{A}, \mathsf{C}]\mathsf{DB}$$

with the aid of which we obtain $[\mathsf{x}^2, \mathsf{p}^2] = 2i\hbar(\mathsf{xp} + \mathsf{px})$, giving

$$\tfrac{d}{dt}\langle\mathsf{x}^2\rangle = \tfrac{1}{m}\langle(\mathsf{xp} + \mathsf{px})\rangle \tag{8}$$

Shifting our attention momentarily from x^2 to $(\mathsf{xp} + \mathsf{px})$, in which we have now an acquired interest, we by an identical argument have

$$\begin{aligned} \tfrac{d}{dt}\langle(\mathsf{xp} + \mathsf{px})\rangle &= \tfrac{1}{2i\hbar m}\langle[(\mathsf{xp} + \mathsf{px}), \mathsf{p}^2]\rangle \\ &= \tfrac{2}{m}\langle\mathsf{p}^2\rangle \end{aligned} \tag{9}$$

and are led to divert our attention once again, from $(\mathsf{xp} + \mathsf{px})$ to p^2. But

$$\begin{aligned} \tfrac{d}{dt}\langle\mathsf{p}^2\rangle &= \tfrac{1}{2i\hbar m}\langle[\mathsf{p}^2, \mathsf{p}^2]\rangle \\ &= 0 \quad \text{so } \langle\mathsf{p}^2\rangle \text{ is a constant; call it } m^2u^2 \end{aligned}$$

by an argument that serves in fact to establish that

$$\text{For a free particle } \langle\mathsf{p}^n\rangle \text{ is constant for } \textit{all} \text{ values of } n. \tag{10}$$

Returning with this information to (9) we obtain

$$\langle(\mathsf{xp}+\mathsf{px})\rangle = 2mu^2t+a$$
$$a \equiv \langle(\mathsf{xp}+\mathsf{px})\rangle_{\text{initial}} \text{ is a constant of integration}$$

which when introduced into (8) gives

$$\langle\mathsf{x}^2\rangle = \tfrac{1}{m}\big\{mu^2t^2+at\big\}+s^2$$
$$s^2 \equiv \langle\mathsf{x}^2\rangle_{\text{initial}} \text{ is a final constant of integration}$$

We conclude that the time-dependence of the centered 2^{nd} moments of a *free* particle can be described

$$\sigma_p^2(t) \equiv \langle(\mathsf{p}-\langle\mathsf{p}\rangle)^2\rangle = m^2(u^2-v^2) \tag{11.1}$$
$$\begin{aligned}\sigma_x^2(t) \equiv \langle(\mathsf{x}-\langle\mathsf{x}\rangle)^2\rangle &= \tfrac{1}{m}\big\{mu^2t^2+at\big\}+s^2-(x_0+vt)^2\\ &= (u^2-v^2)t^2+\tfrac{1}{m}(a-2mvx_0)t+(s^2-x_0^2)\end{aligned} \tag{11.2}$$

Concerning the constants which enter into the formulation of these results, we note that

x_0 and s have the dimensionality of LENGTH
u and v have the dimensionality of VELOCITY
a has the dimensionality of ACTION

and that the values assignable to those constants are subject to some constraint: necessarily (whether one argues from $\sigma_p^2 \geq 0$ or from $\sigma_x^2(t\to\pm\infty)\geq 0$)

$$u^2-v^2 \geq 0$$

while $\sigma_x^2(0)\geq 0$ entails

$$s^2-x_0^2 \geq 0$$

A graph of $\sigma_x^2(t)$ has the form of an up-turned parabola or is linear according as $u^2-v^2 \gtreqless 0$; the latter circumstance is admissible only if $a-2mvx_0=0$, but in the former case the requirement that the roots of $\sigma_x^2(t)=0$ be not real and distinct (i.e., that they be either coincident or imaginary) leads to a sharpened refinement of that admissibility condition:

$$(u^2-v^2)(s^2-x_0^2)-\big[\tfrac{1}{2m}(a-2mvx_0)\big]^2 \geq 0 \tag{12}$$

By quick calculation we find (proceeding from (11.2)) that the least value ever assumed by $\sigma_x^2(t)$ can be described

$$\sigma_x^2(t)\Big|_{\text{least}} = \frac{(u^2-v^2)(s^2-x_0^2)-\big[\tfrac{1}{2m}(a-2mvx_0)\big]^2}{(u^2-v^2)}$$

and so obtain

$$\begin{aligned}\sigma_p^2(t)\sigma_x^2(t) &= m^2(u^2-v^2)\big[(u^2-v^2)t^2+\tfrac{1}{m}(a-2mvx_0)t+(s^2-x_0^2)\big]\\ &\geq m^2(u^2-v^2)(s^2-x_0^2)-\big[\tfrac{1}{2}(a-2mvx_0)\big]^2\end{aligned}\tag{13}$$

In deriving (13) we drew upon the principles of quantum *dynamics*, as they refer to the system $\mathsf{H}=\frac{1}{2m}\mathsf{p}^2$, but imposed no restrictive assumption upon the properties of $|\psi)$; in particular, we did not (as Ehrenfest himself did) assume $(x|\psi)\equiv\psi(x)$ to be Gaussian. A rather different result was achieved by Schrödinger by an argument which draws *not at all* upon dynamics (it exploits little more than the definition $\langle\mathsf{A}\rangle\equiv(\psi|\mathsf{A}|\psi)$ and Schwarz' inequality); if A and B refer to arbitrary observables, and $|\psi)$ to an arbitrary state, then according to Schrödinger[10]

$$\begin{aligned}(\Delta A)^2(\Delta B)^2 &\geq \Big\langle\frac{\mathsf{AB}-\mathsf{BA}}{2i}\Big\rangle^2+\Big\{\Big\langle\frac{\mathsf{AB}+\mathsf{BA}}{2}\Big\rangle-\langle\mathsf{A}\rangle\langle\mathsf{B}\rangle\Big\}^2\\ &\geq \Big\langle\frac{\mathsf{AB}-\mathsf{BA}}{2i}\Big\rangle^2\end{aligned}\tag{14}$$

which in a particular case ($\mathsf{A}\mapsto\mathsf{x}$, $\mathsf{B}\mapsto\mathsf{p}$) entails

$$\sigma_p^2(t)\sigma_x^2(t)\geq(\hbar/2)^2+\Big\{\Big\langle\frac{\mathsf{xp}+\mathsf{px}}{2}\Big\rangle-\langle\mathsf{x}\rangle\langle\mathsf{p}\rangle\Big\}^2\tag{15}$$

Reverting to our established notation, we find

$$\Big\{\text{etc.}\Big\}^2=\Big\{m(u^2-v^2)t+\tfrac{1}{2}(a-2mvx_0)\Big\}^2$$

and observe that the expression on the right *invariably vanishes once*, at time

$$t=-\Big[\frac{a-2mvx_0}{2m(u^2-v^2)}\Big]$$

Which is precisely the time at which, according to (11.2), $\sigma_x^2(t)$ assumes its least value. Evidently (13) will be consistent with (15) if and only if we impose upon the parameters $\{x_0,s,u,v$ and $a\}$ this sharpened—and *non*-dynamically motivated—refinement of (12):

$$(u^2-v^2)(s^2-x_0^2)-\big[\tfrac{1}{2m}(a-2mvx_0)\big]^2\geq(\hbar/2m)^2\tag{16}$$

Notice that we recover (12) if we approach the limit that $m\to\infty$ in such a way as to preserve the finitude of $\frac{1}{2m}(a-2mvx_0)$.

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[10] "Zum Heisenbergschen Unscharfenprinzip," Berliner Berichte, 296 (1930). For discussion which serves to place Schrödinger's result in context, see §7.1 in Jammer's *The Conceptual Development of Quantum Mechanics* (1966). For a more technical discussion which emphasizes the importance of the "correlation term" {etc.}—a term which the argument which appears on p. 109 of Griffiths' text appears to have been designed to circumvent—see the early sections in Bohm's Chapter 10. Or see my own QUANTUM MECHANICS (1967), Chapter III, pp. 51–58.

3. A still simpler example: the "photon". We are in the habit of thinking of the free particle as the "simplest possible" dynamical system. But at present we are concerned with certain *algebraic aspects* of quantum dynamics, and from that point of view it becomes natural to consider the Hamiltonian

$$\mathsf{H} = c\,\mathsf{p} \tag{17}$$

which depends not quadratically but only linearly upon p. We understand c to be a constant with the dimensionality of VELOCITY.[11] Classically, the canonical equations of motion read

$$\dot{x} = c \quad \text{and} \quad \dot{p} = 0 \tag{18}$$

and give

$$x(t) = x_0 + ct \quad \text{and} \quad p(t) = \text{constant}$$

The entities to which the theory refers (lacking any grounds on which to call them "particles," I will call them "photons") invariably move *to the right* with speed c. Quantum mechanically, Ehrenfest's theorem gives

$$\tfrac{d}{dt}\langle\mathsf{p}\rangle = 0 \quad \text{and} \quad \tfrac{d}{dt}\langle\mathsf{x}\rangle = \tfrac{1}{i\hbar}\langle[\mathsf{x}, c\,\mathsf{p}]\rangle = c$$

which exactly reproduce the classical equations (17), and inform us that the 1st moments $\langle\mathsf{x}\rangle$ and $\langle\mathsf{p}\rangle$ move "classically:"

$$\begin{aligned}\langle\mathsf{x}\rangle &= x_0 + ct\\ \langle\mathsf{p}\rangle &= \text{constant: call it } p\end{aligned}$$

Looking to the higher moments, the argument which gave (10) now supplies the information that that indeed $\langle\mathsf{p}^n\rangle$ is constant for *all* values of n, and so also therefore are all the *centered* moments of momentum; so also, in particular, is

$$\sigma_p^2(t) = \text{constant; call it } P^2$$

From

$$\tfrac{d}{dt}\langle\mathsf{x}^2\rangle = \tfrac{1}{i\hbar}\langle[\mathsf{x}^2, c\,\mathsf{p}]\rangle = 2c\langle\mathsf{x}\rangle = 2c(x_0 + ct)$$

we obtain

$$\langle\mathsf{x}^2\rangle = s^2 + 2cx_0t + c^2t^2$$

giving

$$\begin{aligned}\sigma_x^2(t) = \langle\mathsf{x}^2\rangle - \langle\mathsf{x}\rangle^2 &= (s^2 + 2cx_0t + c^2t^2) - (x_0 + ct)^2\\ &= s^2 - x_0^2\\ &= \text{constant}\end{aligned}$$

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[11] One might be tempted to write $P/2m$ in place of c, but it seems extravagant to introduce two constants where one will serve.

By extension of the same line of argument one can show (inductively) that the centered moments $\langle(\mathsf{x}-\langle\mathsf{x}\rangle)^n\rangle$ of *all* orders n are constant. Looking finally to the mean motion of the "correlation operator" $\mathsf{C}\equiv\frac{1}{2}(\mathsf{xp}+\mathsf{px})$ we find

$$\tfrac{d}{dt}\langle\mathsf{C}\rangle=\tfrac{1}{2i\hbar}\langle[(\mathsf{xp}+\mathsf{px}),c\mathsf{p}]\rangle=c\langle\mathsf{p}\rangle=cp$$

giving

$$\langle\mathsf{C}\rangle=a+cpt$$

The motion of the "correlation coefficient"

$$C=\Big\langle\frac{\mathsf{xp}+\mathsf{px}}{2}\Big\rangle-\langle\mathsf{x}\rangle\langle\mathsf{p}\rangle \tag{19}$$

can therefore be described

$$C(t)=(a+cpt)-(x_0+ct)p=a-px_0$$

The correlation coefficient C is, in other words, also constant. We conclude that for the "photonic system"

$$\begin{aligned}\sigma_p^2(t)\sigma_x^2(t)&=\text{constant}\\&=P^2\cdot(s^2-x_0^2)\\&\geq(\hbar/2)^2+(a-px_0)^2\quad\text{according to Schrödinger}\end{aligned}$$

and on these grounds that the parameters $\{x_0,s,P,p$ and $a\}$ are subject to a constraint which can (compare (16)) be written

$$P^2(s^2-x_0^2)-(a-px_0)^2\geq(\hbar/2)^2 \tag{20}$$

From the constancy of the moments of principal interest to us we infer that the "photonic" system is non-dispersive. That same conclusion is supported also by this alternative line of argument: (17) gives rise to a "Schrödinger equation" which can be written $c(\frac{\hbar}{i}\frac{\partial}{\partial x})\psi=i\hbar\frac{\partial}{\partial t}\psi$ or more simply

$$(\partial_x+\tfrac{1}{c}\partial_t)\psi=0$$

and the general solution of which is well known to move "rigidly" (which is to say: non-dispersively) to the right:

$$\psi(x,t)=f(x-ct)$$

Only at (20) does the quantum mechanical photonic system differ in any obvious respect from its classical counterpart. It seems to me curious that the system has not been discussed more widely. The system—which does not admit of Lagrangian formulation—derives some of its formal interest from the circumstance that both T-invariance and P-invariance are broken.

