WHEN DO POSITION AND MOMENTUM DISTRIBUTIONS DETERMINE THE QUANTUM MECHANICAL STATE?

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Received 6 January 1986; revised manuscript received 12 June 1986; accepted for publication 29 July 1986

The condition under which a measured quantum mechanical system is determined by distributions of observables are considered. Two given inequivalent states of the hamiltonian $H = p^2/2m + V(q)$, which have the same position and momentum distribution, serve as a basis for the argumentation.

Recently it was recognized that the standard, Copenhagen interpretation of quantum mechanics contains some unprovable and unnecessary "additions" to the formal apparatus of the theory which itself has turned out to be just a statistical elaboration of any yes–no measurement [1]. Such criticism accentuates some old questions: How does one determine the state of a system that has been prepared in some specified manner? How many physical observables completely determine the state of a system [2]? And what in this case does the state of a system mean [3]? As early as 1933 Pauli wrote: "The mathematical problem, as to whether for given probability densities, the wave function, if such function exists, is always uniquely determined, has still not been investigated in all its generality." [4]. Recently, the problem was reconsidered [3], and the result was obtained that in general such a function, called the "Pauli unique state", does not exist for given probability densities, i.e. observable distributions. It was proved that scattering states are not uniquely determined by their position and momentum distribution (the "Pauli non-unique states") while bound states of the hamiltonian $H = p^2/2m + V(q)$ are [3].

On the other hand, it can easily be checked that the two functions

$$\psi_1 = C \exp\left[-a(q-q_0)^2 + \mathrm{i} p_0(q-q_0)/\hbar\right],$$

and

$$\psi_2 = C \exp\left[-a^*(q-q_0)^2 + \mathrm{i} p_0(q-q_0)/\hbar\right],$$

where $\mathrm{Re}(a) > 0$, and $C = [2\,\mathrm{Re}(a)/\pi]^{1/4}$, have the same position and momentum distributions, simply by comparison of their real parts (which determine the value of the densities $\psi\psi^*$) and the real parts of the correspondent Fourier-transformed wave functions which, after elementary calculations, show up to be proportional to

$$\exp\left[-\mathrm{Re}(a)(p-p_0)^2/4\hbar\,|a|^2\right].$$

(Obviously, we obtain the same result using expressions for mean values: $\langle p\rangle_\psi = \langle\psi\,|\,\hat{p}\,|\,\psi\rangle = -\mathrm{i}\hbar\langle\psi\,|\,\partial/\partial q\,|\,\psi\rangle$, and the analogous one for the position operator with the Fourier-transformed functions.)

We shall prove that the functions ψ_1 and ψ_2 are linearly independent (i.e. inequivalent) by supposing the opposite. In this case they should be multiples of each other:

$$\psi_1 = c\psi_2 = c'\psi_1 \exp\left[2\mathrm{i}\,\mathrm{Im}(a)\left(q^2 - 2q_0 q\right)\right],$$

whence we get $q = \text{const.}$, which is in contradiction with q being a variable. So we conclude that ψ_1 and ψ_2 are mutually inequivalent. An analogous proof is valid for the Fourier-transformed functions.

Next, we are going to show that under very general physical assumptions our functions have the same distributions of the total energy operator $H = p^2/2m + V(q)$.

Let us first consider its kinetic part, whose mean values for ψ_1 and ψ_2 are the same:

$$\begin{aligned}\langle p^2\rangle_{\psi_1} &= -\hbar^2\langle\psi_1|\partial^2/\partial q^2|\psi_1\rangle \\ &= \hbar^2|a|^2/\mathrm{Re}(a) + p_0^2 \\ &= -\hbar^2\langle\psi_2|\partial^2/\partial q^2|\psi_2\rangle = \langle p^2\rangle_{\psi_2}.\end{aligned}$$

Notice the enlargement of the kinetic part of the energy which does not occur in the case of the real gaussian and which stems from the correlation between position and momentum established by the imaginary square terms within ψ_1 and ψ_2. In the corresponding Wigner phase space representation [5] densities are no longer circular but elliptic.

The potential part of the hamiltonian is a multiplication operator $\hat{V}\psi = V(q)\psi$. We suppose that $V(q)$ is a real, non-negative square integrable function. Its mean values are also the same:

$$\begin{aligned}\langle\hat{V}\rangle_{\psi_1} &= \int_{-\infty}^{+\infty}\psi_1^* V(q)\psi_1\,\mathrm{d}q \\ &= \int_{-\infty}^{+\infty}\exp\left[-\mathrm{Re}(a)(q-q_0)^2\right]V(q)\,\mathrm{d}q \\ &= \int_{-\infty}^{+\infty}\psi_2^* V(q)\psi_2\,\mathrm{d}q = \langle\hat{V}\rangle_{\psi_2}.\end{aligned}$$

We could easily generalize the obtained results for $\mathbb{R}^n$ as well as for any Borel subset of $\mathbb{R}^n$ but it would be of no use with the present reasoning.

