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Variance and Covariance in Quantum Mechanics and the Spreading of Position Probability

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A rigorous discussion of the concept of expectation value of an unbounded observable is given, and of its variance. It is shown that if A and B are observables for which the expectations $\langle A^2 \rangle$ and $\langle B^2 \rangle$ exist, and such that $\alpha A + \beta B$ is also an observable for some real numbers α and β, neither of which vanishes, then a quantum mechanical analog of covariance and correlation coefficient can be defined. The quadratic variation with time of the variance of position of a particle moving freely in one dimension is deduced rigorously, assuming only that there is a time at which the variances of position and momentum exist.

1. INTRODUCTION

The close analogy between the spreading of a wave packet and the spreading of a swarm of particles has often been pointed out. In a previous paper (Farina, 1977) this analogy was discussed in some detail. It was shown there that both classically and quantum mechanically the variance of position of a freely moving particle varies quadratically with time, and the formal proofs of this result differ essentially in the noncommutativity of position and momentum in quantum mechanics.

This paper suffered two important limitations. The first of these was the lack of mathematical rigor in the arguments, which were of a formal nature. Secondly, and equally important, was the philosophical nature of the arguments. The paper assumed that the particle was in a pure state. Now our knowledge of states occurring in the real world suggests that they are not usually pure. If we wish our deductions to apply to all such states occurring in nature we must certainly remove this assumption.

In this paper we shall attempt to remove the limitations just mentioned. We shall, in fact, only assume that the variances of the position and momentum exist at one particular time. We shall show with this assumption

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that the expectation value of position varies linearly with time while its variance is a quadratic function of time which tends to infinity when $|t| \to \infty$.

Before we do this, we shall prove some results of a more general nature. Firstly we analyze the meaning of expectation value for bounded and unbounded observables in the light of Gleason's theorem. We then proceed to the basic results, which are the expression of the expectation value in terms of pure states when the variance exists (proposition 1), its converse (proposition 2), and the existence under certain conditions of a quantum mechanical analog of covariance of two observables. Essentially the same analog has also arisen in the proof of a rigorous quantum mechanical central limit theorem (Cushen and Hudson, 1971). Finally, in Sections 6–9, we apply our results to an analysis of the free motion of a particle in one dimension and discuss our conclusions.

2. EXPECTATION VALUE OF A BOUNDED OBSERVABLE

A state Ω of a quantum mechanical system is a probability measure on the lattice $\mathfrak{L}(\mathfrak{h})$ of subspaces of the associated separable Hilbert space $\mathfrak{h}$. Gleason's theorem asserts that, for any state Ω there is a set of positive numbers $\{\lambda_j\}_{j=1}^{J}$ $(J \leqslant \infty)$ and a corresponding set of normalized vectors $\{\psi_j\}_{j=1}^{J} \subseteq \mathfrak{h}$ such that

$$\sum_{j=1}^{J} \lambda_j = 1 \tag{1}$$

and, for any $\mathfrak{M} \in \mathfrak{L}(\mathfrak{h})$

$$\Omega(\mathfrak{M}) = \sum_{j=1}^{J} \lambda_j \| P_{\mathfrak{M}} \psi_j \|^2, \tag{2}$$

$P_{\mathfrak{M}}$ being the projection operator onto $\mathfrak{M}$.

If A is a bounded self-adjoint operator the spectral theorem shows that there exist M, N such that $-\infty < M < N < +\infty$ and

$$A = \int_M^N \lambda \, dE(\lambda) \tag{3}$$

where $\{E(\lambda)\}_{\lambda \in \mathbf{R}}$ is the spectral family of A and the spectrum of A lies inside an interval $[M, N]$ for some $M, N \in \mathbb{R}$. If the probability that A has a value less than or equal to λ is $P(\lambda)$ then by (2)

$$P(\lambda) = \sum_{j=1}^{J} \lambda_j \| E(\lambda) \psi_j \|^2 \tag{4}$$

$P(\lambda)=0$ if $\lambda \leqslant M$ and $P(\lambda)=1$ if $N<\lambda$, and the expectation value $\langle A\rangle$ of A is therefore naturally defined as

$$\langle A\rangle=\int_M^N \lambda\, dP(\lambda)=\int_M^N \lambda\, d\left[\sum_{j=1}^{J} \lambda_j \| E(\lambda)\psi_j \|^2\right] \tag{5}$$

If $J<\infty$ this gives

$$\begin{aligned}\langle A\rangle &= \sum_{j=1}^{J} \lambda_j \int_M^N \lambda\, d\| E(\lambda)\psi_j \|^2 \\ &= \sum_{j=1}^{J} \lambda_j \int_M^N \lambda\, d\langle \psi_j | E(\lambda) | \psi_j\rangle \\ &= \sum_{j=1}^{J} \lambda_j \left\langle \psi_j \middle| \int_M^N \lambda\, dE(\lambda)\psi_j \right\rangle\end{aligned}$$

so by (3)

$$\langle A\rangle=\sum_{j=1}^{J} \lambda_j \langle \psi_j | A | \psi_j\rangle \tag{6}$$

If $J=\infty$ (5) can be written

$$\langle A\rangle=\int_M^N \lambda\, d\left[\lim_{J'\to\infty} \sum_{j=1}^{J'} \lambda_j \| E(\lambda)\psi_j \|^2\right]$$

and by the dominated convergence theorem this yields

$$\begin{aligned}\langle A\rangle &= \lim_{J'\to\infty} \int_M^N \lambda\, d\left[\sum_{j=1}^{J'} \lambda_j \| E(\lambda)\psi_j \|^2\right] \\ &= \lim_{J'\to\infty} \sum_{j=1}^{J'} \lambda_j \int_M^N \lambda\, d\| E(\lambda)\psi_j \|^2 \\ &= \lim_{J'\to\infty} \sum_{j=1}^{J'} \lambda_j \langle \psi_j | A | \psi_j\rangle \\ &= \sum_{j=1}^{\infty} \lambda_j \langle \psi_j | A | \psi_j\rangle\end{aligned}$$

so that (6) is still valid.

