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On Wave Functions in Quantum Mechanics.

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SUMMARY - Some examples and considerations are presented to show that the possibility of determining a quantistic state s by means of the expectations of fundamental observables is doubtful.

PART 2

On Fundamental Observables and Quantistic States.

9. Introduction to Part 2.

Quantum mechanics—more precisely its foundations—can be improved by basing them on primitive notions that are more surely operative and on postulates that are better supported by experiments, as far as the reference to a physical model (involving e.g. electrons) allows. The present work aims at making a step in this direction by giving, in particular, some solutions to the problem considered at the

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outset of N. 1 (Part 1)—cf. the last part of footnote (1) in Part 3, N. 13.

In connection with this task it is of interest to consider Assumption 2.1 which substantially says that a state s of a quantal system $\mathfrak{S}$ (formed with n spinless pairwise distinguishable particles) is determined by the expected values $\mathcal{E}_s(\omega)$ in the usual *direct* sense, of all fundamental observables ω (for $\mathfrak{S}$) in the state s. Indeed it is to remark that on the one hand Assumption 2.1 seems to be often considered as true, while on the other hand

(i) *actual experiments are far from assuring the truth of Assumption* 2.1,

which fact is emphasized in the present work; furthermore the considerations presented in NN. 10, 11 support thesis (e) in N. 1, i.e. that

(ii) *Assumption* 2.1 *is probably false.*

Hence, to fulfil the task above we must help using that assumption, in particular when we define or characterize intuitively states and wave functions. Of course this induces some changes in these basic notions; more precisely the proofs of Theors 4.1 and 2.1 (N. 5) induce us, first, to characterize connex pure states by means of a certain system σ of position and momentum measurements, and then to extend this characterization to general pure states by means of a joinability property—cf. Post .5.1.

The task above will be fulfilled in Part 3 by the construction of an ariomatic theory $\mathcal{T}_1$ of quantum mechanics in hich wave functions are defined, Born's rule need not be postulated, and the fundamental proportionality theorem 2.1 is proved.

Now let us describe the content of Part 2 in more detail. In N. 10 we show by an explicit (admittedly easy) quantistic example that the usual statistical distribution for position and momentum does not determine its wave function up to a constant factor. This example, also used in turn to construct a certain example in N. 16 (Part 3) relevant for the notion of states, shows rigorously the validity of a quantistic analogue for a known indetermination in classical statistical mechanics. Still in N. 10 this indetermination is shown to be very high. This fact is used in N. 11 to support assertion (ii) above, i.e. thesis (e) in N. 1.

(1) We understand $p \cdot q = \sum_{h=1}^{N} p_h q_h$.

10. On a certain impossible characterization of states by the statistical distributions of position and momentum, from the quantistic and classical points of view.

The state of a classical system, $\mathfrak{S}_c$, can be determined by means of precise measurements of its position co-ordinates q_h and conjugate momenta p_h $(h = 1, \ldots, N)$. Then the following conjecture may appear natural: *the state s of the corresponding quantistic system* $\mathfrak{S}$ (N. 4) *is determined by the statistical distributions* $B \to \mathcal{E}_s[\chi_B(q)]$ *and* $B \to \mathcal{E}_s[\chi_B(p)]$ $(B \in \mathcal{B}_n)$, cf. N. 2 in Part 1.

As is usually done, we assume those distributions—which are Lebesgue measures—to have the respective densities $P(q)$ and $\pi(p)$. It is known that a statistical state s_c for the classical analogue $\mathfrak{S}_c$ of $\mathfrak{S}$ is not determined by the corresponding (classical) densities $P_c(q)$ and $\pi_c(p)$; but, if s_c is regular enough, it is determined by the probability density $\varrho(q, p)$ for the result of a simultaneous (precise) measurement of the q_h's and p_h's $(h = 1, \ldots, N)$.