4. Computational features of the general case. One could without difficulty—though I on this occasion won't—construct similarly detailed accounts of the momental dynamics of the systems

$$\begin{aligned} \text{FREE FALL} &: \quad \mathsf{H} = \tfrac{1}{2m}\mathsf{p}^2 + mg\,\mathsf{x} \\ \text{HARMONIC OSCILLATOR} &: \quad \mathsf{H} = \tfrac{1}{2m}\mathsf{p}^2 + m\omega^2\,\mathsf{x}^2 \end{aligned}$$

and, indeed, of any system with a Hamiltonian

$$\mathsf{H} = c_1\mathsf{p}^2 + c_2(\mathsf{xp}+\mathsf{px}) + c_3\mathsf{x}^2 + c_4\mathsf{p} + c_5\mathsf{x} + c_6\mathbf{1}$$

which depends at most quadratically upon the operators x and p. To illustrate problems presented in the more general case I look to the system

$$\mathsf{H} = \tfrac{1}{2m}\mathsf{p}^2 + \tfrac{1}{4}k\,\mathsf{x}^4 \tag{21}$$

The classical equations of motion read

$$\left.\begin{aligned} \dot{p} &= -kx^3 \\ \dot{x} &= \tfrac{1}{m}p \end{aligned}\right\} \tag{22}$$

while Ehrenfest's relations (2) become

$$\left.\begin{aligned} \tfrac{d}{dt}\langle\mathsf{p}\rangle &= -k\langle\mathsf{x}^3\rangle \\ \tfrac{d}{dt}\langle\mathsf{x}\rangle &= \tfrac{1}{m}\langle\mathsf{p}\rangle \end{aligned}\right\} \tag{23.1}$$

The latter are, as Ehrenfest was the first to point out, exact corollaries of the Schrödinger equation $\mathsf{H}|\psi) = i\hbar\frac{\partial}{\partial t}|\psi)$, and they are in an obvious sense "reminiscent" of their classical counterparts. But (23.1) does not provide an *instance* of (22), for the simple reason that $\langle\mathsf{x}^3\rangle$ and $\langle\mathsf{x}\rangle$ are *distinct variables*. More to the immediate point, (23.1) *does not comprise a complete and soluable system* of differential equations.

In an effort to achieve "completeness" we look to

$$\begin{aligned} \tfrac{d}{dt}\langle\mathsf{x}^3\rangle = \tfrac{1}{i\hbar}\langle[\mathsf{x}^3,\mathsf{H}]\rangle &= \tfrac{1}{2mi\hbar}\langle[\mathsf{x}^3,\mathsf{p}^2]\rangle \\ &\qquad [\mathsf{x}^3,\mathsf{p}^2] = [\mathsf{x}^3,\mathsf{p}]\mathsf{p} + \mathsf{p}[\mathsf{x}^3,\mathsf{p}] \\ &\qquad\qquad = 3i\hbar(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2) \\ &= \tfrac{3}{2m}\langle(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2)\rangle \end{aligned} \tag{23.2}$$

and discover that we must add $(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2)$ to our list of variables. We look therefore to

$$\tfrac{d}{dt}\langle(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2)\rangle = \tfrac{1}{i\hbar}\langle[(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2),\mathsf{H}]\rangle$$

By tedious computation

$$\begin{aligned} [(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2),\mathsf{p}^2] &= i\hbar(\mathsf{xp}^2 + 2\mathsf{pxp} + \mathsf{p}^2\mathsf{x}) \\ [(\mathsf{x}^2\mathsf{p} + \mathsf{p}\,\mathsf{x}^2),\mathsf{x}^4] &= -8i\hbar\mathsf{x}^5 \end{aligned}$$

so we have

$$\tfrac{d}{dt}\langle(\mathsf{x}^2\mathsf{p}+\mathsf{p}\,\mathsf{x}^2)\rangle = \tfrac{1}{2m}\langle(\mathsf{x}\mathsf{p}^2+2\mathsf{p}\mathsf{x}\mathsf{p}+\mathsf{p}^2\mathsf{x})\rangle - \tfrac{8}{3}k\langle\mathsf{x}^5\rangle \tag{23.2}$$

but must now add both $\langle(\mathsf{x}\mathsf{p}^2+2\mathsf{p}\mathsf{x}\mathsf{p}+\mathsf{p}^2\mathsf{x})\rangle$ and $\langle\mathsf{x}^5\rangle$ to our list of variables. Pretty clearly (since H introduces factors faster that $[\mathsf{x},\mathsf{p}] = i\hbar\mathbf{1}$ can kill them) equations (23) comprise only the leading members of an *infinite system of coupled first-order linear (!) differential equations*.

Writing down such a system—quite apart from the circumstance that it may require an infinite supply of paper and ink—poses an algebraic problem of a high order, particularly in the more general case

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

$V(\mathsf{x})$ described by power series, or Laplace transform, or. . .

and especially in the most general case $\mathsf{H} = h(\mathsf{x},\mathsf{p})$. But assuming the system to *have* been written down, *solving* such a system poses a mathematical problem which is qualitatively quite distinct both from the problem of solving it's (generally non-linear) classical counterpart

$$\left.\begin{aligned}\dot p &= -V'(x)\\ \dot x &= \tfrac{1}{m}p\end{aligned}\right\} \quad : \quad \text{equivalently} \quad m\ddot x = -V'(x)$$

and from solving the associated Schrödinger equation

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

Distinct from and, we can anticipate, more difficult than. But while the computational utility of the "momental formulation of quantum mechanics" can be expected to be slight except in a few favorable cases, the formalism does by its mere existence pose some uncommon questions which would appear to merit consideration.

5. The momental hierarchy supported by an arbitrary observable. Let A refer to an arbitrary observable. According to (1)

$$\tfrac{d}{dt}\langle\mathsf{A}\rangle = \tfrac{1}{i\hbar}\langle[\mathsf{A},\mathsf{H}]\rangle$$

Noting that if A and B are hermitian then $[\mathsf{A},\mathsf{B}]$ is antihermitian but $\frac{1}{i\hbar}[\mathsf{A},\mathsf{B}]$ is again hermitian (which is to say: an acceptable "observable"), let us agree to write

$$\begin{aligned}\mathsf{A}_0 &\equiv \mathsf{A}\\ \mathsf{A}_1 &\equiv \tfrac{1}{i\hbar}[\mathsf{A},\mathsf{H}]\\ \mathsf{A}_2 &\equiv \tfrac{1}{i\hbar}[\tfrac{1}{i\hbar}[\mathsf{A},\mathsf{H}],\mathsf{H}] \equiv \big(\tfrac{1}{i\hbar}\big)^2\big\{\mathsf{A},\mathsf{H}^2\big\}\\ &\;\vdots\\ \mathsf{A}_{n+1} &\equiv \tfrac{1}{i\hbar}[\mathsf{A}_n,\mathsf{H}] \equiv \big(\tfrac{1}{i\hbar}\big)^n\big\{\mathsf{A},\mathsf{H}^n\big\} \quad : \quad n = 0,1,2,\ldots\end{aligned} \tag{24}$$

The $\mathbf{H}$-induced quantum motion of the "momental heirarchy supported by $\mathbf{A}$" can be described

$$\tfrac{d}{dt}\langle \mathbf{A}_n\rangle = \langle \mathbf{A}_{n+1}\rangle \quad : \quad n = 0, 1, 2, \ldots \tag{25}$$

The heirarchy *truncates* at $n = m$ if and only if it is the case that $\mathbf{A}_{m+1} = \mathbf{0}$ (which entails $\mathbf{A}_n = \mathbf{0}$ for all $n > m$); if and only if, that is to say, $\mathbf{A}_n$ is a constant of the motion. In such a circumstance one has

$$\big(\tfrac{d}{dt}\big)^{m+1}\langle \mathbf{A}\rangle_t = 0$$

which entails that $\langle \mathbf{A}\rangle_t$ is a *polynomial* in t; specifically

$$\langle \mathbf{A}\rangle_t = \sum_{n=0}^{m} \tfrac{1}{n!}\langle \mathbf{A}_n\rangle_0 t^n \tag{26}$$

Several instances of just such a situation have, in fact, already been encountered. For example: let $\mathbf{H}$ have the "photonic" structure (17), and let $\mathbf{A}$ be assigned the meaning $\frac{1}{m!}\mathbf{x}^m$; the resulting heirarchy truncates in after m steps:

$$\begin{aligned}
\mathbf{A}_0 &\equiv \tfrac{1}{m!}\mathbf{x}^m\\
\mathbf{A}_1 &= c^1\tfrac{1}{(m-1)!}\mathbf{x}^{m-1}\\
\mathbf{A}_2 &= c^2\tfrac{1}{(m-2)!}\mathbf{x}^{m-2}\\
\mathbf{A}_3 &= c^3\tfrac{1}{(m-3)!}\mathbf{x}^{m-3}\\
&\vdots\\
\mathbf{A}_m &= c^m\,\mathbf{1} \quad \text{(a physically uninteresting constant of the motion)}\\
\mathbf{A}_n &= \mathbf{0} \quad \text{for } n > m
\end{aligned}$$

In §3 we had occasion to study just such heirarchies in the cases $m = 1$ and $m = 2$, and were—for reasons now clear—led to polynomials in t. We developed there an interest also in the truncated heirarchy

$$\begin{aligned}
\mathbf{A}_0 &\equiv \tfrac{1}{2}(\mathbf{xp} + \mathbf{px})\\
\mathbf{A}_1 &= c\,\mathbf{p}\\
\mathbf{A}_2 &= \mathbf{0}
\end{aligned}$$

Tractability of another sort attaches to heirarchies which, though not truncated, exhibit the property of *cyclicity*, which in its simplest manifestation means that

$$\mathbf{A}_m = \lambda\,\mathbf{A}_0$$

for some λ and some least value of m. Then $\mathbf{A}_{m+q} = \lambda\,\mathbf{A}_q$, $\mathbf{A}_{2m} = \lambda^2\,\mathbf{A}_0$ and

$$\big(\tfrac{d}{dt}\big)^m\langle \mathbf{A}\rangle_t = \lambda\langle \mathbf{A}\rangle_t$$

which again yields to solution by elementary means:

$$\langle \mathsf{A}\rangle_t = \text{sum of exponentials involving the } m^{\text{th}} \text{ roots of } \lambda$$

For example: let H have the generic quadratic structure

$$\mathsf{H} = \tfrac{1}{2}a\,\mathsf{p}^2 + \tfrac{1}{2}b\,\mathsf{x}^2$$

and let A be assigned the meaning x (alternatively p);

$$\begin{array}{ll} \mathsf{A}_0 \equiv \mathsf{x} & \qquad \mathsf{A}_0 \equiv \mathsf{p} \\ \mathsf{A}_1 = a\,\mathsf{p} & \qquad \mathsf{A}_1 = -b\,\mathsf{x} \\ \mathsf{A}_2 = -ba\,\mathsf{x} & \qquad \mathsf{A}_2 = -ab\,\mathsf{p} \\ \quad\vdots & \qquad\quad\vdots \end{array}$$

Each of the preceding hierarchies is cyclic, with period 2 and $\lambda = -ab$. If we set $a = 1/m$ and $b = m\omega^2$ then $\lambda = -\omega^2$, and we obtain results that bear on the quantum mechanics of a *harmonic oscillator*; in particular, we have

$$\left(\tfrac{d}{dt}\right)^2 \langle \mathsf{x}\rangle_t = -\omega^2 \langle \mathsf{x}\rangle_t$$

which informs us that $\langle \mathsf{x}\rangle_t$ oscillates harmonically for *all* $|\psi)$:[12] the standard Gaussian assumption is superfluous. In the limit $\omega \downarrow 0$ (i.e., for $b = 0$) the preceeding heirarchies (instead of being cyclic) truncate, and we obtain results appropriate to the quantum mechanics of a *free particle*. When A is assigned the meaning x^2 (alternatively p^2) we are led to hierarchies

$$\begin{array}{ll} \mathsf{A}_0 \equiv \mathsf{x}^2 & \qquad \mathsf{A}_0 \equiv \mathsf{p}^2 \\ \mathsf{A}_1 = a(\mathsf{xp} + \mathsf{px}) & \qquad \mathsf{A}_1 = -b(\mathsf{xp} + \mathsf{px}) \\ \quad\vdots & \qquad\quad\vdots \end{array}$$

which become *identical to within a factor* at the second step, and it is *thereafter* that the hierarchy continues cyclically

$$\begin{aligned} \mathsf{A}_0 &\equiv \tfrac{1}{2}(\mathsf{xp} + \mathsf{px}) \\ \mathsf{A}_1 &= (a\,\mathsf{p}^2 - b\,\mathsf{x}^2) \\ \mathsf{A}_2 &= -2ab(\mathsf{xp} + \mathsf{px}) \\ &\;\vdots \end{aligned}$$

with period 2 and $\lambda = -4ab$. From the fact that $\frac{d}{dt}\langle \mathsf{x}^2\rangle_t$ is oscillatory it follows that

$$\langle \mathsf{x}^2\rangle_t = \text{constant} + \text{oscillatory part}$$

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[12] This seldom remarked fact was first brought casually to my attention years ago by Richard Crandall.

and from this we conclude it to be a property of harmonic oscillators that (for all $|\psi)$) $\sigma_x^2(t)$ and $\sigma_p^2(t)$ "ripple" with *twice the base frequency of the oscillator*.