It follows that the expectation value of A^2 is

$$\langle A^2\rangle = \sum_{j=1}^{J} \lambda_j \langle \psi_j | A^2 | \psi_j \rangle \tag{7}$$

Since A is a bounded self-adjoint operator (7) can be rewritten

$$\langle A^2\rangle = \sum_{j=1}^{J} \lambda_j \| A\psi_j \|^2 \tag{8}$$

It should be noted that $\langle A\rangle$ depends only on the state, and so is independent of the particular choice of the ψ_j's and λ_j's.

3. EXPECTATION VALUES OF UNBOUNDED OBSERVABLES

If A is unbounded we cannot be sure that (6) is true, or even meaningful. In the first place ψ_j may not be in the domain of A for every j; even if this is the case the series on the right-hand side of (6) may not converge, or may not converge to $\langle A\rangle$. However, we shall show that if $\langle A^2\rangle$ is assumed to exist then ψ_j is in the domain $\mathfrak{D}(A)$ of A for every value of j, and moreover both (6) and (8) are true. To prove (7) would require first proving that ψ_j is in the domain $\mathfrak{D}(A^2)$ of A^2 for every value of j, but as we shall see we do not need to do this.

Firstly we must describe what we mean by saying that the expectation value of an observable represented by the unbounded self-adjoint operator A exists. To say that $\langle A\rangle$ exists means that the Riemann–Stieltjes integral

$$\langle A\rangle = \lim_{\substack{M\to-\infty \\ N\to+\infty}} \int_M^N \lambda \, dP(\lambda) \tag{9}$$

exists, where $P(\lambda)$ is the probability of the observable having a value less than or equal to λ, and the limits $M\to-\infty$ and $N\to+\infty$ are taken in any way.

Now by (4), which is still valid if A is unbounded,

$$\int_M^N \lambda \, dP(\lambda) = \int_M^N \lambda \, d\left[\sum_{j=1}^{J} \lambda_j \| E(\lambda)\psi_j \|^2\right] \tag{10}$$

If we define the bounded self-adjoint operator A_{MN} by

$$A_{MN} = \int_M^N \lambda \, dE(\lambda) \tag{11}$$

we can prove from (10), using precisely the arguments of Section 2, that

$$\int_M^N \lambda \, dP(\lambda) = \sum_{j=1}^{J} \lambda_j \langle \psi_j | A_{MN} | \psi_j \rangle = \langle A_{MN} \rangle \tag{12}$$

by (6) and so (9) implies that

$$\langle A \rangle = \lim_{\substack{M \to -\infty \\ N \to +\infty}} \sum_{j=1}^{J} \lambda_j \langle \psi_j | A_{MN} | \psi_j \rangle = \lim_{\substack{M \to -\infty \\ N \to +\infty}} \langle A_{MN} \rangle \tag{13}$$

where the limit $M \to -\infty$, $N \to +\infty$ may be taken in any way.

In the case of A^2 we note that

$$\begin{aligned}(A_{MN})^2 &= \left[\int_M^N \lambda \, dE(\lambda)\right]^2 \\ &= \int_M^N \lambda^2 \, dE(\lambda) \\ &= (A^2)_{MN}\end{aligned}$$

Therefore

$$\begin{aligned}\langle (A^2)_{MN} \rangle &= \langle (A_{MN})^2 \rangle \\ &= \sum_{j=1}^{J} \lambda_j \langle \psi_j | (A_{MN})^2 | \psi_j \rangle \\ &= \sum_{j=1}^{J} \lambda_j \| A_{MN} \psi_j \|^2 \end{aligned} \tag{14}$$

If $\langle A^2 \rangle$ exists the result proved above shows that the left-hand side of (14) tends to the unique limit $\langle A^2 \rangle$ as $M \to -\infty$ and $N \to +\infty$ however the limits are taken, and so the same applies to the right-hand side.

Suppose $\langle A^2 \rangle$ exists; then

$$\langle A^2 \rangle = \lim_{\substack{M \to -\infty \\ N \to +\infty}} \int_M^N \lambda^2 \, dP(\lambda)$$

where $M \to -\infty$ and $N \to +\infty$ in any way. It follows then that

$$\langle A \rangle = \lim_{\substack{M \to -\infty \\ N \to +\infty}} \int_M^N \lambda \, dP(\lambda)$$

also exists; that is, if $\langle A^2 \rangle$ exists so does $\langle A \rangle$.

We are now in a position to prove the result stated in the first paragraph of this section. We do this next.

4. EXPRESSION OF EXPECTATION VALUE IN TERMS OF PURE STATES

We shall now prove the following:

Proposition 1. If A is an unbounded self-adjoint operator in $\mathfrak{h}$ and $\langle A^2 \rangle$ exists then $\langle A \rangle$ exists and there is a set of positive numbers $\{\lambda_j\}_{j=1}^{J}$ $(J \leqslant \infty)$ and a set of normalized vectors $\{\psi_j\}_{j=1}^{J}$ such that

$$\psi_j \in \mathfrak{D}(A) \qquad (j = 1, \ldots, J)$$

$$\sum_{j=1}^{J} \lambda_j = 1$$

$$\langle A \rangle = \sum_{j=1}^{J} \lambda_j \langle \psi_j | A | \psi_j \rangle \tag{15}$$

$$\langle A^2 \rangle = \sum_{j=1}^{J} \lambda_j \| A\psi_j \|^2 \tag{16}$$

Proof. We have already seen that if $\langle A^2 \rangle$ exists then $\langle A \rangle$ exists. If $-\infty < M < N < +\infty$ A_{MN} is a bounded self-adjoint operator and so we can put $-M = N = i$ $(i = 1, 2, \ldots)$ in (14). We get

$$\langle (A^2)_{-i,i} \rangle = \sum_{j=1}^{J} \lambda_j \| A_{-i,i} \psi_j \|^2 \tag{17}$$