By analogy with the classical theory one aspects the above conjecture to be false. Here we want to prove (rigorously) its falsity by a simple example—to be used also in N. 16—and to this aim we denote the Fourier transform (1) $h^{-N/2}\int_{\mathbf{R}^N} e^{-2\pi i \hbar^{-1} q\cdot p}\psi(q)\,dq$ of ψ by $\hat{\psi}$ or $\psi^\wedge$ and formulate the conjecture above as follows:

CONJECTURE (*to be disproved*). *If for the wave functions ψ and f*

$$(10.1) \qquad |\psi(q)| = |f(q)| \qquad \text{and} \qquad |\hat{\psi}(p)| = |\hat{f}(p)| \qquad \text{a.e.},$$

then ψ and f are proportional, i.e. $\psi = cf$ for some $c \in \mathbf{C}$.

We denote the complex conjugate of z $(\in \mathbf{C})$ by z^* and we first remember after von Neumann that, *for every* $\psi \in \mathcal{H}$ (2),

$$(10.2) \qquad \psi^{\wedge *} = (\psi^* o - I) \qquad \text{where} \qquad (\psi^* o - I)(q) = \psi^*(-q)\,.$$

(2) For the case of the reader we remark that (10.2) holds because, setting $\xi = -q$, for nearly all p we have $(h = 2\pi\hbar)$

$$h^{N/2}\psi^{\wedge *}(p) = \int_{\mathbf{R}^N} \exp\left[\frac{i}{\hbar} q\cdot p\right] \psi^*(q)\,\mathrm{d}q = \\ = \int_{\mathbf{R}^N} \exp\left[-\frac{i}{\hbar}\xi\cdot p\right] \psi^*(-\xi)\,d\xi = h^{N/2}(\psi^* o - I)^\wedge(p)\,.$$

There are infinitely many choices of the functions ψ and f above for which they *are* e.g. *twice continuously differentiable, have connex supports, and fulfil the conditions*

$$(10.3) \qquad \psi(q) = \pm\, \psi(-q) = r(q)\, e^{i\varphi(q)}\,, \qquad \varphi'(q) \not\equiv 0\,, \qquad f = \psi^*\,,$$

where $\varphi(q)$ *and* $r(q)$ *are real functions with the above regularity properties and* (10.3) *holds in the support* Supp (ψ) *of* ψ. It is natural to accept the following

ASSUMPTION 10.1. *Some of the above choices of* ψ *and* f *(possibly with compact supports) represent quantistic states.*

As a consequence we can prove the

THEOR 10.1. *The conjecture above is false in that some wave functions* ψ *and* f *of the kind above fulfil* (10.1) *and are not proportional.*

Indeed by Assumption 10.1 some wave functions ψ and f fulfil the condition above in italics involving (10.3), so that by $(10.3)_4$, $(10.1)_1$ holds. In addition by $(10.2)_2$ and $(10.3)_1$, $\psi^* o - I = \pm\, \psi^*$, so that $(10.2)_1$ becomes $\psi\,\hat{}^* = \pm\, \psi^*\,\hat{}$. Hence

$$|\psi^*\,\hat{}(p)| = |\psi\,\hat{}^*(p)| = |\psi\,\hat{}(p)|$$

which by $(10.3)_4$, yields $(10.1)_2$. By (10.3) we have $f = c\psi$ for no $c \in \boldsymbol{C}$. q.e.d.

* * *

For the afore-mentioned classical system $\mathfrak{S}_c$ we have

$$(10.4) \qquad P_c(q) = \int_{\mathbf{R}^N} \varrho(q, p)\, dp\,, \qquad \pi_c(p) = \int_{\mathbf{R}^N} \varrho(q, p)\, dq$$

and

$$(10.5) \qquad \int_{\mathbf{R}^{2N}} \varrho(q, p)\, dq\, dp = 1\,, \qquad \varrho(q, p) \geqslant 0 \qquad \text{a.e.}\,.$$

Hence

$$(10.6) \qquad \int_{\mathbf{R}^N} P_c(q)\, dq = 1 = \int_{\mathbf{R}^N} \pi_c(p)\, dp\,, \qquad P_c(q) \geqslant 0\,,\ \pi_c(p) \geqslant 0 \qquad \text{a.e.}\,.$$

If P_c and π_c are given and (10.6) holds, then (10.4), and hence (10.5), can be fulfilled—cf. e.g. [3], p. 129—by defining $\varrho(q, p)$ e.g. as follows:

$$\varrho(q, p) = P_c(q)\,\pi_c(p) \,. \tag{10.7}$$

It is useful to realize that the indetermination affecting the solution of (10.4) is very high.

