Classical Statistics Inherent in Pure Quantum States

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The statistics of pure quantum states of the harmonic oscillator is separated into a quantum mechanical and a classical part by associating a classical analog with each quantum state. Several types of states are considered and it is shown that all pure states of the same average energy are equally close to their classical analogs.

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As is well known, a quantum mechanical description, even by a pure state, is a statistical description; whatever the state of the system, the values of certain dynamical variables are predictable only by a probability density. Heisenberg's uncertainty principle precludes a completely deterministic description. However, not all of the uncertainty need be considered to be of quantum mechanical origin. In the case of mixed states, this is, of course, obvious, since a probability—coming from a lack of information that could, in principle, be eliminated—is explicitly introduced into the description. In the case of pure states, it is not so obvious that part of the uncertainty may be considered to be classical. A distinction between—or identification of—types of uncertainty in a quantum-state description will not yield new results in the calculation of expectation values. It will yield, however, a deeper insight into quantum mechanics and its relation to classical theory, and will eliminate a popular misconception to be described later. It is the purpose of the present paper to present and illustrate a method of identifying the classical part of the uncertainty in pure states of the harmonic oscillator. While one may expect the ideas involved to be applicable to other systems also, the widespread use of the harmonic oscillator as a model in many branches of physics makes it a system of fundamental interest in itself.

The method calls for associating with each quantum state a classical phase-space probability density, the "classical analog" of the quantum state. The uncertainties of the classical distribution are then identified as the classical part of the total uncertainty of the quantum state. As will be seen immediately, merely the criteria for constructing the distribution contain sufficient information for identification of the classical part of the uncertainties in the fundamental variables.

An attempt to present a quantum mechanical description as a purely statistical description, in which averages of dynamical variables are obtained by a function analogous to a probability density, encounters two obstacles: the dependence of this function on the ordering of the factors when a product of (quantum mechanical) variables is averaged, and the assumption of negative values by this function for a specific ordering scheme.[1] One can, however, set up criteria for constructing a purely statistical description which comes "closest" to the quantum mechanical description.[2] Consider the harmonic oscillator of frequency ω with coordinate q and momentum p in dimensionless form, the Hamiltonian being $H = \frac{1}{2}\hbar\omega(q^2 + p^2)$. Where distinction between operators and c numbers need be made, operators will be designated by a circumflex (such as $\hat{q}, \hat{p}$, with $[\hat{q}, \hat{p}] = i$) and c numbers by a tilde (such as $\tilde{q}, \tilde{p}$). A classical statistical description is given by a phase-space probability density $P(\tilde{q}, \tilde{p})$, while a pure-state quantum mechanical description is given either by the quantum state $|\psi\rangle$ or by the (equivalent) density matrix $|\psi\rangle\langle\psi|$. Averages—or expectation values—of functions of q and p, say $\varphi(q,p)$, are obtained from the expressions $\langle\varphi(\hat{q},\hat{p})\rangle = \langle\psi|\varphi(\hat{q},\hat{p})|\psi\rangle$, $\langle\varphi(\tilde{q},\tilde{p})\rangle = \iint d\tilde{q}\, d\tilde{p}\, P(\tilde{q},\tilde{p})\varphi(\tilde{q},\tilde{p})$.

The classical analog of the state $|\psi\rangle$ is defined as the probability density $P(\tilde{q}, \tilde{p})$ which meets the following criteria:

$$\langle\tilde{q}\rangle = \langle\hat{q}\rangle, \quad \langle\tilde{p}\rangle = \langle\hat{p}\rangle, \tag{1}$$

$$\Delta\tilde{q} = K\,\Delta\hat{q}, \quad \Delta\tilde{p} = K\,\Delta\hat{p}, \quad V(\tilde{q},\tilde{p}) = K^2 V(\hat{q},\hat{p}), \tag{2}$$

$$\Delta\varphi(\tilde{q},\tilde{p}) \leqslant \Delta\varphi(\hat{q},\hat{p}), \tag{3}$$

where $(\Delta\varphi)^2 = \langle\varphi\rangle^2 - \langle\varphi\rangle^2$, $V(q,p) = \frac{1}{2}\langle qp + pq\rangle - \langle q\rangle\langle p\rangle$, $K^2 = -1[(\Delta\hat{q})^2 + (\Delta\hat{p})^2]^{-1}$, the equality sign in (3) applies only when the right-hand side vanishes, $\varphi(\hat{q},\hat{p})$ is any Hermitian polynomial in $\hat{q}$ and $\hat{p}$, and $\varphi(\tilde{q},\tilde{p})$ is the corresponding c-number function.[3]