Now put $T_i = \langle (A^2)_{-i,i} \rangle$, $t_{ij} = \lambda_j \| A_{-i,i} \psi_j \|^2$ $(j = 1, \ldots, J)$. The conditions (i)–(iii) of the theorem proved in the appendix are satisfied if $T = \langle A^2 \rangle$, and so by conclusion (iv) of the theorem

$$t_{ij} = \lambda_j \| A_{-i,i} \psi_j \|^2$$

has a limit as $i \to \infty$. Since $\lambda_j > 0$

$$\| A_{-i,i} \psi_j \|^2 = \lambda_j^{-1} t_{ij}$$

has a finite limit as $i \to \infty$ for $j = 1, \ldots, J$. Further

$$\| A_{-i,i}\psi_j \|^2 = \left\| \int_{-i}^{i} \lambda \, dE(\lambda)\psi_j \right\|^2$$

$$= \int_{-i}^{i} \lambda^2 \| dE(\lambda)\psi_j \|^2$$

$$= \int_{-i}^{i} \lambda^2 \, d\| E(\lambda)\psi_j \|^2$$

so it follows by the spectral theorem for an unbounded self-adjoint operator (Helmberg, 1969) that $\psi_j \epsilon \mathfrak{D}(A)$ $(j = 1, \ldots, J)$.

Now

$$t_j = \lim_{i \to \infty} t_{ij} = \lim_{i \to \infty} \lambda_j \| A_{-i,i}\psi_j \|^2 = \lambda_j \| A\psi_j \|^2$$

and so (16) follows from conclusion (v) of the theorem of the appendix.

To prove (15) first note that

$$\langle A_{0,i} \rangle = \sum_{j=1}^{J} \lambda_j \langle \psi_j | A_{0,i} | \psi_j \rangle \tag{18}$$

$$\langle A_{-i,0} \rangle = \sum_{j=1}^{J} \lambda_j \langle \psi_j | A_{-i,0} | \psi_j \rangle \tag{19}$$

Since $\langle A \rangle$ exists both $\langle A_{0,i} \rangle$ and $\langle A_{-i,0} \rangle$ tend to finite limits as $i \to \infty$. Since also

$$A_{-i,i} = A_{-i,0} + A_{0,i}$$

we have

$$\langle A \rangle = \lim_{i \to \infty} \langle A_{-i,i} \rangle = \lim_{i \to \infty} \langle A_{-i,0} \rangle + \lim_{i \to \infty} \langle A_{0,i} \rangle \tag{20}$$

and

$$\langle \psi_j | A | \psi_j \rangle = \lim_{i \to \infty} \langle \psi_j | A_{-i,0} | \psi_j \rangle + \lim_{i \to \infty} \langle \psi_j | A_{0,i} \psi_j \rangle \tag{21}$$

Now (18) satisfies the conditions (i)–(iii) of the theorem of the appendix with

$$T_i = \langle A_{0,i} \rangle, \qquad t_{ij} = \lambda_j \langle \psi_j | A_{0,i} | \psi_j \rangle, \qquad T = \lim_{i \to \infty} \langle A_{0,i} \rangle$$

while (19) satisfies the same conditions of the same theorem if

$$T_i = -\langle A_{-i,0}\rangle, \qquad t_{ij} = -\lambda_j\langle\psi_j|A_{-i,0}|\psi_j\rangle, \qquad T = -\lim_{i\to\infty}\langle A_{-i,0}\rangle$$

Hence

$$\lim_{i\to\infty}\langle A_{0,i}\rangle = \sum_{j=1}^{J}\lim_{i\to\infty}\lambda_j\langle\psi_j|A_{0,i}|\psi_j\rangle$$

$$\lim_{i\to\infty}\langle A_{-i,0}\rangle = \sum_{j=1}^{J}\lim_{i\to\infty}\lambda_j\langle\psi_j|A_{-i,0}|\psi_j\rangle$$

If we add these last two results and use (20) and (21) we obtain (15). ■

5. THE CONVERSE OF PROPOSITION 1, AND COVARIANCE

The following question now naturally arises. Suppose the right-hand side of (16) exists. Does it then follow that $\langle A^2\rangle$ exists? The answer is yes, as the following result shows.

Proposition 2. Suppose A is an observable with the property that $\psi_j \in \mathfrak{D}(A)$ for $j=1,2,\ldots,J$. Then if

$$S = \sum_{j=1}^{J}\lambda_j\|A\psi_j\|^2$$

exists both $\langle A^2\rangle$ and $\langle A\rangle$ exist. Moreover, $\langle A\rangle$ and $\langle A^2\rangle$ are given by (15) and (16), respectively.

Proof. From (12) with A replaced by A^2 and λ by λ^2, and (14),

$$\int_M^N \lambda^2\, dP(\lambda) = \langle (A^2)_{MN}\rangle = \sum_{j=1}^{J}\lambda_j\|A_{MN}\psi_j\|^2 \tag{22}$$

Since $\psi_j \in \mathfrak{D}(A)(j=1,\ldots,J)$ we have $\|A_{MN}\psi_j\|^2 \leqslant \|A\psi_j\|^2$. Hence (22) implies

$$\int_M^N \lambda^2\, dP(\lambda) \leqslant \sum_{j=1}^{J}\lambda_j\|A\psi_j\|^2 = S \tag{23}$$

As $M\to-\infty$ and $N\to+\infty$ in any way the left-hand side of (23) cannot decrease, and it is bounded above by S. It therefore has a unique limit, and so $\langle A^2 \rangle$ exists.