Hierarchies into which $\mathbf{0}$ intrudes are necessarily truncated, and those which contain a repeated element are necessary cyclic, but in general one can expect a hierarchy to be neither truncated nor cyclic. In the general case one has

$$\langle \mathbf{A}\rangle_t = \sum_{n=0}^{\infty} \tfrac{1}{n!}\langle \mathbf{A}_n\rangle_0 t^n \quad \text{within some radius of convergence} \tag{27}$$

which does give back (26) when the hierarchy truncates, does sum up nicely in cyclic cases,[13] and can be construed to be a generating function for the expectation values of the members of the hierarchy. This, however, becomes a potentially useful point of view only if one (from what source?) has independent knowledge of $\langle \mathbf{A}\rangle_t$. I note in passing that at (27) we have recovered a result which is actually standard; in the Heisenberg picture one writes

$$\mathbf{A}_t = e^{-\frac{1}{i\hbar}\mathbf{H}t}\mathbf{A}_0 e^{+\frac{1}{i\hbar}\mathbf{H}t}$$

to describe quantum motion, and makes use of the operator identity

$$\begin{aligned} &= \sum_{n=0}^{\infty} \tfrac{1}{n!}\big(\tfrac{1}{i\hbar}\big)^n \big\{\mathbf{A},\mathbf{H}^n\big\} t^n \\ &\equiv \sum_{n=0}^{\infty} \tfrac{1}{n!}\mathbf{A}_n t^n \end{aligned} \tag{28}$$

from which (27) can be recovered as an immediate corollary.

6. Reconstruction of the wave function from momental data.[14] While $\langle \mathbf{A}\rangle$ is a "moment" in the sense that it describes the expected mean (1^{st} moment) of a set of A-measurements, I propose henceforth to reserve for that term a more restrictive meaning. I propose to call the numbers $\langle \mathbf{x}^n\rangle$—which by standard usage are the moments of probability distribution $|\psi^*(x)\psi(x)|$—"moments of the wave function," though the wave function $\psi(x)$ is by nature a probability *amplitude*. In that extended sense, so also are the numbers $\langle \mathbf{p}^n\rangle$ "moments of the wave function." But so also are some other numbers. My assignment is to describe the least population of such numbers sufficient to the purpose at hand (reconstruction of the wave function), and then to show how they in fact achieve that objective. It proves convenient to consider those problems in reverse order, and to begin with review of some classical probability theory:

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[13] Note that while $\mathbf{A}_n = \mathbf{0}$ implies truncation, the $|\psi)$-dependent circumstance $\langle \mathbf{A}_n\rangle = 0$ does not; similarly, $\mathbf{A}_n = \lambda\mathbf{A}_0$ implies cyclicity but $\langle \mathbf{A}_n\rangle = \lambda\langle \mathbf{A}_n\rangle$ does not.

[14] Time is passive in the following discussion (all I have to say should be understood to hold *at each moment*), so allusions to t will be dropped from my notation.

Let $P(x,p)$ be some bivariate distribution function. The marginal moments $\langle x^m\rangle$ and $\langle p^n\rangle$ can be described in terms of the associated marginal distribution functions $f(x)\equiv\int P(x,p)\,dp$ and $g(p)\equiv\int P(x,p)\,dx$

$$\langle x^m\rangle = \int x^m f(x)\,dx \quad\text{and}\quad \langle p^n\rangle = \int p^n g(p)\,dp$$

If x and p are statistically independent random variables then $P(x,p)$ contains no information not already present in $f(x)$ and $g(p)$; indeed, one has

$$P(x,p) = f(x)g(p) \quad\text{giving}\quad \langle x^m p^n\rangle = \langle x^m\rangle\langle p^n\rangle \;:\; x \text{ and } p \text{ independent}$$

But that is a very special situation; the general expectation must be that x and p are statistically dependent. Then $P(x,p)$ contains information not present in $f(x)$ and $g(p)$, the mixed moments $\langle x^m p^n\rangle$ individually contain information not present within the set of marginal moments, and one must be content to write

$$\langle x^m p^n\rangle = \iint x^m p^n P(x,p)\,dxdp$$

That $f(x)$ can be reconstructed from the data $\{\langle x^m\rangle : m = 0,1,2,\ldots\}$, and $g(p)$ from the data $\{\langle p^n\rangle : n = 0,1,2,\ldots\}$, has in effect been remarked already in §1; form

$$F(\beta) \equiv \sum_{m=0}^{\infty} \tfrac{1}{m!}\langle x^m\ \rangle\big(\tfrac{i}{\hbar}\beta x\big)^m = \big\langle e^{\frac{i}{\hbar}\beta x}\big\rangle = \int e^{\frac{i}{\hbar}\beta x} f(x)\,dx$$

Then

$$f(x) = \tfrac{1}{h}\int e^{-\frac{i}{\hbar}\beta x} F(\beta)\,d\beta$$

and similarly

$$g(p) = \tfrac{1}{h}\int e^{-\frac{i}{\hbar}\alpha p} G(\alpha)\,d\alpha$$

where $G(\alpha) \equiv \big\langle e^{\frac{i}{\hbar}\alpha p}\big\rangle$. The question now arises: How (if at all) can one reconstruct $P(x,p)$ from the data $\{\langle x^m p^n\rangle\}$? The answer is: By straightforward extension of the procedure just described. Group the mixed moments according to their net order

$$\begin{array}{c} 1 \\ \langle x\rangle \quad \langle p\rangle \\ \langle x^2\rangle \quad \langle xp\rangle \quad \langle p^2\rangle \\ \langle x^3\rangle \quad \langle x^2p\rangle \quad \langle xp^2\rangle \quad \langle p^3\rangle \\ \vdots \end{array}$$

and form

$$\begin{aligned} Q(\alpha,\beta) &\equiv \sum_{k=0}^{\infty} \tfrac{1}{k!}\big(\tfrac{i}{\hbar}\big)^k \Big\{ \sum_{n=0}^{k} \tbinom{k}{n} \big\langle x^n p^{k-n}\big\rangle \beta^n \alpha^{k-n} \Big\} \\ &= \sum_{k=0}^{\infty} \tfrac{1}{k!}\big(\tfrac{i}{\hbar}\big)^k \big\langle (\alpha p + \beta x)^k \big\rangle = \big\langle e^{\frac{i}{\hbar}(\alpha p+\beta x)} \big\rangle \\ &= \iint e^{\frac{i}{\hbar}(\alpha p+\beta x)} P(x,p)\, dx dp \end{aligned}$$

Immediately

$$P(x,p) = \tfrac{1}{h^2} \iint e^{-\frac{i}{\hbar}(\alpha p+\beta x)} \underbrace{\big\langle e^{\frac{i}{\hbar}(\alpha p+\beta x)} \big\rangle}_{\text{moment data } \langle x^m p^n\rangle \text{ resides here}} dq dy \tag{29}$$

If x and p are statistically independent, then $\big\langle e^{\frac{i}{\hbar}(\alpha p+\beta x)}\big\rangle = \big\langle e^{\frac{i}{\hbar}\alpha p}\big\rangle\big\langle e^{\frac{i}{\hbar}\beta x}\big\rangle$ and we recover $P(x,p) = f(x)g(p)$.

My present objective is to construct the *quantum counterpart* of the preceding material, and for that purpose the so-called "phase space formulation of quantum mechanics" provides the natural tool. This lovely theory, though it has been available for nearly half a century,[15] remains—except to specialists in quantum optics[16] and a few other fields—much less well known than it deserves to be. I digress now, therefore, to review its relevant essentials:

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[15] Seeds of the theory were planted by Hermann Weyl (see Chapter IV, §14 in his *Gruppentheorie und Quantenmechanik* (2^{nd} edition, 1930)) and Eugene Wigner: "On the quantum correction for thermodynamic equilibrium," Phys. Rev. **40**, 749 (1932). Those separately motivated ideas were fused and systematically elaborated in a classic paper by J. E. Moyal (who worked in collaboration with the British statistician M. E. Bartlett): "Quantum mechanics as a statistical theory," Proc. Camb. Phil. Soc. **45**, 92 (1949). The foundations of the subject were further elaborated in the 1950's by T. Takabayasi ("The formulation of quantum mechanics in terms of ensembles in phase space," Prog. Theo. Phys. **11**, 341 (1954)), G. A. Baker Jr. ("Formulation of quantum mechanics in terms of the quasi-probability distribution induced on phase space," Phys. Rev. **109**, 2198 (1958)) and others. For a fairly detailed account of the theory and many additional references, see my QUANTUM MECHANICS (1967), Chapter 3, pp. 27–32 and pp. 99 *et seq.* or the Reed College thesis of Thomas Banks: "The phase space formulation of quantum mechanics" (1969).

[16] L. Mandel & E. Wolf, in *Optical coherence and quantum optics* (1995), make only passing reference (at p. 541) to the phase space formalism. But Mark Beck (see below) has supplied these references: Ulf Leonhardt, *Measuring the Quantum State of Light* (1997); M. Hillery, R. F. O'Connell, M. O. Scully and E. P. Wigner, "Distribution functions in physics: fundamentals," Phys. Rep. **106**, 121 (1984).

To the question "What is the self-adjoint operator A that should, for the purposes of quantum mechanical application, be associated with the classical observable $A(x,p)$?" a variety of answers have been proposed.[17] The rule of association (or correspondence procedure) advocated by Weyl can be described

$$\begin{aligned} A(x,p) &= \iint a(\alpha,\beta)e^{\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta \\ &\Big\downarrow \text{ WEYL TRANSFORMATION} \\ \mathsf{A} &= \iint a(\alpha,\beta)e^{\frac{i}{\hbar}(\alpha \mathsf{p}+\beta \mathsf{x})}\,d\alpha d\beta \end{aligned} \tag{30}$$

It was to the wonderful properties of the operators $\mathsf{E}(\alpha,\beta)\equiv e^{\frac{i}{\hbar}(\alpha\mathsf{p}+\beta\mathsf{x})}$ that Weyl sought to draw attention.[18] Those entail in particular that if

$$\mathsf{A}\xleftarrow[\text{Weyl}]{} A(x,p) \qquad\text{and}\qquad \mathsf{B}\xleftarrow[\text{Weyl}]{} B(x,p)$$

then

$$\text{trace}\,\mathsf{AB} = \tfrac{1}{h}\iint A(x,p)B(x,p)\,dxdp \tag{31}$$

and permit this description of the *inverse* Weyl transformation:

$$\mathsf{A}\xrightarrow[\text{Weyl}]{} A(x,p) = \iint \Big\{\tfrac{1}{h}\text{trace}\,\mathsf{AE}^{+}(\alpha,\beta)\Big\}e^{\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta \tag{32}$$

Those facts acquire their relevance from the following observations: familiarly, $\langle\mathsf{A}\rangle = (\psi|\mathsf{A}|\psi)$ can be written

$$\langle\mathsf{A}\rangle = \text{trace}\,\mathsf{A}\boldsymbol{\rho}$$
$$\boldsymbol{\rho}\equiv|\psi)(\psi| \text{ is the } \textit{density matrix} \text{ associated with the state } |\psi)$$

Writing

$$\mathsf{A}\xrightarrow[\text{Weyl}]{} A(x,p) \qquad\text{and}\qquad \boldsymbol{\rho}\xrightarrow[\text{Weyl}]{} h\cdot P_\psi(x,p)$$

one therefore has

$$\langle\mathsf{A}\rangle = \iint A(x,p)P_\psi(x,p)\,dxdp \tag{33}$$

[17] See J. R. Shewell, "On the formation of quantum mechanical operators," AJP **27**, 16 (1959).