The meaning of the first criterion is obvious. The second and third criteria require that the classical uncertainty be less than the quantum mechanical uncertainty unless the latter vanishes, a recognition of the fact that ideal quantum measurements produce uncertainties, in general, while (ideal) classical measurements do not.[4] The criteria refer to quantities evaluated at a given time. The time independence of criteria (1) and (2) can be demonstrated simply. With the notation $q(0) \equiv q_0$, etc., the equations of motion $\dot{q} = \omega p$ and $\dot{p} = -\omega q$ are solved by

$$q(t) = q_0 \cos\omega t + p_0 \sin\omega t,$$

$$p(t) = p_0 \cos\omega t - q_0 \sin\omega t,$$

which yield

$$[\Delta q(t)]^2 = (\Delta q_0)^2 \cos^2\omega t + (\Delta p_0)^2 \sin^2\omega t + V(q_0, p_0) \sin\omega t \cos\omega t,$$

$$[\Delta p(t)]^2 = (\Delta q_0)^2 \sin^2\omega t + (\Delta p_0)^2 \cos^2\omega t - V(q_0, p_0) \sin\omega t \cos\omega t,$$

$$V(q(t), p(t)) = [(\Delta p_0)^2 - (\Delta q_0)^2] \sin\omega t \cos\omega t + V(q_0, p_0) \cos 2\omega t.$$

These relationships are valid both classically and quantum mechanically. Furthermore, K is a constant of motion, since

$$\tfrac{1}{2}\hbar\omega[(\Delta\hat{q})^2 + (\Delta\hat{p})^2] = \langle H(\hat{q}, \hat{p})\rangle - H(\langle q\rangle, \langle p\rangle).$$

Thus, if criteria (1) and (2) are valid initially, they are valid for all time. The above discussion of time dependence utilizes the Heisenberg picture, quantum mechanically, and its equivalent, classically. The Schrödinger picture and its classical equivalent may also be used, in which case P rotates clockwise with angular velocity ω, while q and p are time independent.

It is instructive to examine the implications of the criteria concerning the energy. One can write

$$\langle\tilde{H}\rangle - H(\langle q\rangle, \langle p\rangle) = K^2[\langle\hat{H}\rangle - H(\langle q\rangle, \langle p\rangle)],$$

which yields

$$\langle\tilde{H}\rangle = \langle\hat{H}\rangle - \tfrac{1}{2}\hbar\omega.$$

We see that the average energy of the classical analog is just that of the quantum state reduced by the zero-point energy. In view of the fact that the zero-point energy is of purely quantum mechanical origin, this is a physically reasonable result.

The limits of K are also of interest. From $\Delta\hat{q}\Delta\hat{p} \geq \frac{1}{2}$ (the uncertainty principle in present notation) we have $(\Delta\hat{q})^2 + (\Delta\hat{p})^2 \geq 1$, which implies $0 \leq K \leq 1$. Since K is the fraction of the uncertainty of the quantum state which may be regarded as classical, this means that the classical analog can be completely deterministic, a result that we should reasonably expect.