It now follows from Proposition 1 (Section 4) that $\langle A \rangle$ also exists, and that $\langle A \rangle$ and $\langle A^2 \rangle$ are given by (15) and (16), respectively. ■

We shall use this result to define the quantum mechanical analog of covariance. In order to do this we first prove two preliminary results.

Proposition 3. If A and B are observables such that both $\langle A^2 \rangle$ and $\langle B^2 \rangle$ exist, then the sums

$$\sum_{j=1}^{J} \lambda_j \langle A\psi_j | B\psi_j \rangle, \qquad \sum_{j=1}^{J} \lambda_j \langle B\psi_j | A\psi_j \rangle \tag{24}$$

both exist. If $J = \infty$ either series is absolutely convergent.

Proof. Since $\langle A^2 \rangle$ and $\langle B^2 \rangle$ exist it follows from Proposition 1 (Section 4) that $\psi_j \in \mathfrak{D}(A) \cap \mathfrak{D}(B)$ for $j = 1, \dots, J$. Hence the result is obvious if $J < \infty$.

Suppose now that $J = \infty$, and J' is a positive integer. By repeated application of Schwarz's inequality

$$\begin{aligned}\sum_{j=1}^{J'} |\lambda_j \langle A\psi_j | B\psi_j \rangle| &= \sum_{j=1}^{J'} \lambda_j |\langle A\psi_j | B\psi_j \rangle| \\ &\leqslant \sum_{j=1}^{J'} \lambda_j \|A\psi_j\| \|B\psi_j\| \\ &= \sum_{j=1}^{J'} \left(\lambda_j^{1/2} \|A\psi_j\|\right)\left(\lambda_j^{1/2} \|B\psi_j\|\right) \\ &\leqslant \left(\sum_{j=1}^{J'} \lambda_j \|A\psi_j\|^2 \right)^{1/2} \left(\sum_{j=1}^{J'} \lambda_j \|B\psi_j\|^2 \right)^{1/2} \end{aligned} \tag{25}$$

The right-hand side of (25) tends monotonically to $\langle A^2 \rangle \langle B^2 \rangle$ as $J' \to +\infty$ by Proposition 1, and so the left-hand side converges when $J' \to \infty$. Thus the first series of (24) converges absolutely. That the second does so also follows by taking complex conjugates of the first. ■

Proposition 4. Suppose that A and B are observables such that

(i) $\langle A^2 \rangle$ and $\langle B^2 \rangle$ both exist,

(ii) $\alpha A + \beta B$ is an observable, where α, β are nonzero real numbers.

Then

(iii) $\langle(\alpha A+\beta B)\rangle$ and $\langle(\alpha A+\beta B)^2\rangle$ both exist

and

(iv) $$\langle(\alpha A+\beta B)\rangle=\alpha\langle A\rangle+\beta\langle B\rangle \tag{26}$$

$$\langle(\alpha A+\beta B)^2\rangle=\alpha^2\langle A^2\rangle+\alpha\beta\langle AB+BA\rangle+\beta^2\langle B^2\rangle \tag{27}$$

where

$$\langle AB+BA\rangle=\sum_{j=1}^{J}\lambda_j\left[\langle A\psi_j|B\psi_j\rangle+\langle B\psi_j|A\psi_j\rangle\right] \tag{28}$$

is dependent only on the state of the system, being independent of the choice of the λ_j's and the ψ_j's.

Proof. Since $\psi_j \in \mathcal{D}(A)\cap\mathcal{D}(B)=\mathcal{D}(\alpha A+\beta B)$ for each $j=1,\dots,J$ it follows that, if J' is a positive integer and $J'\leqslant J$, then

$$\begin{aligned}\sum_{j=1}^{J'}\|(\alpha A+\beta B)\psi_j\|^2 &= \alpha^2\sum_{j=1}^{J'}\|A\psi_j\|^2 \\ &\quad+\alpha\beta\sum_{j=1}^{J'}\lambda_j\left[\langle A\psi_j|B\psi_j\rangle+\langle B\psi_j|A\psi_j\rangle\right] \\ &\quad+\beta^2\sum_{j=1}^{J'}\lambda_j\|B\psi_j\|^2\end{aligned}$$

If $J<\infty$ we can put $J=J'$. If $J=\infty$ we let $J'\to+\infty$; since by Propositions 1 and 3 the right-hand side tends to a limit it follows that the left-hand side also tends to a limit. Consequently Proposition 2 implies that $\langle(\alpha A+\beta B)\rangle$ and $\langle(\alpha A+\beta B)^2\rangle$ exist, being given by (15) and (16) with A replaced by $\alpha A+\beta B$. Thus

$$\begin{aligned}\langle(\alpha A+\beta B)\rangle &= \sum_{j=1}^{J}\lambda_j\langle\psi_j|\alpha A+\beta B|\psi_j\rangle \\ &=\alpha\sum_{j=1}^{J}\lambda_j\langle\psi_j|A|\psi_j\rangle+\beta\sum_{j=1}^{J}\lambda_j\langle\psi_j|B|\psi_j\rangle \\ &=\alpha\langle A\rangle+\beta\langle B\rangle\end{aligned}$$

while

$$\langle(\alpha A+\beta B)^2\rangle = \sum_{j=1}^{J} \lambda_j \|(\alpha A+\beta B)\psi_j\|^2$$

$$= \alpha^2 \sum_{j=1}^{J} \lambda_j \|A\psi_j\|^2 + \alpha\beta \sum_{j=1}^{J} \lambda_j\left[\langle A\psi_j | B\psi_j\rangle + \langle B\psi_j | A\psi_j\rangle\right]$$

$$+ \beta^2 \sum_{j=1}^{J} \lambda_j \|B\psi_j\|^2$$

$$= \alpha^2\langle A^2\rangle + \alpha\beta\langle AB+BA\rangle + \beta^2\langle B^2\rangle$$