[18] Among those many wonderful properties are the *trace-wise orthonormality* property

$$\text{trace}\,\mathsf{E}(\alpha,\beta)\mathsf{E}^{+}(\bar\alpha,\bar\beta) = h\delta(\alpha-\bar\alpha)\delta(\beta-\bar\beta)$$

from which it follows in particular that

$$\text{trace}\,\mathsf{E}(\alpha,\beta) = h\delta(\alpha)\delta(\beta)$$

where by application of (32) we have

$$P_\psi(x,p) = \tfrac{1}{h^2}\iint (\psi|e^{-\frac{i}{\hbar}(\alpha\mathsf{p}+\beta\mathsf{x})}|\psi)e^{\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta \tag{34}$$

which can by fairly quick calculation be brought to the form

$$P_\psi(x,p) = \tfrac{2}{h}\int \psi^*(x+\xi)\,e^{2\frac{i}{\hbar}p\xi}\,\psi(x-\xi)\,d\xi \tag{35}$$

At (35) we have recovered the famous "Wigner distribution function," which Wigner in 1932 was content simply to pluck from his hat.[19] The function $P_\psi(x,p)$—which in the phrase space formalism serves to describe the "state" of the quantum system, but is invariable real-valued—possesses many of the properties one associates with the term "distribution function;" one finds, for example, that

$$\iint P_\psi(x,p)\,dxdp = 1$$

$$\int P_\psi(x,p)\,dp = |\psi(x)|^2 \quad\text{and}\quad \int P_\psi(x,p)\,dx = |\varphi(p)|^2$$

where $\varphi(p) \equiv (p|\psi)$ is the Fourier transform of $\psi(x) \equiv (x|\psi)$. And even more to the point: the Wigner distribution enters at (33) into an equation which is formally identical to the equation used to define the expectation value $\langle A(x,p)\rangle$ in *classical* (statistical) mechanics. But $P_\psi(x,p)$ possess also some "weird" properties—properties which serve to encapsulate important respects in which quantum statistics is non-standard, quantum mechanics non-classical

$P_\psi(x,p)$ is not precluded from assuming *negative values*
$P_\psi(x,p)$ is *bounded*: $|P_\psi(x,p)| \leq 2/h$
$P_\psi(x,p) = |\psi(x)|^2\cdot|\varphi(p)|^2$ is *impossible*

and for those reasons (particularly the former) is called a "quasi-distribution" by some fastidious authors.

From the marginal moments $\{\langle\mathsf{x}^n\rangle : n = 0,1,2,\ldots\}$ it is possible (by the classical technique already described) to reconstruct $|\psi(x)|^2$ *but not the wave function* $\psi(x)$ *itself*, for the data set contains no *phase* information. A similar remark pertains to the reconstruction of $\varphi(p)$ from $\{\langle\mathsf{p}^m\rangle : m = 0,1,2,\ldots\}$. But $\psi(x)$ and its "Wigner transform" $P_\psi(x,p)$ are equivalent objects in the sense that they contain identical stores of information; from $P_\psi(x,p)$ it *is* possible to recover $\psi(x)$, by a technique which I learned from Mark Beck[20] and will

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[19] Or perhaps from the hat of Leo Szilard; in a footnote Wigner reports that "This expression was found by L. Szilard and the present author some years ago for another purpose," but cites no reference.

[20] Private communication. Mark does not claim to have himself invented the trick in question, but it was, so far as I am aware, unknown to the founding fathers of this field.

describe in a moment. The importance (for us) of this fact lies in the following observation:

> Momental data sufficient to determine $P_\psi(x,p)$ is sufficient also to determine $\psi(x)$, to with an unphysical over-all phase factor.

The construction of $\psi(x) \xleftarrow[\text{Wigner}]{} P_\psi(x,p)$ (Beck's trick) proceeds as follows: By Fourier transformation of (35) obtain

$$\begin{aligned}\int P_\psi(x,p)e^{-2\frac{i}{\hbar}p\hat{\xi}}\,dp &= \int \psi^*(x+\xi)\,\delta(\xi-\hat{\xi})\psi(x-\xi)\,d\xi\\ &= \psi^*(x+\hat{\xi})\,\psi(x-\hat{\xi})\end{aligned}$$

Select a point a at which $\int P_\psi(a,p)\,dp = \psi^*(a)\,\psi(a) \neq 0$.[21] Set $\hat{\xi} = a - x$ to obtain

$$\int P_\psi(x,p)e^{-2\frac{i}{\hbar}p(a-x)}\,dp = \psi^*(a)\,\psi(2x-a)$$

and by notational adjustment $2x - a \mapsto x$ obtain

$$\begin{aligned}\psi(x) &= [\psi^*(a)]^{-1}\cdot\int P_\psi(\tfrac{x+a}{2},p)\,e^{\frac{i}{\hbar}p(x-a)}\,dp \qquad (36)\\ &\downarrow\\ &= [\psi^*(0)]^{-1}\cdot\int P_\psi(\tfrac{x}{2},p)\,e^{\frac{i}{\hbar}px}\,dp \quad\text{in the special case } a=0\end{aligned}$$

where the prefactor is, in effect, a normalization constant, fixed to within an arbitrary phase factor.

Returning to the question which originally motivated this discussion—What least set of momental data is sufficient to determine the state of the quantum system?—we are in position now to recognize that an answer was implicit already in (34), which (taking advantage of the reality of the Wigner distribution, and in order to regain contact with notations used by Moyal) I find it convenient at this point to reexpress

$$P_\psi(x,p) = \tfrac{1}{h^2}\iint M_\psi(\alpha,\beta)e^{-\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta \qquad (38)$$

$$M_\psi(\alpha,\beta) \equiv (\psi|e^{\frac{i}{\hbar}(\alpha\mathsf{p}+\beta\mathsf{x})}|\psi) = (\psi|\mathsf{E}(\alpha,\beta)|\psi) \qquad (39)$$

Evidently

$$\mathsf{E}(\alpha,\beta) = \sum_{k=0}^{\infty}\tfrac{1}{k!}\big(\tfrac{i}{\hbar}\big)^k\Big\{\sum_{n=0}^{k}\mathsf{M}_{k-n,n}\alpha^{k-n}\beta^n\Big\} \qquad (40)$$

$$\begin{aligned}\mathsf{M}_{m,n} &\equiv \sum_{\text{all orderings}} m\ \mathsf{p}\text{-factors and } n\ \mathsf{x}\text{-factors} \qquad (41)\\ &= \text{sum of } \tbinom{m+n}{n} \text{ terms altogether}\end{aligned}$$

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[21] Such a point is, by $\int \psi^*(x)\,\psi(x)\,dx = 1$, certain to exist. It is often most convenient (but not always possible) to—with Beck—set $a = 0$.

so it is the momental set $\{\langle \mathsf{M}_{n,m}\rangle\}$ that provides the answer to our question.

Looking now in more detail to the primitive operators $\mathsf{M}_{m,n}$, the operators of low order can be written

$$\begin{aligned}
\mathsf{M}_{0,0} &= \mathbf{1}\\[4pt]
\mathsf{M}_{1,0} &= \mathsf{p}\\
\mathsf{M}_{0,1} &= \mathsf{x}\\[4pt]
\mathsf{M}_{2,0} &= \mathsf{pp}\\
\mathsf{M}_{1,1} &= \mathsf{px}+\mathsf{xp}\\
\mathsf{M}_{0,2} &= \mathsf{xx}\\[4pt]
\mathsf{M}_{3,0} &= \mathsf{ppp}\\
\mathsf{M}_{2,1} &= \mathsf{ppx}+\mathsf{pxp}+\mathsf{xpp}\\
\mathsf{M}_{1,2} &= \mathsf{pxx}+\mathsf{xpx}+\mathsf{xxp}\\
\mathsf{M}_{0,3} &= \mathsf{xxx}\\
&\ \vdots
\end{aligned}$$

It is hardly surprising—yet not entirely obvious—that

$$\frac{1}{\text{number of terms}}\mathsf{M}_{m,n} \xleftarrow[\text{Weyl}]{} p^m x^n \tag{42}$$

I say "not entirely obvious" because by original definition $\mathsf{A} \xleftarrow[\text{Weyl}]{} A(x,p)$ assumes $A(x,p)$ to be Fourier transformable, which polynomials are not.[22] I digress now to indicate how by natural extension the Weyl transform acquires its surprising robustness and utility.

Any operator presented in the form

$$\mathsf{A} = \text{sum of powers of } \mathsf{x} \text{ and } \mathsf{p} \text{ operators}$$

can, by virtue of the fundamental commutation relation, be written in many ways. In particular, any A can, by repeated use of $\mathsf{xp} = \mathsf{px} + i\hbar\mathbf{1}$, be brought to "$\mathsf{px}$-ordered form" (else "$\mathsf{xp}$-ordered form") in which all p-operators stand left of all x-operators (else the reverse). I find it convenient to write (idiosyncratically)

$$\left.\begin{aligned}
{}_{\mathsf{x}}\big[F(x,p)\big]_{\mathsf{p}} &\equiv \text{result of } \mathsf{xp}\text{-ordered substitution into } F(x,p)\\
{}_{\mathsf{p}}\big[F(x,p)\big]_{\mathsf{x}} &\equiv \text{result of } \mathsf{px}\text{-ordered substitution into } F(x,p)
\end{aligned}\right\} \tag{43}$$

[22] On the other hand, that definition —(30)—is built upon an assertion

$$e^{\frac{i}{\hbar}(\alpha\,\mathsf{p}+\beta\mathsf{x})} \xleftarrow[\text{Weyl}]{} e^{\frac{i}{\hbar}(\alpha p+\beta x)}$$

from which (42) appears to follow as an immediate implication.

and, inversely, to let $F_{xp}(x,p)$ denote the function which yields F *by* xp*-ordered substitution*:

$$\begin{aligned}\mathsf{F} &= {}_{\mathsf{x}}\big[F_{xp}(x,p)\big]_{\mathsf{p}} && (44)\\ &= {}_{\mathsf{p}}\big[F_{px}(x,p)\big]_{\mathsf{x}} \quad : \quad \text{reverse-ordered companion of the above}\end{aligned}$$

For example, if

$$\mathsf{F} \equiv \mathsf{xpx} = \mathsf{x}^2\mathsf{p} - i\hbar\mathsf{x} = \mathsf{px}^2 + i\hbar\mathsf{x}$$

then

$$F_{xp}(x,p) = x^2p - i\hbar x \quad \text{but} \quad F_{px}(x,p) = x^2p + i\hbar x$$

Some sense of (at least one source of) the frequently great computational utility of "ordered display" can be gained from the observation that

$$\begin{aligned}(x|\mathsf{F}|y) &= \int (x|\mathsf{F}|p)dp(p|y) \quad : \quad \text{MIXED REPRESENTATION TRICK}\\ &= \tfrac{1}{\sqrt{h}}\int F_{xp}(x,p)e^{-\frac{i}{\hbar}py}\,dp \qquad (45)\\ &= \int (x|p)dp(p|\mathsf{F}|y)\\ &= \tfrac{1}{\sqrt{h}}\int e^{+\frac{i}{\hbar}xp}F_{px}(y,p)\,dp\end{aligned}$$

One of the principal recommendations of Weyl's procedure is that it lends itself so efficiently to the analysis of operator ordering/re-ordering problems; if A and B *commute with their commutator* (as, in particular, x and p do) then[23]

$$e^{\mathsf{A}+\mathsf{B}} = e^{+\frac{1}{2}[\mathsf{A},\mathsf{B}]}\cdot e^{\mathsf{B}}e^{\mathsf{A}} = e^{-\frac{1}{2}[\mathsf{A},\mathsf{B}]}\cdot e^{\mathsf{A}}e^{\mathsf{B}}$$

which entail

$$e^{\frac{i}{\hbar}(\alpha\mathsf{p}+\beta\mathsf{x})} = \begin{cases} e^{+\frac{1}{2}\frac{i}{\hbar}\alpha\beta}\cdot e^{\frac{i}{\hbar}\beta\mathsf{x}}e^{\frac{i}{\hbar}\alpha\mathsf{p}} & : \quad \mathsf{xp}\text{-ordered display}\\ e^{-\frac{1}{2}\frac{i}{\hbar}\alpha\beta}\cdot e^{\frac{i}{\hbar}\alpha\mathsf{p}}e^{\frac{i}{\hbar}\beta\mathsf{x}} & : \quad \mathsf{px}\text{-ordered display}\end{cases} \qquad (46)$$

Returning with this information to (30) we have

---

[23] The following are among the most widely known of the identities which issue from "Campbell-Baker-Hausdorff theory," which originates in the pre-quantum mechanical mathematical work of J. E. Campbell (1898), H. F. Baker (1902) and F. Hausdorff (1903), but attracted wide interest only after the invention of quantum mechanics. For a good review and references to the classical literature, see R. M. Wilcox, "Exponential operators and parameter differentiation in quantum mechanics," J. Math. Phys. **8**, 962 (1967). Or "An operator ordering technique with quantum mechanical applications" (1966) in my COLLECTED SEMINARS.

$$
\begin{aligned}
A(x,p) &= \iint a(\alpha,\beta)e^{\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta \\
&\Big\updownarrow \text{Weyl} \\
\mathbf{A} &= \iint a(\alpha,\beta)e^{\frac{i}{\hbar}(\alpha\mathbf{p}+\beta\mathbf{x})}\,d\alpha d\beta \\
&= \iint a(\alpha,\beta)e^{+\frac{1}{2}\frac{i}{\hbar}\alpha\beta}\cdot e^{\frac{i}{\hbar}\beta\mathbf{x}}e^{\frac{i}{\hbar}\alpha\mathbf{p}}\,d\alpha d\beta \\
&= {}_{\mathbf{x}}\Big[\exp\big\{\tfrac{1}{2}\tfrac{\hbar}{i}\tfrac{\partial^2}{\partial x\partial p}\big\}A(x,p)\Big]_{\mathbf{p}}
\end{aligned}
$$

from which we learn that

$$
\left.
\begin{aligned}
A_{xp}(x,p) &= \exp\big\{+\tfrac{1}{2}\tfrac{\hbar}{i}\tfrac{\partial^2}{\partial x\partial p}\big\}A(x,p) \\
A_{px}(x,p) &= \exp\big\{-\tfrac{1}{2}\tfrac{\hbar}{i}\tfrac{\partial^2}{\partial x\partial p}\big\}A(x,p)
\end{aligned}
\right\}
\tag{47}
$$

Suppose (which is to revisit a previous example) we were to take $A(x,p) = px^2$; then (47) asserts

$$
\begin{aligned}
A(x,p) \equiv px^2 \xrightarrow[\text{Weyl}]{} \mathbf{A} &= \mathbf{x}^2\mathbf{p} - i\hbar\mathbf{x} \\
&= \mathbf{p}^2\mathbf{x} + i\hbar\mathbf{x}
\end{aligned}
$$

while by explicit calculation we find

$$
\begin{aligned}
&= \mathbf{x}\mathbf{p}\mathbf{x} \\
&= \tfrac{1}{3}(\mathbf{p}\mathbf{x}\mathbf{x} + \mathbf{x}\mathbf{p}\mathbf{x} + \mathbf{x}\mathbf{x}\mathbf{p}) \equiv \tfrac{1}{3}\mathbf{M}_{1,2}
\end{aligned}
$$

Here we have brought patterned order and efficiency to a calculation which formerly lacked those qualities, and have at the same time shown how the Weyl correspondence comes to be applicable to polynomial expressions.