Several types of quantum states widely used to describe the harmonic oscillator will now be considered. The first is an energy state, defined by $H|n\rangle = (n + \frac{1}{2})\hbar\omega|n\rangle$. Since there is no uncertainty in the quantum mechanical energy, there can be no uncertainty in the classical energy, according to criterion (3), and the above relationship between $\langle\tilde{H}\rangle$ and $\langle\hat{H}\rangle$ shows that $\tilde{H}$ is precisely $n\hbar\omega$. Furthermore, since the criteria are stationary, the classical analog must be stationary.[3] The only probability density of precise energy that is stationary is a microcanonical ensemble of infinitesimal energy width. We consider, therefore, the applicability of the criteria to the microcanonical ensemble of energy $n\hbar\omega$. With use of polar coordinates given by $\tilde{q} = r\cos\theta$, $\tilde{p} = r\sin\theta$, this ensemble is described by $P(r, \theta) = (2\pi r_0)^{-1} \times \delta(r - r_0)$, where $r_0 = (2n)^{1/2}$, and classical averages are calculated by

$$\langle\varphi(\tilde{q}, \tilde{p})\rangle = (2\pi)^{-1}\int_0^{2\pi} d\theta\, \varphi(r_0\cos\theta, r_0\sin\theta).$$

Note that $\langle q\rangle = \langle p\rangle = \langle qp + pq\rangle = 0$ both classically and quantum mechanically, so that criterion (1) is satisfied. Also, $(\Delta\hat{q})^2 = (\Delta\hat{p})^2 = n + \frac{1}{2}$, $(\Delta\tilde{q})^2 = (\Delta\tilde{p})^2 = n$, $K^2 = n(n + \frac{1}{2})^{-1}$, so that criterion (2) is satisfied. As for criterion (3), a proof that it is satisfied in its complete generality has not yet been found, and we consider only several illustrations. Noting that $\langle q^{2m+1}\rangle = 0$, we obtain $(\Delta q^{2m+1})^2 = \langle q^{2(2m+1)}\rangle$. From the angular integration above, we get $\langle\tilde{q}^{2m}\rangle = n^m(2m)!\,2^{-m}(m!)^{-2}$. It can be shown that $\langle\hat{q}^{2m}\rangle$ is a polynomial in n of order m, with the highest-order term being equal to $\langle\tilde{q}^{2m}\rangle$, and the lower-order terms being positive. For instance, $\langle\hat{q}^6\rangle = \frac{1}{8}(20n^3 + 30n^2 + 40n + 15)$, while $\langle\tilde{q}^6\rangle = \frac{5}{2}n^3$. We therefore have $\Delta(\tilde{q}^{2m+1}) < \Delta(\hat{q}^{2m+1})$. An identical argument applies to $\Delta(p^{2m+1})$. Other examples, not too tedious to calculate explicitly, are consistent with criterion (3), and one may conjecture that it is satisfied generally. It is of interest to note that the term of highest order in the polynomial (in n) obtained for the expectation value of a product of m factors $\hat{q}$ and r factors $\hat{p}$, in any order, can be shown to be identical to $\langle\tilde{q}^m\tilde{p}^r\rangle$. Thus, the statistics of the energy state becomes identical to that of the microcanonical ensemble for large n.

We proceed, next, to coherent states, defined by $2^{-1/2}(\hat{q} + i\hat{p})|\alpha\rangle = \alpha|\alpha\rangle$, α being a complex number. These are a special class of minimal wave packets, for which not only the minimum uncertainty condition, $\Delta\hat{q}\Delta\hat{p}=\frac{1}{2}$, but also the condition $(\Delta\hat{q})^2+(\Delta\hat{p})^2=1$ holds. Here $K=0$, so that there exists no uncertainty at all in the classical description. The classical analog is, therefore, completely deterministic. The precise values of q and p are given by $q'=2^{-1/2}(\alpha+\alpha^*)$, $p'=-2^{-1/2}\times i(\alpha-\alpha^*)$, and the probability density is $P(\tilde{q},\tilde{p})=\delta(\tilde{q}-q')\delta(\tilde{p}-p')$. Obviously, all criteria for the classical analog are satisfied.