If neither α nor β vanish

$$\langle AB+BA\rangle = (\alpha\beta)^{-1}\left[\langle(\alpha A+\beta B)^2\rangle - \alpha^2\langle A^2\rangle - \beta^2\langle B^2\rangle\right]$$

The right-hand side of this equation depends only on the state, being independent of the particular choice of λ_j's and ψ_j's. It follows that the same is true of the left-hand side. ■

We are now in a position to define covariance. Suppose $\langle A^2\rangle$ and $\langle B^2\rangle$ exist, and $\alpha A+\beta B$ is an observable for some $\alpha, \beta \in \mathbb{R}$ where α and β are both nonzero. Then

$$\langle(A-\langle A\rangle)^2\rangle = \int_{-\infty}^{+\infty} (\lambda-\langle A\rangle)^2\, dP(\lambda)$$

$$= \int_{-\infty}^{+\infty} \lambda^2\, dP(\lambda) - 2\langle A\rangle \int_{-\infty}^{+\infty} \lambda\, dP(\lambda) + \langle A\rangle^2$$

$$= \langle A^2\rangle - \langle A\rangle^2$$

also exists; similarly $(B-\langle B\rangle)^2$ exists. It follows that

$$\operatorname{Cov}(A, B) = \tfrac{1}{2}\langle(A-\langle A\rangle)(B-\langle B\rangle) + (B-\langle B\rangle)(A-\langle A\rangle)\rangle$$

$$= \frac{1}{2}\sum_{j=1}^{J} \lambda_j\left[\langle(A-\langle A\rangle)\psi_j | (B-\langle B\rangle)\psi_j\rangle\right.$$

$$\left. + \langle(B-\langle B\rangle)\psi_j | (A-\langle A\rangle)\psi_j\rangle\right] \tag{29}$$

exists and is independent of the particular choice of the λ_j's and ψ_j's, depending only on the state. It is natural to define this as the covariance of A and B by analogy to classical statistics.

It is an immediate consequence of (25) that

$$|\mathrm{Cov}(A,B)| \leqslant \langle A^2\rangle^{1/2}\langle B^2\rangle^{1/2}$$

Hence if ρ is defined by

$$\rho = \frac{\mathrm{Cov}(A,B)}{\langle A^2\rangle^{1/2}\langle B^2\rangle^{1/2}}$$

$-1 \leqslant \rho \leqslant +1$, and ρ is the quantum mechanical analog of correlation coefficient.

6. POSITION AND MOMENTUM OF A FREE PARTICLE

Let us consider the free motion of a particle of mass μ. For simplicity we assume the motion is one-dimensional, since generalization to higher dimensions is straightforward. We shall use our results to prove that if the variances of position and momentum exist at a particular time then they exist for all times, and are related quadratically in the time. Before we do this we need some preliminary results, which we shall derive in this section.

We shall denote the position and momentum operators by x and p, respectively, and the domain of an operator by $\mathfrak{D}(A)$, as before. With these definitions we define operators x_t and p_t by

$$\mathfrak{D}(x_t) = \{\psi \in \mathfrak{h} : U_t\psi \in \mathfrak{D}(x)\}, \qquad x_t\psi = U_t^* x U_t \psi \tag{30}$$

$$\mathfrak{D}(p_t) = \{\psi \in \mathfrak{h} : U_t\psi \in \mathfrak{D}(p)\}, \qquad p_t\psi = U_t^* p U_t \psi \tag{31}$$

in (30) and (31) U_t denotes the evolution operator for free motion in one dimension, while the Hilbert space $\mathfrak{h}$ is $\mathfrak{L}_2(\mathbb{R})$.

In the Fourier transformed space

$$\mathfrak{D}(p) = \left\{\psi \in \mathfrak{h} : \int_{-\infty}^{+\infty} |\mathfrak{F}\psi(p')|^2\, dp' < \infty\right\} \tag{32}$$

where $\mathfrak{F}$ denotes the Fourier transform. Further, $\forall \psi \in \mathfrak{h}$ and $\forall p' \in \mathbb{R}$,

$$\mathfrak{F}U_t\psi(p') = \exp\left(-\frac{ip'^2 t}{2\mu}\right)\mathfrak{F}\psi(p') \tag{33}$$

while

$$\mathfrak{D}(x)=\left\{\psi\in\mathfrak{h}:\int_{-\infty}^{+\infty}|x|^2|\psi(x)|^2\,dx<\infty\right\} \tag{34}$$

It follows from (32) and (33) that if $\psi\in\mathfrak{D}(p)$ then $U_t\psi\in\mathfrak{D}(p)$, and so $\psi\in\mathfrak{D}(p_t)$. Further,

$$p_t\psi=p\psi \qquad \forall\psi\in\mathfrak{D}(p) \tag{35}$$

Suppose now that ψ is a vector of $\mathfrak{h}$ which belongs to the domains of both p and x, and consider

$$\psi_t(\theta)=\exp(ip\theta)U_t\psi$$

where θ is an arbitrary real number. For any $p'\in\mathbb{R}$ we have

$$\begin{aligned}\mathfrak{F}U_t\exp(ix\theta)\psi(p')&=\exp\left(\frac{-ip'^2t}{2\mu}\right)\mathfrak{F}\exp(ix\theta)\psi(p')\\&=\exp\left(-\frac{ip'^2t}{2\mu}\right)\mathfrak{F}\psi(p'-\theta)\end{aligned} \tag{36}$$