7. A shift of emphasis—from moments to their generating function. We began with an interest—Ehrenfest's interest—in (the quantum dynamical motion of) only a pair of moments ($\langle\mathbf{x}\rangle$ and $\langle\mathbf{p}\rangle$), but in consequence of the structure of (2) found that a collateral interest in *mixed moments of all orders* was thrust upon us. Here I explore implications of some commonplace wisdom:

> *When one has interest in properties of an infinite set of objects, it is often simplest and most illuminating to look not to the objects individually but to their* generating function.

I look now, therefore, in closer detail to properties of a function which we have already encountered—to what I call the "Moyal function"

$$
\begin{aligned}
M_\psi(\alpha,\beta) \equiv (\psi|e^{\frac{i}{\hbar}(\alpha\mathbf{p}+\beta\mathbf{x})}|\psi) &= (\psi|\mathbf{E}(\alpha,\beta)|\psi) \\
&= \langle\mathbf{E}(\alpha,\beta)\rangle \text{ with } \mathbf{E}(\alpha,\beta) \text{ unitary}
\end{aligned}
\tag{48}
$$

which was seen at (38) to be precisely the *Fourier transform of the Wigner distribution*, and therefore to be (by performance of Beck's trick) a repository of all the information borne by $|\psi)$.

To describe the motion of all mixed moments at once we examine the time derivative of $M_\psi(\alpha,\beta)$, which by (1) can be described

$$\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) = \tfrac{1}{i\hbar}\langle[\mathsf{E}(\alpha,\beta),\mathsf{H}]\rangle \tag{49}$$

Proceeding on the assumption that

$$\mathsf{H} \underset{\text{Weyl}}{\longleftarrow} H(x,p) = \iint h(\tilde\alpha,\tilde\beta)e^{\frac{i}{\hbar}(\tilde\alpha p+\tilde\beta x)}\,d\tilde\alpha d\tilde\beta$$

we have

$$\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) = \tfrac{1}{i\hbar}\iint h(\tilde\alpha,\tilde\beta)\langle[\mathsf{E}(\alpha,\beta),\mathsf{E}(\tilde\alpha,\tilde\beta)]\rangle\,d\tilde\alpha d\tilde\beta$$

But it is[24] an implication of (46) that

$$\begin{aligned}[\mathsf{E}(\alpha,\beta),\mathsf{E}(\tilde\alpha,\tilde\beta)] &= \underbrace{(e^{\vartheta}-e^{-\vartheta})}\cdot\mathsf{E}(\alpha+\tilde\alpha,\beta+\tilde\beta) \\ &\qquad = 2i\sin\vartheta \;\;:\;\; \vartheta\equiv\tfrac{1}{2\hbar}(\alpha\tilde\beta-\beta\tilde\alpha)\end{aligned} \tag{50}$$

so we can write

$$\begin{aligned}\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) &= \tfrac{2}{\hbar}\iint h(\tilde\alpha,\tilde\beta)\sin\big(\tfrac{\alpha\tilde\beta-\beta\tilde\alpha}{2\hbar}\big)\cdot M_\psi(\alpha+\tilde\alpha,\beta+\tilde\beta)\,d\bar\alpha d\bar\beta \\ &= \tfrac{2}{\hbar}\iint h(\tilde\alpha-\alpha,\tilde\beta-\beta)\sin\big(\tfrac{\alpha\tilde\beta-\beta\tilde\alpha}{2\hbar}\big)\cdot M_\psi(\tilde\alpha,\tilde\beta)\,d\tilde\alpha d\tilde\beta \\ &= \iint \mathfrak{T}(\alpha,\beta;\tilde\alpha,\tilde\beta)\cdot M_\psi(\tilde\alpha,\tilde\beta)\,d\tilde\alpha d\tilde\beta \end{aligned} \tag{51.1}$$

$$\mathfrak{T}(\alpha,\beta;\tilde\alpha,\tilde\beta) \equiv \tfrac{2}{\hbar}h(\tilde\alpha-\alpha,\tilde\beta-\beta)\sin\big(\tfrac{\alpha\tilde\beta-\beta\tilde\alpha}{2\hbar}\big) \tag{51.2}$$

Equation (51.1)—which formally resembles (and is ultimately equivalent to) this formulation of Schrödinger equation

$$\tfrac{\partial}{\partial t}(x|\psi) = \int (x|\mathsf{H}|\tilde x)d\tilde x(\tilde x|\psi)$$

—is, in effect, a giant system of coupled first-order differential equations in the mixed moments of all orders; it asserts that the time derivatives of those moments are linear combinations of their instantaneous values, and that it is the responsibility of the Hamiltonian to answer the question "*What* linear combinations?" and thus to distinguish one dynamical system from another.

[24] See Chapter 3, p. 112 of QUANTUM MECHANICS (1967) for the detailed argument.

By Fourier transformation one at length[24] recovers

$$\begin{aligned}\tfrac{\partial}{\partial t}P_\psi(x,p) &= \tfrac{2}{\hbar}\sin\Big\{\tfrac{\hbar}{2}\big[\big(\tfrac{\partial}{\partial x}\big)_H\big(\tfrac{\partial}{\partial p}\big)_P - \big(\tfrac{\partial}{\partial x}\big)_P\big(\tfrac{\partial}{\partial p}\big)_H\big]\Big\}H(x,p)P_\psi(x,p) \qquad (52)\\ &= \underbrace{\big\{\tfrac{\partial H}{\partial x}\tfrac{\partial}{\partial p} - \tfrac{\partial H}{\partial p}\tfrac{\partial}{\partial x}\big\}P_\psi(x,p)}_{\text{Poisson bracket }[H,P_\psi]} + \text{“quantum corrections” of order } O(\hbar^2)\end{aligned}$$

which is the "phase space formulation of Schrödinger's equation" in its most frequently encountered form.

Equation (52) makes latent good sense in all cases $H(x,p)$, and explicit good sense in simple cases; for example: in the "photonic case" $H = cp$ (see again §3) one obtains

$$\tfrac{\partial}{\partial t}P_\psi(x,p) = -c\tfrac{\partial}{\partial x}P_\psi(x,p) \tag{53.1}$$

while for an oscillator $H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2x^2$ we find

$$\begin{aligned}\tfrac{\partial}{\partial t}P_\psi(x,p) &= \big\{m\omega^2x\tfrac{\partial}{\partial p} - \tfrac{1}{m}p\tfrac{\partial}{\partial x}\big\}P_\psi(x,p) &(53.2)\\ &\downarrow\\ &= -\tfrac{1}{m}p\tfrac{\partial}{\partial x}P_\psi(x,p) \quad \text{in the “free particle limit” } \omega\downarrow 0 &(53.3)\end{aligned}$$

I postpone discussion of the *solutions* of those equations (but draw immediate attention to the fact that each of those cases is so quadratically simple that *"quantum corrections" are entirely absent*)...in order to draw attention to my immediate point, which is that *in each of those cases (51) is meaningless*, for the simple reason that none of those Hamiltonians is Fourier transformable; in each case $h(\alpha,\beta)$ fails to exist. In a first effort to work around this problem, let us back up to (49) and consider again the case $H = cp$: then

$$\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) = c\tfrac{1}{i\hbar}\langle[\mathsf{E}(\alpha,\beta),\mathsf{p}]\rangle \tag{54}$$

It is an implication of (50) that

$$\begin{aligned}[\mathsf{E}(\alpha,\beta), e^{\frac{i}{\hbar}\bar\alpha\mathsf{p}}] &= \sum_{k=0}^\infty \tfrac{1}{k!}\big(\tfrac{i}{\hbar}\bar\alpha\big)^k[\mathsf{E}(\alpha,\beta),\mathsf{p}^k] = \mathbf{0} + \bar\alpha\cdot\tfrac{i}{\hbar}[\mathsf{E}(\alpha,\beta),\mathsf{p}] + \cdots\\ &= 2i\sin\big\{\tfrac{-\beta\bar\alpha}{2\hbar}\big\}\mathsf{E}(\alpha+\bar\alpha,\beta) = \bar\alpha\cdot\big(-\tfrac{i}{\hbar}\beta\big)\mathsf{E}(\alpha,\beta) + \cdots\end{aligned}$$

from which we infer

$$[\mathsf{E}(\alpha,\beta),\mathsf{p}] = -\beta\,\mathsf{E}(\alpha,\beta) \tag{55}$$

Returning with this information to (54) we have

$$\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) = -\tfrac{1}{i\hbar}c\beta M_\psi(\alpha,\beta) \tag{56}$$

which can be cast in the form (51.1) with $\mathfrak{T}(\alpha,\beta;\tilde\alpha,\tilde\beta) = -\frac{1}{i\hbar}c\delta(\tilde\alpha-\alpha)\delta(\tilde\beta-\beta)\tilde\beta$. The implication appears to be that we should in general expect $\mathfrak{T}(\alpha,\beta;\tilde\alpha,\tilde\beta)$ to have the character not of a function but of a *distribution*.

It is in preparation for discussion of less trivial cases (free particle and oscillator) that I digress now to explore some consequences of the identity (55),[25] which can be written

$$\mathbf{E}(\alpha,\beta)\,\mathbf{p} = (\mathbf{p}-\beta\mathbf{1})\mathbf{E}(\alpha,\beta)$$

or again as the "shift rule" (most familiar in the case $\alpha = 0$)

$$\mathbf{E}(\alpha,\beta)\,\mathbf{p}\,\mathbf{E}^{-1}(\alpha,\beta) = (\mathbf{p}-\beta\mathbf{1})$$

Immediately

$$\mathbf{E}(\alpha,\beta)\,\mathbf{p}^m\,\mathbf{E}^{-1}(\alpha,\beta) = (\mathbf{p}-\beta\mathbf{1})^m$$

or again

$$[\mathbf{E}(\alpha,\beta),\mathbf{p}^m] = \{(\mathbf{p}-\beta\mathbf{1})^m - \mathbf{p}^m\}\,\mathbf{E}(\alpha,\beta)$$

which—because {etc.} introduces "dangling $\mathbf{p}$-operators" except in the cases $m = 0$ and $m = 1$—does, as it stands, not quite serve our purposes. It is, however, an implication of (46) that

$$\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\alpha}\big)^m\,\mathbf{E}(\alpha,\beta) = (\mathbf{p}-\tfrac{1}{2}\beta\mathbf{1})^m\,\mathbf{E}(\alpha,\beta)$$

and therefore that

$$\begin{aligned}\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\alpha}-\tfrac{1}{2}\beta\big)^m\,\mathbf{E}(\alpha,\beta) &= (\mathbf{p}-\beta\mathbf{1})^m\,\mathbf{E}(\alpha,\beta)\\ \big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\alpha}+\tfrac{1}{2}\beta\big)^m\,\mathbf{E}(\alpha,\beta) &= \mathbf{p}^m\,\mathbf{E}(\alpha,\beta)\end{aligned}$$

So we obtain

$$[\mathbf{E}(\alpha,\beta),\mathbf{p}^m] = \Big\{\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\alpha}-\tfrac{1}{2}\beta\big)^m - \big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\alpha}+\tfrac{1}{2}\beta\big)^m\Big\}\,\mathbf{E}(\alpha,\beta) \tag{57.1}$$

$$= \begin{cases} \mathbf{0} & : \quad m=0 \\ -\beta\,\mathbf{E}(\alpha,\beta) & : \quad m=1 \\ -2\frac{\hbar}{i}\beta\frac{\partial}{\partial\alpha}\mathbf{E}(\alpha,\beta) & : \quad m=2 \\ & \;\vdots \end{cases}$$

and, by similar argument,[26]

$$[\mathbf{E}(\alpha,\beta),\mathbf{x}^n] = \Big\{\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\beta}+\tfrac{1}{2}\alpha\big)^n - \big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\beta}-\tfrac{1}{2}\alpha\big)^n\Big\}\,\mathbf{E}(\alpha,\beta) \tag{57.2}$$

---

[25] We want—minimally—to be in position to say useful things about the commutators $[\mathbf{E}(\alpha,\beta),\mathbf{p}^2]$ and $[\mathbf{E}(\alpha,\beta),\mathbf{x}^2]$.