The last type of pure state that we consider is a minimal wave packet which is not a coherent state, that is, $\Delta\hat{q}\,\Delta\hat{p}=\frac{1}{2}$, but $(\Delta\hat{q})^2+(\Delta\hat{p})^2>1$. In this case, $\Delta\hat{q}\,\Delta\hat{p}$ does not remain constant, as for coherent states, but oscillates with frequency 4ω above the value $\frac{1}{2}$. It is useful to describe the quantum state by its wave function in both the q and p representation:

$$\psi(q)=\sigma^{-1/2}\pi^{-1/4}\exp[-\tfrac{1}{2}\sigma^{-2}(q-q_1)^2+ip_1q],$$
$$\psi(p)=\sigma^{1/2}\pi^{-1/4}\exp[-\tfrac{1}{2}\sigma^{2}(p-p_1)^2-iq_1p].$$

[The wave packet must be Gaussian[5]; the special case of $\sigma=1$ is a coherent state with $\alpha=2^{-1/2}(q_1+ip_1)$.] We have, in this case, $\langle\hat{q}\rangle=q_1$, $\langle\hat{p}\rangle=p_1$, $(\Delta\hat{q})^2=\frac{1}{2}\sigma^2$, $(\Delta\hat{p})^2=\frac{1}{2}\sigma^{-2}$, $V(\hat{q},\hat{p})=0$, $K^2=(\sigma^2-1)^2\times(\sigma^4+1)^{-1}$. It is of interest to note the energy uncertainty,

$$(\Delta\hat{H})^2=(\hbar\omega)^2[\tfrac{1}{2}(\sigma^2q_1^{\,2}+\sigma^{-2}p_1^{\,2})+\tfrac{1}{8}(\sigma^2-\sigma^{-2})^2].$$

We consider, as the classical analog, the Gaussian density

$$P(\tilde{q},\tilde{p})=\frac{1}{\pi K^2}\exp\left[-\frac{1}{K^2}\left(\frac{(\tilde{q}-q_1)^2}{\sigma^2}+\sigma^2(\tilde{p}-p_1)^2\right)\right].$$

This yields $\langle\tilde{q}\rangle=q_1$, $\langle\tilde{p}\rangle=p_1$, $(\Delta\tilde{q})^2=\frac{1}{2}K^2\sigma^2$, $(\Delta\tilde{p})^2=\frac{1}{2}K^2\sigma^{-2}$, $V(\tilde{q},\tilde{p})=0$, and the energy uncertainty is given by

$$(\Delta\tilde{H})^2=(\hbar\omega)^2[\tfrac{1}{2}K^2(\sigma^2q_1^{\,2}+\sigma^{-2}p_1^{\,2})+\tfrac{1}{8}K^4(\sigma^4+\sigma^{-4})].$$

It is seen that criteria (1) and (2) are satisfied. As in the case of energy states, we consider only specific examples related to criterion (3). One such example is the uncertainty in energy. Inspection shows $\Delta\tilde{H}<\Delta\hat{H}$. Other, particularly simple, examples are furnished by the functions q^m and p^m. Quantum mechanically, uncertainties in these functions are determined by the Gaussian densities $|\psi(q)|^2$ and $|\psi(p)|^2$, respectively, while classically, they are determined by the same densities narrowed by the factor K.

We discuss, now, mixed quantum states, which may be defined by an ensemble of pure quantum states, over which the average obtained from each pure state is again averaged for the final result.[6] Formally, the mixed state can be described by a diagonal density matrix, $\rho_{\text{mixed}}=\sum_i p_i\rho_i$, where $\rho_i=|\psi_i\rangle\langle\psi_i|$, the $|\psi_i\rangle$'s are an orthonormal set of states, and p_i is the probability of finding the system in the state $|\psi_i\rangle$. We follow exactly the same procedure with the classical analogs, and let the classical analog of the mixed state be $P(\tilde{q},\tilde{p})_{\text{mixed}}=\sum_i p_iP_i(\tilde{q},\tilde{p})$, where $P_i(\tilde{q},\tilde{p})$ is the classical analog of the state $|\psi_i\rangle$.