(36) shows that if $\psi\in\mathfrak{D}(p)$ then $U_t\exp(ix\theta)\psi\in\mathfrak{D}(p)$ also. Further,

$$\begin{aligned}\mathfrak{F}\exp(ix\theta)U_t\psi(p')&=\mathfrak{F}U_t\psi(p'-\theta)\\&=\exp\left[-\frac{i(p'-\theta)^2t}{2\mu}\right]\mathfrak{F}\psi(p'-\theta)\\&=\exp\left(-\frac{i\theta^2t}{2\mu}\right)\exp\left(\frac{ip'\theta t}{\mu}\right)\mathfrak{F}U_t\exp(ix\theta)\psi(p')\end{aligned}$$

so

$$\exp(ix\theta)U_t\psi=\exp\left(-\frac{i\theta^2t}{2\mu}\right)\exp\left(\frac{ip\theta t}{\mu}\right)U_t\exp(ix\theta)\psi \tag{37}$$

Now $\psi\in\mathfrak{D}(x)$ and $U_t\exp(ix\theta)\psi\in\mathfrak{D}(p)$, hence by Stone's theorem (37) implies that $U_t\psi\in\mathfrak{D}(x)$ and, further, that we can strongly differentiate (37) with respect to θ. If we do this and then set $\theta=0$ we obtain

$$xU_t\psi=\frac{pt}{\mu}U_t\psi+U_tx\psi$$

We have seen that $v = p/\mu$ commutes with U_t, hence if we operate on this with U_t^* and use (30) we obtain

$$x_t\psi = (x + vt)\psi \tag{38}$$

7. THE EXPECTATION VALUE OF MOMENTUM AND POSITION

We shall assume that at some time the expectation values $\langle x^2\rangle$ and $\langle p^2\rangle$ for a freely moving particle both exist. Without loss of generality we can assume this time to be $t=0$. According to Gleason's theorem the state at $t=0$ is a convex linear combination of pure states given by (2), say. Our previous results show that $\langle x\rangle$ and $\langle v\rangle = \langle p\rangle/\mu$ both exist, and that $\psi_j \in \mathfrak{D}(x)\cap\mathfrak{D}(p)$ for $j=1,\ldots,J$. Further,

$$\langle x\rangle = \sum_{j=1}^{J} \lambda_j \langle\psi_j | x | \psi_j\rangle \tag{39}$$

$$\langle v\rangle = \frac{\langle p\rangle}{\mu} = \sum_{j=1}^{J} \lambda_j \langle\psi_j | v | \psi_j\rangle = \sum_{j=1}^{J} \lambda_j \left\langle \psi_j \middle| \frac{p}{\mu} \middle| \psi_j \right\rangle \tag{40}$$

$$\langle x^2\rangle = \sum_{j=1}^{J} \lambda_j \| x\psi_j\|^2 \tag{41}$$

$$\langle v^2\rangle = \sum_{j=1}^{J} \lambda_j \| v\psi_j\|^2 \tag{42}$$

Now at time t the state, instead of being given by (2), is given by

$$\Omega_t(\mathfrak{M}) = \sum_{j=1}^{J} \lambda_j \| P_{\mathfrak{M}} U_t \psi_j \|^2 \tag{43}$$

Consider, then, the operator p_t defined by (31). As we saw in Section 6, since $\psi_j \in \mathfrak{D}(p)(j=1,\ldots,J)$ it follows that $U_t\psi_j \in \mathfrak{D}(p)$. Further, using (31) and (35)

$$\| pU_t\psi_j\|^2 = \|U_t^* pU_t\psi_j\|^2 = \| p_t\psi_j\|^2 = \| p\psi_j\|^2$$

and so

$$\sum_{j=1}^{J} \lambda_j \| pU_t\psi_j\|^2 = \sum_{j=1}^{J} \lambda_j \| p\psi_j\|^2 = \langle p^2\rangle$$

exists. According to Proposition 2 this implies that the expectation values $\langle p \rangle_t$ and $\langle p^2 \rangle_t$ exist at time t, and moreover

$$\langle p \rangle_t = \sum_{j=1}^{J} \lambda_j \langle U_t\psi_j | p | U_t\psi_j \rangle = \sum_{j=1}^{J} \lambda_j \langle \psi_j | p_t | \psi_j \rangle$$

$$= \sum_{j=1}^{J} \lambda_j \langle \psi_j | p | \psi_j \rangle = \langle p \rangle$$

$$\langle p^2 \rangle_t = \sum_{j=1}^{J} \lambda_j \| pU_t\psi_j \|^2 = \sum_{j=1}^{J} \lambda_j \| U_t^* p U_t \psi_j \|^2$$

$$= \sum_{j=1}^{J} \lambda_j \| p\psi_j \|^2 = \langle p^2 \rangle$$

Thus the expectation values of p and p^2 are unaltered.

In Section 6 we saw that $U_t\psi_j \in \mathfrak{D}(x)$ for $j = 1, \dots, J$. Further, if J' is a positive integer and $J' \leqslant J$,

$$\sum_{j=1}^{J'} \lambda_j \| xU_t\psi_j \|^2 = \sum_{j=1}^{J'} \lambda_j \| U_t^* x U_t \psi_j \|^2 = \sum_{j=1}^{J'} \lambda_j \| x_t \psi_j \|^2$$

$$= \sum_{j=1}^{J'} \lambda_j \| (x + vt)\psi_j \|^2$$

$$= \sum_{j=1}^{J'} \lambda_j \| x\psi_j \|^2 + t \sum_{j=1}^{J'} \lambda_j \left[\langle x\psi_j | v\psi_j \rangle + \langle v\psi_j | x\psi_j \rangle \right]$$

$$+ t^2 \sum_{j=1}^{J'} \lambda_j \| v\psi_j \|^2 \tag{44}$$

If $J < \infty$ we can put $J' = J$ in (44), and this shows that

$$\sum_{j=1}^{J} \lambda_j \| xU_t\psi_j \|^2 \tag{45}$$

exists. If $J = \infty$ we can let $J' \to \infty$ in (44). In this case the first and third terms tend to $\langle x^2 \rangle$ and $t^2 \langle v^2 \rangle$, respectively, and since $\langle x^2 \rangle$ and $\langle v^2 \rangle$ both exist it follows from Proposition 3 that the second term on the right-hand side of (44) also tends to a finite limit. In other words (45) is still true when $J=\infty$.