[26] It is simpler to make substitions $\mathbf{p}\mapsto+\mathbf{x}$, $\mathbf{x}\mapsto-\mathbf{p}$, $\alpha\mapsto+\beta$, $\beta\mapsto-\alpha$ (which by design preserve both $[\mathbf{x},\mathbf{p}]$ and the definition of $\mathbf{E}(\alpha,\beta)$) into the results already in hand.

Returning with this information to the case of an oscillator, we have

$$
\begin{aligned}
\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) &= \tfrac{1}{i\hbar}\big\langle \tfrac{1}{2m}\big[\mathbf{E}(\alpha,\beta),\mathbf{p}^2\big] + \tfrac{1}{2}m\omega^2\big[\mathbf{E}(\alpha,\beta),\mathbf{x}^2\big]\big\rangle \\
&= \tfrac{1}{i\hbar}\big\langle\big\{\tfrac{1}{2m}\big(-2\tfrac{\hbar}{i}\beta\tfrac{\partial}{\partial\alpha}\big) + \tfrac{1}{2}m\omega^2\big(+2\tfrac{\hbar}{i}\alpha\tfrac{\partial}{\partial\beta}\big)\big\}\mathbf{E}(\alpha,\beta)\big\rangle \\
&= \big\{\tfrac{1}{m}\beta\tfrac{\partial}{\partial\alpha} - m\omega^2\alpha\tfrac{\partial}{\partial\beta}\big\}M_\psi(\alpha,\beta) \qquad (58.1)\\
&\downarrow \\
&= \tfrac{1}{m}\beta\tfrac{\partial}{\partial\alpha}M_\psi(\alpha,\beta) \quad \text{in the “free particle limit”} \qquad (58.2)
\end{aligned}
$$

Equations (56) and (58) are as simple as—and bear a striking resemblance to—their Wignerian counterparts (53). But to render (58.2)—say—into the form (51) we would have to set $\mathcal{T}(\alpha,\beta;\tilde\alpha,\tilde\beta) = -\frac{1}{m}\delta'(\tilde\alpha-\alpha)\delta(\tilde\beta-\beta)\tilde\beta$, in conformity with our earlier conclusion concerning the generally distribution-like character of the kernel $\mathcal{T}(\alpha,\beta;\tilde\alpha,\tilde\beta)$. The absence of $\hbar$-factors on the right sides of (58) is consonant with the absence of "quantum corrections" on the right sides of (53), but makes a little surprising the (dimensionally enforced) $1/i\hbar$ that appears on the right side of (56). One could but I won't... undertake now to describe the analogs of (58) which arise from $H(x,p) = \frac{1}{2m}p^2 + V(x)$ and from Hamiltonians of still more general structure. Instead, I take this opportunity to underscore what has been *accomlished* at (58.1). By explicit expansion of the expression on the left we have

$$
\begin{aligned}
\tfrac{\partial}{\partial t}M_\psi(\alpha,\beta) = \tfrac{\partial}{\partial t}\Big\{&\langle\mathbf{1}\rangle + \tfrac{i}{\hbar}\big[\alpha\langle\mathbf{p}\rangle + \beta\langle\mathbf{x}\rangle\big] \\
&+ \tfrac{1}{2}\big(\tfrac{i}{\hbar}\big)^2\big[\alpha^2\langle\mathbf{p}^2\rangle + \alpha\beta\langle\mathbf{p}\mathbf{x}+\mathbf{x}\mathbf{p}\rangle + \beta^2\langle\mathbf{x}^2\rangle\big] + \cdots\Big\}
\end{aligned}
$$

while expansion of the expression on the right gives

$$
\begin{aligned}
&\big\{\tfrac{1}{m}\beta\tfrac{\partial}{\partial\alpha} - m\omega^2\alpha\tfrac{\partial}{\partial\beta}\big\}M_\psi(\alpha,\beta) \\
&\quad= \tfrac{i}{\hbar}\big[\tfrac{1}{m}\beta\langle\mathbf{p}\rangle - m\omega^2\alpha\langle\mathbf{x}\rangle\big] \\
&\qquad+ \tfrac{1}{2}\big(\tfrac{i}{\hbar}\big)^2\big[\tfrac{1}{m}2\alpha\beta\langle\mathbf{p}^2\rangle + \big(\tfrac{1}{m}\beta^2 - m\omega^2\alpha^2\big)\langle\mathbf{p}\mathbf{x}+\mathbf{x}\mathbf{p}\rangle - m\omega^2 2\alpha\beta\langle\mathbf{x}^2\rangle\big] + \cdots
\end{aligned}
$$

Term-by-term identification gives rise to a system of equations:

$$
\begin{aligned}
\alpha^1 &: \quad \tfrac{d}{dt}\langle\mathbf{p}\rangle = -m\omega^2\langle\mathbf{x}\rangle \\
\beta^1 &: \quad \tfrac{d}{dt}\langle\mathbf{x}\rangle = \tfrac{1}{m}\langle\mathbf{p}\rangle \\
\alpha^2 &: \quad \tfrac{d}{dt}\langle\mathbf{p}^2\rangle = -m\omega^2\langle\mathbf{x}\mathbf{p}+\mathbf{p}\mathbf{x}\rangle \\
\alpha\beta &: \quad \tfrac{d}{dt}\langle\mathbf{x}\mathbf{p}+\mathbf{p}\mathbf{x}\rangle = \tfrac{2}{m}\langle\mathbf{p}^2\rangle - 2m\omega^2\langle\mathbf{x}^2\rangle \\
\beta^2 &: \quad \tfrac{d}{dt}\langle\mathbf{x}^2\rangle = \tfrac{1}{m}\langle\mathbf{x}\mathbf{p}+\mathbf{p}\mathbf{x}\rangle \\
&\ \ \vdots
\end{aligned}
$$

which in the "free particle limit" become

$$
\begin{aligned}
\alpha^1 \quad &: \quad \tfrac{d}{dt}\langle \mathbf{p}\rangle = 0\\
\beta^1 \quad &: \quad \tfrac{d}{dt}\langle \mathbf{x}\rangle = \tfrac{1}{m}\langle \mathbf{p}\rangle\\
\alpha^2 \quad &: \quad \tfrac{d}{dt}\langle \mathbf{p}^2\rangle = 0\\
\alpha\beta \quad &: \quad \tfrac{d}{dt}\langle \mathbf{x}\mathbf{p}+\mathbf{p}\mathbf{x}\rangle = \tfrac{2}{m}\langle \mathbf{p}^2\rangle\\
\beta^2 \quad &: \quad \tfrac{d}{dt}\langle \mathbf{x}^2\rangle = \tfrac{1}{m}\langle \mathbf{x}\mathbf{p}+\mathbf{p}\mathbf{x}\rangle\\
&\ \vdots
\end{aligned}
$$

These are precisely the results achieved in §2 by other means. It seems, on the basis of such computation, fair to assert that *equations of type (58) provide a succinct expression of Ehrenfest's theorem in its most general form.*[27]

Let us agree, in the absence of any standard terminology, to call (52) the "Wigner equation," and its Fourier transform—the generalizations of (56)/(58)—the "Moyal equation." Evidently solution of Moyal's equation—a single partial differential equation—is equivalent to (though poses a very different mathematical problem from) the solution of the coupled systems of ordinary differential "moment equation" of the sort anticipated in §4 and encountered just above.[28] In the next section I look to the. . .

8. Solution of Moyal's equation in some representative cases. Look first to the "photonic system" $H(x,p) = cp$. Solutions of the Wigner equation (53.1) can be described

$$
\begin{aligned}
P_\psi(x,p;t) &= \exp\big\{-ct\tfrac{\partial}{\partial x}\big\}P_\psi(x,p;0)\\
&= P_\psi(x-ct,p;0)
\end{aligned}
\tag{59.1}
$$

while the associated Moyal equation (56) promptly yields

$$
M_\psi(\alpha,\beta;t) = e^{\frac{i}{\hbar}c\beta t}\cdot M_\psi(\alpha,\beta;0) \tag{59.2}
$$

[27] It should in this connection be observed that the equations to which we have been led, though rooted in formalism based upon the Weyl correspondence, have in the end a stand-alone validity, and are therefore released from the criticism that there exist plausible alternatives to Weyl's rule (see again the paper by J. L. Shewell to which I made reference in footnote 17), and that its adoption is in some sense an arbitrary act. A similar remark pertains to other essential features of the phase space formalism.

[28] One is reminded in this connection of the partial differential *wave equation* that arises by a "refinement procedure" from the system of ordinary differential equations that describe the motion of a discrete lattice. And it becomes in this light natural to ask: "Does Moyal's equation admit of representation as the field equation implicit in some Lagrange density? Does it provide, on other words, an instance of a Lagrangian field theory?"

These simple results are simply interrelated—if (compare (38))

$$P_\psi(x,p;0) = \tfrac{1}{h^2}\iint M_\psi(\alpha,\beta;0)e^{-\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta$$

then (59.2) immediately entails (59.1)—but cast no light on a fundamental question which I must for the moment be content to set aside: What general *constraints/side conditions* does theory impose upon the functions $P_\psi(x,p;0)$ and $M_\psi(\alpha,\beta;0)$?

Looking next to the oscillator: equations (53.2) and (58.1), which have already been remarked to "bear a striking resemblance to" one another, are in fact structurally identical; whether one proceeds by notational adjustment

$$\begin{aligned}&\{x\mapsto u, +p/m\omega\mapsto v\}\text{ from (53.2)}\\ &\{\alpha\mapsto u, -\beta/m\omega\mapsto v\}\text{ from (58.1)}\end{aligned}$$

one obtains an equation of the form

$$\tfrac{\partial}{\partial t}F(u,v) = \omega\big\{u\tfrac{\partial}{\partial v} - v\tfrac{\partial}{\partial u}\big\}F(u,v)$$

The differential operator within braces is familiar from angular momentum theory as the generator of rotation on the (u,v)-plane; immediately

$$\begin{aligned}F(u,v;t) &= \exp\big\{\big[u\tfrac{\partial}{\partial v} - v\tfrac{\partial}{\partial u}\big]\omega t\big\}F(u,v;0)\\ &= F(u\cos\omega t - v\sin\omega t, u\sin\omega t + v\cos\omega t;0)\end{aligned}$$

—the accuracy of which can be confirmed by quick calculation. So we have

$$P_\psi(x,p;t) = P_\psi\big(x\cos\omega t-(p/m\omega)\sin\omega t,\, m\omega x\sin\omega t+p\cos\omega t;0\big) \tag{60.1}$$

which, though entirely and accurately quantum mechanical in its meaning, conforms well to the familiar classical fact that $H_{\text{oscillator}}(x,p)$ generates synchronous elliptical circulation on the phase plane. Similarly (or by Fourier transformation)

$$M_\psi(\alpha,\beta;t) = M_\psi\big(\alpha\cos\omega t+(\beta/m\omega)\sin\omega t,\, -m\omega\alpha\sin\omega t+\beta\cos\omega t;0\big) \tag{60.2}$$

according to which the circulation on the (α,β)-plane is *relatively retrograde—as one expects it to be*.[29] Information concerning the time-dependence of the n^{th}-order moments can now be extracted from

$$\big\langle(\alpha\mathbf{p}+\beta\mathbf{x})^n\big\rangle_t = \big\langle\big([\alpha\cos\omega t+(\beta/m\omega)\sin\omega t]\,\mathbf{p} + [-m\omega\alpha\sin\omega t+\beta\cos\omega t]\,\mathbf{x}\big)^n\big\rangle_0 \tag{61}$$

[29] The simple source of that expectation:

$$\text{If } \langle x\rangle = \int xP(x)\,dx \text{ then } \int xP(x+a)\,dx = \langle x\rangle - a \;\;:\;\; \text{compare the signs!}$$

Evidently and remarkably, the n^{th}-order moments move *among themselves* — independently of any reference to the motion of moments of any other order. And Fourier analysis of their motion will (consistently with a property of $\sigma_x^2(t)$ reported in §5, and in consequence ultimately of De Moive's theorem) reveal terms of frequencies $\omega, 2\omega, 3\omega, \ldots n\omega$.