Lastly, we stress that, given the above-proved inequivalence of ψ_1 and ψ_2, they cannot be observationally equivalent in general. In order to prove this claim one can be tempted to use a projector $\hat{P}$ on ψ_1 and ψ_2, defined so as to satisfy: $\langle\psi_2|\psi_1\rangle = \langle\psi_2|\hat{P}|\psi_2\rangle$, and try to show that: $\langle\hat{P}\rangle_{\psi_1} \neq \langle\hat{P}\rangle_{\psi_2}$ [#1]. However, we cannot do this because, though inequivalent, ψ_1 and ψ_2 are not orthogonal to each other,

$$\begin{aligned}\langle\psi_2|\psi_1\rangle &= \int_{-\infty}^{+\infty}\psi_2^*\psi_1\,\mathrm{d}q \\ &= \frac{\sqrt{|a|+\mathrm{Re}(a)} + \mathrm{i}\sqrt{|a|-\mathrm{Re}(a)}}{\sqrt{2|a|}} \\ &= \langle\psi_1|\psi_2\rangle^*.\end{aligned}$$

The proof can receive the following elaboration.

Since ψ_1 and ψ_2 are linearly independent there exist ψ^1 and ψ^2 which are biorthogonal to ψ_1 and ψ_2, i.e. which satisfy: $\langle\psi^i|\psi_j\rangle = \langle\psi_j|\psi^i\rangle = \delta^i_j$, $i, j = 1, 2$ [6], and we can define projectors on ψ^1 and ψ^2 as $\hat{P}_1 = |\psi^1\rangle\langle\psi_1|$, $\hat{P}_2 = |\psi^2\rangle\langle\psi_2|$. Thus, on the one hand we get

$$\begin{aligned}&\langle\hat{P}_1\rangle_{\psi_2} = \langle\psi_2|\hat{P}_1|\psi_2\rangle = \langle\psi_2|\psi^1\rangle\langle\psi_1|\psi_2\rangle = 0, \\ &\langle\hat{P}_2\rangle_{\psi_1} = \langle\psi_1|\hat{P}_2|\psi_1\rangle = 0,\end{aligned}$$

on the other hand it is

$$\langle\hat{P}_1\rangle_{\psi_1} = \langle\psi_1|\psi^1\rangle\langle\psi_1|\psi_1\rangle = \langle\hat{P}_2\rangle_{\psi_2} = 1.$$

Therefore:

$$\langle\hat{P}_1\rangle_{\psi_2} \neq \langle\hat{P}_1\rangle_{\psi_1}, \quad \langle\hat{P}_2\rangle_{\psi_1} \neq \langle\hat{P}_2\rangle_{\psi_2},$$

i.e. the projectors $\hat{P}_1$ and $\hat{P}_2$ do not give the same distribution for ψ_1 and ψ_2. The question of actual feasibility of the corresponding experiments is, however, beyond the scope of this paper.

Let us now remind ourselves of the afore-mentioned discrepancy between our result and those of others [3] according to which no bounded state of our hamiltonian could be represented by a complex gaussian. The limitation follows from the fact that the proof given in ref. [3] tacitly assumes that the uncertainty relation reaches its lower limit. This is the well-known "textbook requirement" that the gaussian be minimal, i.e. that it admits the minimal possible value of the uncertainty relation. Namely, if we require that the equality sign in the uncertainty relation is obtainable for a chosen state, then the coefficient a in our gaussian cannot be but real. Recalling, however, that there is only one idealized case, i.e. the harmonic oscillator, in which the uncertainty relation can gain its minimal value, we feel free to conclude that there is no proper physical reason which would force us to stick to the real gaussian, i.e. to the minimality

[#1] I gratefully acknowledge that the use of the projector $\hat{P}$ for the clarification on this point has been suggested by a referee of this journal.

requirement imposed on the uncertainty relation. Thus it seems that functions which do not satisfy the requirement, among them the complex gaussian, are worth investigating.

There is still one side which prompts such investigation. If we consider a quantum object restricted to a bounded region, a sharp clash between the individual and statistical uncertainty relations emerges (the former being infinite), no matter which suitable function we use to describe the object [7]. Therefore, what we need is a function which is properly defined in an unbounded region as well, i.e. which belongs to $\mathscr{L}_2(-\infty, +\infty)$. And it is well known that the commonly used function $\psi_0 = \exp(\mathrm{i}\, p_0 q/\hbar)$ does not belong to $\mathscr{L}_2(-\infty, +\infty)$ (because $\int_{-\infty}^{+\infty} \psi_0^* \psi_0 \, \mathrm{d}q \nless \infty$).

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