The description of mixed states by a diagonal density matrix in the representation of an orthogonal set of states has been extended to a description in a representation of coherent states, which are only approximately orthogonal, in a certain sense.[7] The density matrix in this "P representation" is given by

$$\rho=\int\int P(\alpha,\alpha^*)|\alpha\rangle\langle\alpha|d^2\alpha,$$

the integration being over the complex α plane. For $P(\alpha,\alpha^*)$ positive, this density matrix may be regarded as that of a mixed state. Its classical analog is described, in accordance with the above procedure and the fact that the classical analog of a coherent state is a δ function, by $P(\alpha,\alpha^*)$, with $\alpha=2^{-1/2}(\tilde{q}+i\tilde{p})$. In this connection, it is interesting to examine the mixed state for which $P(\alpha,\alpha^*)=(2\pi k)^{-1}\delta(|\alpha|-k)$, where k is a positive constant. This is a mixture of coherent states of energy expectation value $(k^2+\frac{1}{2})\hbar\omega$ and uniformly distributed phases. The analog is a microcanonical ensemble of energy $k^2\hbar\omega$, the same analog as that of an energy state if k^2 is integral. The resemblance of this state to an energy state should not be surprising, since the former is a stationary state with the same $\Delta\hat{q}$ and $\Delta\hat{p}$ as those of the latter, for $k^2=n$. However, $\Delta H=\hbar\omega k$ for the mixed state, while $\Delta H=0$, of course, for the energy state.

There exists a popular conception[8,9] that coherent states are more "classical" than other quantum states of the harmonic oscillator. In the light of the present discussion, reasonable measures of "classicality" and "quantum mechanicality" are given by C and Q, respectively, where $C=\langle\tilde{H}\rangle/\langle\hat{H}\rangle$ and $Q=(\langle\hat{H}\rangle-\langle\tilde{H}\rangle)/\langle\hat{H}\rangle$. One sees immediately that $C=1-\frac{1}{2}\hbar\omega/\langle\hat{H}\rangle$ and $Q=\frac{1}{2}\hbar\omega/\langle\hat{H}\rangle$, which is, essentially, a formulation of the correspondence principle. We conclude, therefore, that for a given $\langle\hat{H}\rangle$, all types of states are equally classical or equally quantum mechanical. In the present context, there exists no justification for considering coherent states to be more classical than other states; all pure states (of given

$\langle\hat{H}\rangle$) are equally "close" to their respective classical analogs.

The concept of "collapse of the wave packet" may be given plausible interpretation in light of the present ideas. Let a particle be in a given initial quantum state. If an ideal measurement is made of a dynamical variable of which the initial state is not an eigenstate, then the postmeasurement state will be the collapsed wave packet, an eigenstate of the variable measured. Looking at the classical analogs of both states, we see one probability distribution collapse into another on measurement. Now, such a change in a statistical ensemble is entirely consistent with classical probability theory, and represents a change of information. Thus, the collapse of the wave packet may be regarded as due to a combination of a change of information (as far as the classical statistics contained in the quantum description is concerned) and to a disturbance of the system (consistent with the minimal form of the uncertainty principle) inherent in an ideal quantum measurement.

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[1] J. E. Moyal, Proc. Cambridge Philos. Soc. 45, 99 (1949).

[2] D. Agmon and I. R. Senitzky, in *Statistical Physics—Statphys 13,* edited by D. Cabib, C. G. Kuper, and I. Riess (Hilger, Bristol, England, 1978), outline an earlier version of some of the present ideas.

[3] Criteria (1)–(3) are to be considered the *only* criteria, in the sense that all other information is to be minimized. It will be seen that for certain states these criteria are sufficient to determine a unique probability density. Whether they are sufficient for all states is an open question. However, the understanding that all other information must be minimized—that is, that the density be the most probable one consistent with the criteria—appears to assure uniqueness. See, for instance, Amnon Katz, *Principles of Statistical Mechanics* (Freeman, San Francisco, 1967), Chaps. II and IV.

[4] Since criteria (3) are the weakest set of conditions consistent with this fact, it is reasonable to conjecture that they permit the existence of a probability density. Existence in specific cases will be demonstrated; a general proof of existence has not yet been found.

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