When one attempts to bring patterned computational order to the detailed implications of (61)—which, I repeat, was obtained by solution of Moyal's equation in the oscillatory case—one is led spontaneously to the reinvention of some standard apparatus. It is natural to attempt to display "synchronous elliptical circulation on the phase plane" as simple phase advancement on a suitably constructed complex plane—natural therefore to notice that the dimensionless construction $\frac{1}{\hbar}(\alpha\mathsf{p}+\beta\mathsf{x})$ can be displayed

$$\tfrac{1}{\hbar}(\alpha\mathsf{p}+\beta\mathsf{x}) = a\boldsymbol{a} + b\boldsymbol{b}$$

provided the dimensionless objects on the right are defined

$$\begin{aligned}
a &\equiv a_1 + ia_2 \equiv \sqrt{\tfrac{m\omega}{2\hbar}}\,\alpha + i\tfrac{1}{\sqrt{2\hbar m\omega}}\,\beta\\
b &\equiv a_1 - ia_2 \equiv a^*\\
\boldsymbol{a} &\equiv \boldsymbol{a}_1 + i\boldsymbol{a}_2 \equiv \tfrac{1}{\sqrt{2\hbar m\omega}}\,\mathsf{p} - i\sqrt{\tfrac{m\omega}{2\hbar}}\,\mathsf{x}\\
\boldsymbol{b} &\equiv \boldsymbol{a}_1 - i\boldsymbol{a}_2 \equiv \boldsymbol{a}^+
\end{aligned}$$

The motion (elliptical circulation) of α and β

$$\begin{aligned}
\alpha &\longmapsto \alpha\cos\omega t + (\beta/m\omega)\sin\omega t\\
\beta &\longmapsto -m\omega\alpha\sin\omega t \;+\; \beta\cos\omega t
\end{aligned}$$

becomes in this notation very easy to describe

$$a \longmapsto ae^{-i\omega t}$$

and so also, therefore, does the motion of $\big\langle(\alpha\mathsf{p}+\beta\mathsf{x})^n\big\rangle$; we have

$$\big\langle(a\boldsymbol{a}+b\boldsymbol{b})^n\big\rangle_t = \big\langle(ae^{-i\omega t}\boldsymbol{a}+be^{+i\omega t}\boldsymbol{b})^n\big\rangle_0 \tag{62}$$

which, by the way, shows very clearly where the higher frequency components come from. But this is in (reassuring) fact very old news, for $\boldsymbol{a}$ and $\boldsymbol{b}$ are familiar as the ↓ and ↑ "ladder operators" described by Dirac in §34 of his *Principles of Quantum Mechanics*; they have the property that

$$[\boldsymbol{a},\boldsymbol{b}] = \mathbf{1}$$

and permit the oscillator Hamiltonian to be described

$$\mathsf{H} = \hbar\omega\big\{\boldsymbol{b}\boldsymbol{a} + \tfrac{1}{2}\mathbf{1}\big\}$$

Working in the Heisenberg picture, one therefore has

$$\dot{\boldsymbol{a}} = \tfrac{1}{i\hbar}[\boldsymbol{a}, \mathsf{H}] = -i\omega\boldsymbol{a} \quad \text{giving} \quad \begin{aligned} \boldsymbol{a}(t) &= e^{-i\omega t}\boldsymbol{a}(0) \\ \boldsymbol{b}(t) &= e^{+i\omega t}\boldsymbol{b}(0) \end{aligned}$$

of which (?) can be considered a corollary. It is interesting to notice, pursuant to a previous remark concerning higher frequency components, that if

$$\mathsf{A} \equiv \text{product of } m \ \boldsymbol{b}\text{-factors and } n \ \boldsymbol{a}\text{-factors } \textit{in any order}$$

then

$$\dot{\mathsf{A}} = i(m-n)\omega\mathsf{A} \quad \text{giving} \quad \mathsf{A}(t) = e^{i(m-n)\omega t}\mathsf{A}(0)$$

It is, in short, quite easy to obtain detailed information about how the motion of all numbers of the type $\langle\mathsf{A}\rangle$. But only exceptionally are such numbers of direct physical interest, since only exceptionally is A hermitian (representative of an *observable*), and the extraction of information concerning the motion of (x, p)-moments can be algebraically quite tedious. Quantum opticians (among others) have, however, stressed the *general* theoretical utility, in connection with *many* of the questions that arise from the phase space formalism, of operators imitative of $\boldsymbol{a}$ and $\boldsymbol{b}$.

In the "free particle limit" equations (60) read

$$P_\psi(x, p; t) = P_\psi(x - \tfrac{1}{m}pt, p; 0) \tag{63.1}$$

$$M_\psi(\alpha, \beta; t) = M_\psi(\alpha + \tfrac{1}{m}\beta t, \beta; 0) \tag{63.2}$$

Verification that (63.1) does in fact satisfy the "free particle Wigner equation" (53.3), and that (63.2) does satisfy the associated Moyal equation (58.2), is too immediate to write out. From the latter one obtains (compare (61))

$$\big\langle(\alpha\mathsf{p} + \beta\mathsf{x})^n\big\rangle_t = \big\langle([\alpha + \tfrac{1}{m}\beta t]\mathsf{p} + \beta\mathsf{x})^n\big\rangle_0 \tag{64}$$

which provides an elegantly succinct summary of material developed by clumbsy means in §2. But the definitions of $\boldsymbol{a}$ and $\boldsymbol{b}$ become, in this limit, meaningless; that fact touches obliquely on the reason that I found it simplest to treat the oscillator first.

9. When is $P_\psi(x, p)$ a "possible" Wigner function? When, within standard quantum mechanics, we write $\mathsf{H}|\psi) = i\hbar\frac{\partial}{\partial t}|\psi)$ we usually—and when we write $\langle\mathsf{A}\rangle = (\psi|\mathsf{A}|\psi)$ we invariably—understand $|\psi)$ to be subject to the side condition $(\psi|\psi) = 1$. That condition is universal, rooted in the interpretive foundations of the theory.[30] My present objective—responsive to a question posed already in connection with (59)—is to describe conditions which attach with similar

[30] I will not concern myself here with the boundary, differentiability, continuity, single-valuedness and other conditions which which in individual problems attach typically and so consequentially to (for example) $\psi(x) \equiv (x|\psi)$.

universality to the functions $P_\psi(x,p)$ and $M_\psi(\alpha,\beta)$, and which collectively serve to distinguish admissible functions from "impossible" ones.

The issue is made relatively more interesting by the circumstance that the Wigner distribution provides a representation of the "density matrix" $\boldsymbol{\rho}$, and $\boldsymbol{\rho}$ embodies a richer concept of "state" than does $|\psi)$. In this sense: $|\psi)$ refers to the state of an individual *system*, while $\boldsymbol{\rho}$ refers to the state of a statistically described *ensemble of systems*.[31] We imagine it to be the case[32] that systems drawn from such an ensemble will be[33]

$$\begin{aligned}&\text{in state } |\psi_1) \text{ with probability } p_1\\ &\text{in state } |\psi_2) \text{ with probability } p_2\\ &\qquad\vdots\\ &\text{in state } |\psi_k) \text{ with probability } p_k\\ &\qquad\vdots\end{aligned}$$

Under such circumstances we expect to write

$$\begin{aligned}\langle \mathsf{A}\rangle &= \sum_k p_k(\psi_k|\mathsf{A}|\psi_k) \qquad (65.1)\\ &= \text{ordinary mean of the quantum means}\end{aligned}$$

to describe the expected mean of a series of A-measurements. Exceptionally—when all members of the ensemble are in the *same* state $|\psi)$—the "ordinary" aspect of the averaging process is rendered moot, and we have

$$= 0 + 0 + \cdots + 0 + (\psi|\mathsf{A}|\psi) + 0 + \cdots \qquad (65.2)$$

It is of this "pure case" (the alternative, and more general, case being the "mixed case") that quantum mechanics standardly speaks. Density matrix theory springs from the elementary observation that (65.1) can be expressed

$$\langle \mathsf{A}\rangle = \text{trace}\, \mathsf{A}\boldsymbol{\rho} \qquad (66)$$

$$\boldsymbol{\rho} \equiv \sum_k |\psi_k)p_k(\psi_k| \qquad (67)$$

$$p_k \text{ are non-negative, subject to the constraint } \textstyle\sum p_k = 1$$

[31] Commonly one omits all pedantic reference to an "ensemble," and speaks as though simply uncertain of what state the system is actually in; "It might be in that state, but is more likely to be in this state. . . "

[32] But under what circumstances, and on what observational grounds, could we *establish* it to be the case?

[33] *Found* to be? How? Quantum mechanics itself keeps fuzzing up the idea at issue, simple though it appears at first sight to be. And fuzzy language, though difficult to avoid, only compounds the problem. It is for this reason that I am inclined to take exception to the locution "measuring the quantum state" (to be distinguished from "*preparing* the quantum state"?) which has recently become fashionable, and is used even in the title of one of the publications cited in footnote 15.

from which (65.2) can be recovered as a specialized instance. The operator $\boldsymbol{\rho}$ is hermitian;[34] we are assured therefore that its eigenvalues ρ_k are real and its eigenstates $|\rho_k)$ orthogonal. It is, however, usually a mistake to confuse ρ_k with p_k, $|\rho_k)$ with $|\psi_k)$, the spectral representation $\boldsymbol{\rho} = \sum |\rho_k)\rho_k(\rho_k|$ of $\boldsymbol{\rho}$ with (67); those associations can be made if and only if the states $|\psi_k)$ present in the ensemble are *orthogonal*, which *may* be the case,[35] and by many authors is *casually assumed* to be the case,[36] but in general such an assumption would do violence to the physics.

Let us supppose—in order to keep the notation as simple as possible, and the computation as explicitly detailed—that our ensemble contains a mixture of only two states:

$$\boldsymbol{\rho} = |\psi)p(\psi| + |\phi)q(\phi| \quad \text{with} \quad p + q = 1$$

Operators of the construction $\mathsf{P}_\psi \equiv |\psi)(\psi|$ are hermitian *projection* operators: $\mathsf{P}_\psi^2 = \mathsf{P}_\psi$. Specifically, P_ψ projects $|\alpha) \longrightarrow (\psi|\alpha) \cdot |\psi)$ onto the one-dimensional subspace (or "ray") in state space which contains $|\psi)$ as its normalized element. Generally

$$\text{trace (projection operator)} = \text{dimension of space onto which it projects}$$

so the calculation $\text{trace}\, \mathsf{P}_\psi = \sum (n|\psi)(\psi|n) = (\psi|\big\{\sum |n)(n|\big\}|\psi) = (\psi|\psi) = 1$ yields a result which might, in fact, have been anticipated, and puts us in position to write

$$\begin{gathered} \boldsymbol{\rho} = p\,\mathsf{P}_\psi + q\,\mathsf{P}_\phi \\ \downarrow \\ \text{trace}\,\boldsymbol{\rho} = p + q = 1 \quad : \quad \text{all cases} \end{gathered} \tag{68}$$

More informatively,

$$\begin{aligned} \boldsymbol{\rho}^2 &= p^2\,\mathsf{P}_\psi + q^2\,\mathsf{P}_\phi + pq(\mathsf{P}_\psi\mathsf{P}_\phi + \mathsf{P}_\phi\mathsf{P}_\psi) \\ &\downarrow \\ \text{trace}\,\boldsymbol{\rho}^2 &= p^2 + q^2 + 2pq\,\underbrace{(\psi|\phi)(\phi|\psi)} \\ &\qquad\qquad 0 \le (\psi|\phi)(\phi|\psi) \le 1 \quad \text{by Schwarz' inequality} \end{aligned}$$

[34] And therefore latently an "observable," though originally intended to serve quite a different theoretical function; $\boldsymbol{\rho}$ is associated with the state of the ensemble, not with any device with which we may intend to probe the ensemble. One can, however, readily imagine a quantum "theory of measurement with devices of imperfect resolution" in which $\boldsymbol{\rho}$-line constructs *are* associated with devices rather than states.

[35] And *will* be the case if the ensemble came into being by action of a measurement device.

[36] Such an assumption greatly simplifies certain arguments, but permits one to establish only weak instances of the general propositions in question.