It follows from (45) and Proposition 2 that $\langle x\rangle_t$ and $\langle x^2\rangle_t$ exist, and moreover

$$\begin{aligned}\langle x\rangle_t &= \sum_{j=1}^{J} \langle U_t\psi_j | x | U_t\psi_j\rangle \\ &= \sum_{j=1}^{J} \langle \psi_j | x_t | \psi_j\rangle \\ &= \sum_{j=1}^{J} \langle \psi_j | x+vt | \psi_j\rangle \\ &= \sum_{j=1}^{J} \langle \psi_j | x | \psi_j\rangle + t\sum_{j=1}^{J} \langle \psi_j | v | \psi_j\rangle\end{aligned}$$

that is,

$$\langle x\rangle_t = \langle x\rangle + t\langle v\rangle \tag{46}$$

8. THE SPREADING OF POSITION PROBABILITY

At time $t=0$ the quantities $\langle x^2\rangle$ and $\langle v^2\rangle$ exist by hypothesis. As pointed out in Section 5 this means that the quantities

$$\operatorname{Var} x = \left\langle (x-\langle x\rangle)^2 \right\rangle \tag{47}$$

$$\operatorname{Var} v = \left\langle (v-\langle v\rangle)^2 \right\rangle \tag{48}$$

also exist at time $t=0$. Thus $x-\langle x\rangle$ and $v-\langle v\rangle$ satisfy the conditions of Proposition 3 so

$$\begin{aligned}\operatorname{Cov}(x,v) = \sum_{j=1}^{J} \frac{1}{2}\lambda_j\big[&\langle (x-\langle x\rangle)\psi_j | (v-\langle v\rangle)\psi_j\rangle \\ &+ \langle (v-\langle v\rangle)\psi_j | (x-\langle x\rangle)\psi_j\rangle\big]\end{aligned} \tag{49}$$

also exists. If $\alpha(x-\langle x\rangle)-\beta(v-\langle v\rangle)$ is assumed to be an observable for some α and β in $\mathbb{R}$, both nonzero, Proposition 4 implies that Cov(x, v) is independent of the choice of ψ_j's and λ_j's, but as we shall see we do not need to make this assumption.

Now $U_t\psi_j \in \mathfrak{D}(x) = \mathfrak{D}(x - \langle x\rangle)$ $(j = 1, \dots, J)$, and using (46)

$$\begin{aligned}
\|(x-\langle x\rangle_t)U_t\psi_j\|^2 &= \|U_t^*(x-\langle x\rangle_t)U_t\psi_j\|^2 \\
&= \|(x_t-\langle x\rangle_t)\psi_j\|^2 \\
&= \|[(x+vt)-(\langle x\rangle+t\langle v\rangle)]\psi_j\|^2 \\
&= \|(x-\langle x\rangle)\psi_j + t(v-\langle v\rangle)\psi_j\|^2 \\
&= \|(x-\langle x\rangle)\psi_j\|^2 + \big[\big\langle (x-\langle x\rangle)\psi_j \big| (v-\langle v\rangle)\psi j\big\rangle \\
&\qquad + \big\langle (v-\langle v\rangle)\psi_j \big| (x-\langle x\rangle)\psi_j\big\rangle\big]t \\
&\quad + \|(v-\langle v\rangle)\psi_j\|^2 t^2
\end{aligned} \tag{50}$$

Now for $J \leqslant \infty$

$$\operatorname{Var} x = \sum_{j=1}^{J} \lambda_j \|(x-\langle x\rangle)\psi_j\|^2$$

$$\operatorname{Var} v = \sum_{j=1}^{J} \lambda_j \|(v-\langle v\rangle)\psi_j\|^2$$

Hence the right-hand side of (50) can be summed from $j=1$ to $j=J$ using (49) even if $J=\infty$. The same can therefore be done to the left-hand side. Thus by Proposition 2 the variance $(\operatorname{Var} x)_t$ of x at time t exists, and moreover

$$(\operatorname{Var} x)_t = \operatorname{Var} x + 2t\operatorname{Cov}(x, v) + t^2 \operatorname{Var} v \tag{51}$$

We have thus established the existence and quadratic variation with time of $(\operatorname{Var} x)_t$ subject only to the assumption that Var x and Var v exist at time $t=0$.

If $t \neq 0$ equation (51) can be rewritten

$$\operatorname{Cov}(x, v) = \frac{1}{2t}(\operatorname{Var} x)_t - \frac{1}{2t}\operatorname{Var} x - \frac{t}{2}\operatorname{Var} v \tag{52}$$

The right-hand side of (52) is independent of the particular choice of λ_j's and ψ_j's. Since it is independent of time it depends only on the state Ω of the system at time $t=0$. It follows that $\mathrm{Cov}(x, v)$ depends only on Ω, which is not immediately obvious from its definition (49). As anticipated earlier in this section we do not need to assume that $\alpha x+\beta v$ is an observable to reach this conclusion in this case.