THEOR. 10.2. *Let P_c and π_c be piece-wise continuous functions in $L^1(\mathbf{R}^N)$, that fulfil* (10.6); *and let Γ be the class of the piece-wise continuous functions $\tau(q, p)$ that fulfil conditions* (10.4) *in ϱ. Then Γ contains a family with infinitely many* (*continuous*) *parameters, i.e. Γ includes a manifold of infinite dimension.*

Indeed the function ϱ defined by (10.7) is piece-wise continuous, (10.5) holds, hence for some value (a, b) of (q, p) and some positive real numbers k and ε we have

$$\varrho(q, p) > k \text{ for } |q_h - a_h| < \varepsilon \text{ and } |p_h - b_h| \leqslant \varepsilon \;\; (h = 1, \dots, N) \,. \tag{10.8}$$

Ler c_r and γ_r be two arbitrary successions of real numbers for which

$$\sum_{r=1}^{\infty} c_r = 1 \,, \quad \sum_{r=1}^{\infty} \gamma_r = 1 \,, \quad c_r \geqslant 0 \,, \; \gamma_r \geqslant 0 \;\; (r = 1, 2, \dots) \,; \tag{10.9}$$

furthermore set

$$S_{rs}(q, p) = \prod_{h=1}^{N} \sin 2r\pi \frac{q_h - a_h}{\varepsilon} \sin 2s\pi \frac{p_h - b_h}{\varepsilon} \tag{10.10}$$

and

$$\sigma(q, p) = \begin{cases} k \sum_{r,s=1}^{\infty} c_r \gamma_s \varrho_{rs}(q, p) & \text{if } |q_h - a_h| \leqslant \varepsilon \geqslant |p_h - b_h| \;\; (h = 1, \dots, N) \,, \\ 0 & \text{otherwise} \,. \end{cases} \tag{10.11}$$

Then the series in (10.11) is absolutely convergent and—cf. (10.8)—

$$|\sigma(q, p)| \leqslant \varrho(q, p) \,, \qquad \int_{\mathbf{R}^N} \sigma(q, p)\, dp = 0 = \int_{\mathbf{R}^N} \sigma(q, p)\, dq \,. \tag{10.12}$$

Now we set

$$\tau(q, p) = \varrho(q, p) + \sigma(q, p) ,$$

so that by (10.12), $(10.5)_2$, and (10.4)

$$(10.14) \qquad \tau(q, p) \geqslant 0 , \quad \int_{\mathbf{R}^N} \tau(q, p)\, dp = P_c(q) , \quad \int_{\mathbf{R}^N} \tau(q, p)\, dq = \pi_c(p) ,$$

i.e. τ fulfils conditions (10.4) and $(10.5)_2$ in ϱ. The same can be said of condition $(10.5)_1$ in ϱ by $(10.14)_2$ and $(10.6)_1$. q.e.d.

11. Considerations of a negative kind on the problem of defining wave functions by means of surely fundamental observables.

Let Ω' be a subset of the class Ω of the observables of $\mathfrak{S}$ (at some instant τ) and let Ω'' be the set of the fundamental observables in Ω'. We say that ψ is an *Ω'-function* of the state s (for $\mathfrak{S}$ at τ) if for every $\omega \in \Omega''$

$$(11.1) \qquad \mathcal{E}_s[\chi_B(\omega)] = \langle \psi | E^\omega(B) \psi \rangle \qquad \text{for all } B \in \mathfrak{B}_1 ,$$

where E^ω is the spectral measure E^A of the self-adjoint operator $A = A_{(\omega)}$ representing ω. Obviously *the Ω'-functions are the Ω''-functions* (3).

Let us call the set Ω' ($\subseteq \Omega$) *determinative* (*weakly determinative*) if for every pure (pure connex) state s (N. 1) all Ω'-functions of s are mutually proportional, so that (Theor. 2.1) they are the wave functions of the same states s.