But $p^2 + q^2 = (p+q)^2 - 2pq = 1 - 2pq$, so if we write $(\psi|\phi)(\phi|\psi) \equiv \cos^2\theta$ we have

$$\begin{aligned}\text{trace}\,\boldsymbol{\rho}^2 &= 1 - 2pq\sin^2\theta \le 1\\ &\downarrow\\ &= 1 \text{ if \& only if } \begin{cases} p=1 \;\&\; q=0\text{: the ensemble is pure; else}\\ p=0 \;\&\; q=1\text{: the ensemble is again pure; else}\\ \sin\theta = 0 : |\psi) \sim |\phi) \text{ so the ensemble is again pure}\end{cases}\end{aligned}$$

Evidently

$$\boldsymbol{\rho} \text{ refers to a } \left\{\begin{matrix}\text{pure}\\ \text{mixed}\end{matrix}\right\} \text{ensemble according as} \left\{\begin{matrix}\text{trace}\,\boldsymbol{\rho}^2 = 1\\ \text{trace}\,\boldsymbol{\rho}^2 < 1\end{matrix}\right\} \tag{69}$$

It follows that in the pure case $\boldsymbol{\rho}$ is projective; one has

$$\boldsymbol{\rho}^2 = \boldsymbol{\rho} \Longleftrightarrow \text{trace}\,\boldsymbol{\rho}^2 = 1 \text{ in the pure case} \tag{70}$$

but to write $\boldsymbol{\rho}^2 < \boldsymbol{\rho}$ in the mixed case is to write (some frequently encountered) mathematical nonsense. The conclusions reached above hold generally (i.e., when the ensemble contains *more* than two states) but I will not linger to write out the demonstrations. Instead I look (because the topic is so seldom treated) to the *spectral* properties of $\boldsymbol{\rho}$:

Notice first that every state $|\rho)$ which stands $\perp$ to the space spanned by $|\psi)$ and $|\phi)$ is killed by $\boldsymbol{\rho}$—is, in other words, an eigenstate with zero eigenvalue:

$$\boldsymbol{\rho}\,|\rho) = 0 \quad \text{if } |\rho) \;\perp\; \text{both } |\psi) \text{ and } |\phi)$$

The problem before us is, therefore, actually only 2-dimensional. Relative to some orthonormal basis $\{|1), |2)\}$ in the 2-space spanned by $|\psi)$ and $|\phi)$ we write

$$\begin{aligned}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} &\quad:\quad \text{coordinate representation of } |\psi)\\ \begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} &\quad:\quad \text{coordinate representation of } |\phi)\end{aligned}$$

In that language the associated projection operators P_ψ and P_ϕ acquire the matrix representations

$$\mathbb{P}_\psi \equiv \begin{pmatrix}\psi_1\psi_1^* & \psi_1\psi_2^*\\ \psi_2\psi_1^* & \psi_2\psi_2^*\end{pmatrix} \quad\text{and}\quad \mathbb{P}_\phi \equiv \begin{pmatrix}\phi_1\phi_1^* & \phi_1\phi_2^*\\ \phi_2\phi_1^* & \phi_2\phi_2^*\end{pmatrix}$$

giving $\boldsymbol{\rho} \longrightarrow \mathbb{R} = p\mathbb{P}_\psi + q\mathbb{P}_\phi$. Looking now to

$$\det(\mathbb{R} - \rho\mathbb{I}) = \rho^2 - \rho\cdot\text{trace}\,\mathbb{R} + \det\mathbb{R}$$

we have trace $\mathbb{R} = p + q = 1$ and, by quick calculation,

$$\begin{aligned}\det\mathbb{R} &= pq\big\{\psi_1\psi_1^*\phi_2\phi_2^* + \psi_2\psi_2^*\phi_1\phi_1^* - \psi_1\phi_1^*\phi_2\psi_2^* - \psi_2\phi_2^*\phi_1\psi_1^*\big\}\\ &= pq\big\{(\psi|\psi)(\phi|\phi) - (\psi|\phi)(\phi|\psi)\big\}\\ &= pq\sin^2\theta\end{aligned}$$

giving $\det(\mathbb{R} - \rho\mathbb{I}) = \rho^2 - \rho + pq\sin^2\theta$. The eigenvalues of $\mathbb{R}$ can therefore be described

$$\left.\begin{matrix}\rho_1\\ \rho_2\end{matrix}\right\} = \tfrac{1}{2}\big\{1 \pm \sqrt{1 - 4pq\sin^2\theta}\,\big\} \tag{71.1}$$

$$= \tfrac{1}{2}\big\{(p+q) \pm \sqrt{(p+q)^2 - 4pq\sin^2\theta}\,\big\} \tag{71.2}$$

$$= \tfrac{1}{2}\big\{(p+q) \pm \sqrt{(p-q)^2 + 4pq\cos^2\theta}\,\big\} \tag{71.3}$$

Evidently

$$\text{each eigenvalue is real and non-negative} \tag{72.1}$$

$$\text{sum of eigenvalues} = p + q = 1 \tag{72.2}$$

I distinguish now several cases:

• If $pq\sin^2\theta = 0$ because p (else q) vanishes[37]—which is to say: if $\mathbb{R}$ is projective, and the ensemble therefore pure—then (71.1) gives

$$\rho_1 = 1 \quad\text{and}\quad \rho_2 = 0$$

which conforms nicely to the general proposition that if $\mathbb{P}$ is projective ($\mathbb{P}^2 = \mathbb{P}$) then

$$\begin{aligned}&\det(\,\mathbb{P} - \lambda\mathbb{I}\,)\\ &\quad= (1-\lambda)^{\text{dimension of image space}}\cdot(0-\lambda)^{\text{dimension of its annihilated complement}}\end{aligned}$$

In the case ($p = 1$ & $q = 0$) we obtain descriptions of the associated eigenvectors

$$\mathbb{R}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = 1\cdot\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \quad\text{and}\quad \mathbb{R}\begin{pmatrix}+\psi_2^*\\ -\psi_1^*\end{pmatrix} = 0\cdot\begin{pmatrix}+\psi_2^*\\ -\psi_1^*\end{pmatrix}$$

which are transparently orthonormal. Trivial adjustments yield statements appropriate to the complementary case ($p = 0$ & $q = 1$).

• If $pq \neq 0$ but $|\psi) \perp |\phi)$ then (71.3) gives

$$\rho_1 = p \quad\text{and}\quad \rho_2 = q$$

[37] I dismiss as physically uninteresting the possibility $\sin\theta = 0$, since it has been seen to lead to phony mixtures $|\phi) = e^{i(\text{arbitrary phase})}|\psi)$.

And it is under such circumstances evident that

$$\mathbb{R}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = p\cdot\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \quad\text{and}\quad \mathbb{R}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} = q\cdot\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}$$

• In the general case ($pq \neq 0$ & $(\psi|\phi) \neq 0$) it becomes excessively tedious (even in the 2-dimensional case) to write out explicit descriptions of the eigenvectors. We are assured, however, that they exist, and are orthonormal, and that in terms of them the density matrix acquires a spectral representation of the form

$$\boldsymbol{\rho} = |\rho_1)\rho_1(\rho_1| + |\rho_2)\rho_2(\rho_2| + \sum_{k=3}^{\infty}|\rho_k)0(\rho_k| \tag{73}$$

where $\{|\rho_k)\}$ is some/any basis in that portion of state space which annihilated by $\boldsymbol{\rho}$, the space of states absent from the mixture to which $\boldsymbol{\rho}$ refers. But (73) permits/invites *reconceptualization of the mixture*: we imagine ourselves to have mixed states $|\psi)$ and $|\phi)$ with probabilities p and q, but according to (73) we might equally well[38]—in the sense that we would have obtained identical physical results if we had—mixed states $|\rho_1)$ and $|\rho_2)$ with probabilities ρ_1 and ρ_2. Equation (73) describes an "equivalent mixture" which was "present like a spectre"[39] in the original mixture, and which I will call the "ghost." It is from the ghost that we acquire access to the "arguments from orthonormality" which are standard to the literature, but which at the beginning of this discussion[36] I was at pains to disallow; thus, taking $\sum$ to range over the ghost states present in the mixture,

$$\boldsymbol{\rho} = \sum|\rho_k)\rho_k(\rho_k| \quad\Longrightarrow\quad \text{trace }\boldsymbol{\rho} = \sum\rho_k = 1 \tag{74.1}$$

$$\downarrow$$

$$\boldsymbol{\rho}^2 = \sum|\rho_k)\rho_k^2(\rho_k| \quad\Longrightarrow\quad \text{trace }\boldsymbol{\rho}^2 = \sum\rho_k^2 \leq 1 \tag{74.2}$$

with equality if an only if the mixture is in fact pure. Consistently with the latter claim: working from (71.1) we find

$$\text{trace }\boldsymbol{\rho}^2 = \Big\{\rho_1^2 + \rho_2^2 = 1 - pq\sin^2\theta\Big\} \leq 1$$

which is precisely the result from which we extracted (69).

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[38] At least if this CONJECTURE stands: *Statements of the form (72) pertain generally—no matter how many states we mix, in what proportions, and no matter what may be the inner-product relationships among them.* The point at issue is of an entirely mathematical—not a physical—nature, and will clearly require methods more powerful than the elementary methods that served me in the 2-dimensional case.

[39] Recall that the word "spectrum" derives historically from Newton's claim that colored light is "present like a spectre" in the mixture we call white light.

We confront now this uncommon question: *What mixtures are equivalent in the sense that—and physically indistinguishable because—they share the same ghost?* We will suppose the states present in the mixture to span an n-dimensional space; in its ghostly representation the density matrix then reads

$$\boldsymbol{\rho} = \sum_{k=1}^{n} |\rho_k)\rho_k(\rho_k|$$

where by assumption none of the eigenvalues ρ_k vanishes. They are the roots, therefore, of a polynomial of the form

$$\prod_{k=1}^{n}(\rho - \rho_k) = \rho^n + c_1\rho^{n-1} + \cdots + c_{n-1}\rho + c_n = 0$$

with $c_1 = -\text{trace}\,\boldsymbol{\rho} = -1$ and $c_n = (-)^n\text{det}\,\boldsymbol{\rho} \neq 0$ (else 0 would join the set of eigenvalues, and the dimension of the mixture would be reduced). Now let $\{|\psi_1), |\psi_2), \ldots, |\psi_n)\}$ refer to *any* set of normalized states that span the mixture, and form the complex numbers $z_{jk} \equiv (\psi_j|\psi_k) : j \neq k$, which are $n(n-1)$ in number. Form

$$\tilde{\boldsymbol{\rho}} \equiv \sum_{k=1}^{n} |\psi_k)p_k(\psi_k|$$

where the non-negative real numbers p_k are subject to the constraint $\sum p_k = 1$. Construct the associated characteristic polynomial

$$\text{det}\,(\rho\,\mathbf{1} - \tilde{\boldsymbol{\rho}}) = \rho^n - \rho^{n-1} + \tilde{c}_2\rho^{n-2} + \cdots + \tilde{c}_{n-1}\rho + \tilde{c}_n$$

Specifically, we have where

$$\begin{aligned} \tilde{c}_2 &= \tilde{c}_2(\text{independent } p_i\text{'s and } z_{jk}\text{'s}) \\ &\vdots \\ \tilde{c}_n &= \tilde{c}_n(\text{independent } p_i\text{'s and } z_{jk}\text{'s}) \end{aligned}$$

To achieve equivalence in the strong sense $\tilde{\boldsymbol{\rho}} = \boldsymbol{\rho}$ it is necessary that $\tilde{\boldsymbol{\rho}}$ and $\boldsymbol{\rho}$ have *identical spectra*; we are led therefore to these $n-1$ conditions on a total of $(n-1) + n(n-1) = n^2 - 1$ variables:

$$\left.\begin{aligned} \tilde{c}_2(\text{independent } p_i\text{'s and } z_{jk}\text{'s}) &= c_2 \\ \tilde{c}_3(\text{independent } p_i\text{'s and } z_{jk}\text{'s}) &= c_3 \\ &\vdots \\ \tilde{c}_n(\text{independent } p_i\text{'s and } z_{jk}\text{'s}) &= c_n \end{aligned}\right\} \tag{75}$$

In the case $n = 2$ these become a single condition on three variables:

$$p, \quad z_{12} \equiv (\psi_1|\psi_2) \quad \& \quad z_{21} \equiv (\psi_2|\psi_1)$$

Specifically (see again the calculation that led to (71)), we have

$$p(1-p)\big\{(\rho_1+\rho_2)-z_{12}z_{21}\big\}=\rho_1\rho_2$$

giving

$$\begin{aligned} p &= \tfrac{1}{2}\Big\{1\pm\sqrt{1-4K}\Big\} \quad \text{with} \quad K\equiv\frac{\rho_1\rho_2}{(\rho_1+\rho_2)-z_{12}z_{21}} \text{ and } (\rho_1+\rho_2)=1\\ &= \tfrac{1}{2}\Big\{(\rho_1+\rho_2)\pm\sqrt{(\rho_1+\rho_2)-4\rho_1\rho_2/(1-z_{12}z_{21})}\,\Big\}\end{aligned}$$

If in particular the selected states $|\psi_1)$ and $|\psi_2)$ happen to be orthogonal (if, in other words, $z_{21}\equiv z_{12}^*=0$) then we recover

$$p=\rho_1 \quad \text{and} \quad q\equiv 1-p=\rho_2$$

and have achieved "weak equivalence"

$$\tilde{\boldsymbol{\rho}}=|\psi_1)\rho_1(\psi_1|+|\psi_2)\rho_2(\psi_2| \qquad \sim \qquad \boldsymbol{\rho}=|\rho_1)\rho_1(\rho_1|+|\rho_2)\rho_2(\rho_2|$$