We conclude by noting that the covariance of x and p at time t may be defined by

$$[\mathrm{Cov}(x, v)]_t=\sum_{j=1}^{J} \frac{1}{2}\lambda_j\left[\langle(x-\langle x\rangle_t)U_t\psi_j|(v-\langle v\rangle)U_t\psi_j\rangle\right.$$
$$\left.+\langle(v-\langle v\rangle)U_t\psi_j|(x-\langle x\rangle_t)U_t\psi_j\rangle\right] \tag{53}$$

Proposition 3 ensures the existence of this quantity. Using (38) and (46) we have

$$\begin{aligned}
&\langle(x-\langle x\rangle_t)U_t\psi_j|(v-\langle v\rangle)U_t\psi_j\rangle\\
&\quad=\langle(x_t-\langle x\rangle_t)\psi_j|(v-\langle v\rangle)\psi_j\rangle\\
&\quad=\langle[(x-\langle x\rangle)+(v-\langle v\rangle)t]\psi_j|(v-\langle v\rangle)\psi_j\rangle\\
&\quad=\langle(x-\langle x\rangle)\psi_j|(v-\langle v\rangle)\psi_j\rangle+t\|(v-\langle v\rangle)\psi_j\|^2
\end{aligned}$$

hence (53) yields, using (49),

$$[\mathrm{Cov}(x, v)]_t=\mathrm{Cov}(x, v)+t\,\mathrm{Var}\,v \tag{54}$$

Thus $[\mathrm{Cov}(x, v)]_t$ varies linearly with time. Equation (54) also shows that it is independent of the particular choice of the ψ_j's and λ_j's.

The quantum mechanical analog ρ_t of the correlation coefficient at time t is defined by

$$\rho_t=\frac{[\mathrm{Cov}(x, v)]_t}{[(\mathrm{Var}\,x)_t\mathrm{Var}\,v]^{1/2}} \tag{55}$$

It is easy to see that ρ_t varies monotonically from -1 to $+1$ as t increases from $-\infty$ and $+\infty$. As shown elsewhere (Farina, 1977) this result also holds classically. In fact if a crowd of runners is traveling along a straight line with constant speeds which are not all equal, the speeds will anticorrelate with position when $t\to-\infty$, and correlate with position as $t\to+\infty$.

9. DISCUSSION

We have applied the laws of quantum mechanics in a mathematically rigorous way to a statistical ensemble of particles moving freely in one dimension, and deduced the quadratic dependence on time of the variance of position. The generalization to free motion in space is straightforward (Farina, 1977).

It is important to note that we have made no model of the particles. We do not, for example, regard our ensemble as made up of wave packets. Our only assumptions are the laws of nonrelativistic quantum mechanics and the existence of the variances of position and momentum at one time in the ensemble.

To assume that wave packets are real must always raise problems. Why should particles always be in pure states? When are the packets minimal—was it at the birth of the universe? Our deduction has made no such assumptions, and so avoids these philosophical difficulties.

Although the quadratic variance with time of $\operatorname{Var} x$ is well known, this paper provides, to the best of its author's knowledge, the first derivation of this result which is mathematically, physically, and philosophically rigorous. The author believes that the definition of correlation coefficient between possibly incompatible observables given here is also new.

Our deduction is something that is capable, at least in principle, of experimental test. Pulses of particles are produced in the laboratory, and in theory at least their statistics can be studied. At no stage do wave packets come into our discussion as physical objects. They enter only as mathematical terms (the $U_t\psi_j$'s) in expressions for the measurable expectation values. Each $U_t\psi_j$ spreads out, this being the special case when $J=1$. The spreading out of the individual "wave packets," which are mathematical functions and not physical objects, then imposes itself on the observable expectation values by means of the convex sum whose existence is assured by Gleason's theorem.

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APPENDIX

In this appendix we prove the following:

Theorem. Suppose t_{ij} ($i=1,2,\ldots$; $j=1,2,\ldots,J$; $J\leqslant\infty$) is a set of nonnegative numbers with the following properties:

(i) For each $i = 1, 2, \ldots$ the sum

$$T_i = \sum_{j=1}^{J} t_{ij}$$

exists.

(ii) For each $j = 1, 2, \ldots$ t_{ij} is a nondecreasing function of i.

(iii) When i tends to infinity T_i tends to the finite limit T.

Then

(iv) For each $j = 1, 2, \ldots$ t_{ij} tends to a finite limit t_j as $i \to \infty$.

(v) $$T = \lim_{i \to \infty} T_i = \sum_{j=1}^{J} t_j$$

Proof. Firstly we note that by (ii) T_i is a nondecreasing function of i, and so by (i) and (iii)

$$t_{ij} \leqslant T_i \leqslant T$$

Hence by (ii) t_{ij} has a finite limit, t_j say, as $i \to \infty$, which is (iv). If $J < \infty$ (v) follows from (i) and (iii) by letting $i \to \infty$, so without loss of generality we can replace J by ∞ in (i).

Now for each $J = 1, 2, \ldots$ (i) implies

$$\sum_{j=1}^{J} t_{ij} \leqslant T_i$$

If we let $i \to \infty$ and use (iv)

$$\sum_{j=1}^{J} t_j \leqslant T$$

Since $t_{ij} \geqslant 0$ it follows that $t_j \geqslant 0$, and so the left-hand side of this inequality is a nondecreasing function of J. It therefore converges as $J \to \infty$ to a finite quantity, and moreover

$$\sum_{j=1}^{\infty} t_j \leqslant T \tag{A.1}$$

Given $\epsilon > 0$ (i) implies that there is a positive integer $J = J(i, \epsilon)$ such that

$$T_i - \epsilon \leqslant \sum_{j=1}^{J} t_{ij} \tag{A.2}$$

Since t_{ij} is a nondecreasing function of i for each j and $t_{ij} \to t_j$ as $i \to \infty$ we have

$$t_{ij} \leqslant t_j \qquad (j = 1, 2, \ldots)$$

so from (A.2)

$$T_i - \epsilon \leqslant \sum_{j=1}^{J} t_j$$

Each $t_j \geqslant 0$ so this implies

$$T_i - \epsilon \leqslant \sum_{j=1}^{\infty} t_j$$

If we let $i \to \infty$ and use (iii) we get

$$T - \epsilon \leqslant \sum_{j=1}^{\infty} t_j \tag{A.3}$$

Since ϵ is an arbitrary positive number (A.1) and (A.3) imply

$$T = \sum_{j=1}^{\infty} t_j$$

which is (v).

The above is an elementary proof. In fact, the theorem is the monotone convergence theorem in the special case when the measure is the discrete counting measure.

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