The set $\Omega_1 = \{Q_1, \ldots, Q_N\} = \{Q_i\}$ is obviously not even weakly determinative. The same holds for $\Omega_2 = \{Q_1, P_1, \ldots, Q_N, P_N\}$, as is shown by two suitable states ψ and $f = \psi^*$ considered in the first part of N. 10.

According to the aims of this work—cf. the problem at the outset of N. 1—it would be useful to find an at least weakly determinative class Ω' formed with observables that are surely fundamental—cf.

(3) By using the terminology in [2], p. 170, the Ω'-functions of a state s can be characterized as the wave functions of the states equivalent to s with respect to the closure S of the class of the operators $\chi_B(A)$ where A represents an observable in Ω'' and $B \in \mathfrak{B}_1$.

footnote (1) in Part 1. However this seems rather impossible by the following considerations. At least we are far from being able to proving the existence of such a determinaive class.

The second example in N. 10 shows that, for an arbitrary choice of our quantal system $\mathfrak{S}$, in classical statistical mechanics the analogue of the following quantistic condition (on $\mathfrak{S}$) holds:

The Ω_2-functions of some state s of $\mathfrak{S}$ are Ω_2-functions of infinitely many other states of $\mathfrak{S}$.

This may push people to think that (i) by analogy the above quantistic condition itself is true, and (ii) no finite (weakly) determinative subsets of Ω exist, in general. At this point it is natural to ask whether there are (infinite) determinative sets and whether they include the Jordan algebra Ω_3 generated by Ω_2; we mean the least set Ω_3 for which (*a*) $\Omega_2 \subseteq \Omega_3$ and (*b*) if $A, B \in \Omega_3$ and $\lambda \in \boldsymbol{C}$, then $A + B$, λA, and $A \circ B \in \Omega_3$ where

$$A \circ B = \tfrac{1}{4}(A + B)^2 - \tfrac{1}{4}(A - B)^2 . \tag{11.2}$$

It may be preferable to consider, instead of Ω_3, the Jordan algebra Ω_3' generated by the (infinite) set Ω_2':

$$\Omega_2' = \{E^A(B) : A \in \Omega_2, B \in \mathfrak{B}_1\} \tag{11.3}$$

in that Ω_2' (hence Ω_3') contains only bounded operators.

Since the Jordan product $A \circ B$ is commutative but not associative, and

$$2A \circ B^2 = AB^2 + B^2A , \quad 4(A \circ B) \circ B = 2A \circ B^2 + 2BAB , \tag{11.4}$$

if A and B do not commute, we generally have

$$A \circ B^2 - (A \circ B) \circ B = \tfrac{1}{4}(AB^2 + B^2A - 2BAB) \neq 0 . \tag{11.5}$$

Let us now remember the first point of Bohr's analysis of physical phenomena—cf. [3], vol. 1, p. 153: « no matter how far the phenomena trascend the scope of classical physics, their account must be expressed in classical terms ». In this connection we can remark that, on the one hand, the operators $A \circ B^2$ and $(A \circ B) \circ B$ are distinct, so that they express distinct observables; in spite of this, on the other hand for $A = Q_1$ and $B = P_1$ those operators must reasonably be regarded as representing the coinciding classical magnitudes $q_1 p_1^2$ and $(q_1 p_1) p_1$.

The considerations above push people to think that $q_1 p_1^2$ is not fundamental and the same holds for most polinomials in $q_1, p_1, \ldots$ $\ldots, q_N, p_N$. With some exceptions the values of these polinomials can be measured, according to classical physics, only through measurements of q_h and p_h $(h = 1, \ldots, N)$, and the same can be said of the functions $f(q_1, p_1, \ldots, q_N, p_N)$ of these magnitudes. This strengthens the point of view above and pushes us to extend it, i.e. to assert that *the whole set Ω of observables is not (weakly) determinative.* This implies the falsity of Assumption 2.1, i.e. thesis (*e*) in N. 1—cf. assertions (i) and (ii) in N. 9.

The intuitive considerations above, of a negative character, increase the interest of the Definition 16.1 of wave functions suggested by Theor 2.1 and carried out in NN. 13-16 (Part 3). However they are not essential for this interest, as we said in N. 1.)

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