YU ISSN 0015—3206
FZKAAA 20 (1) 59 (1988)

LETTER TO THE EDITOR

I. A POSSIBILITY TO FORMULATE QUANTUM MECHANICS IN TERMS OF THE PROBABILITY DENSITY FUNCTIONS IN PHASE SPACE

NURUDIN BIJEDIĆ and DRAGAN LALOVIĆ

Department of Mathematical Physics and Biophysics, Institute for Nuclear Sciences »Boris Kidrič« Vinča, 11001 Belgrade, POB 522, Yugoslavia

Received 23 February 1987

Revised manuscript received 1 July 1987

UDC 530.145

Original scientific paper

We show that all essential results of the non-relativistic quantum mechanics of one spinless particle can be expressed directly in terms of the probability density functions in the phase space. This is achieved by representing density matrix $\hat{\varrho}$, which corresponds to a state ψ of the Hilbert space, in the basis of minimal wave packets, and by using a special feature of this representation which hitherto has not been noticed and exploited.

The two essential aspects of the quantum mechanics, its statistical character and the uncertainty relations, in the existing formulation of the theory are taken into account only indirectly through the introduction of the Hilbert space. Neither the vectors nor the operators of the Hilbert space have direct physical meaning. In the present paper we show that in the case of one spinless particle, all essential results of the nonrelativistic quantum mechanics can be obtained within a theory formulated directly in terms of the probability density functions in the phase space. Here, we shall treat the case of one dimension, the generalization to higher dimensions being obvious.

Since in the theory that we are going to formulate the uncertainty relations can not be taken into account through the commutation relations (no Hilbert space in our theory), it is clear that they must be incorporated directly in the probability density function. For this reason it is natural to start with the density matrix $\hat{\varrho}$ of the ordinary quantum mechanics represented in a special basis which takes the uncertainty relations explicitly into account. The members of this basis are the well known »minimal packets«, extensively used by von Neumann[1)] in the treatment of simultaneous measurement of canonically conjugated variables. In the coordinate representation they have the following form (with $\hbar = 1$)

$$\langle q|Q\,P\rangle \equiv \psi_{Q,P}(q) = \left(\frac{b}{\pi}\right)^{1/4} \exp\left\{-\frac{b}{2}(q-Q)^2 + iqP\right\}. \qquad (1)$$

As pointed out by von Neumann, these functions form a complete set, though not orthogonal. The members of this set represent the states in which the average values and the dispersions of the position and the momentum are $Q, \sqrt{\frac{1}{2b}}$ and $P, \sqrt{\frac{b}{2}}$, respectively. The parameter b may take any positive value satisfying $0 < b < +\infty$. Every member of this set is a simultaneous eigenfunction of a pair of commuting operators (to each member there corresponds a particular pair), one of which simulates the position operator, and has the eigenvalue Q, and the other simulates the momentum operator, and has the eigenvalue P. This basis (which we shall call *phase space representation*) is the appropriate one for the description of the situations in which the position and the momentum of a particle are simultaneously measured, but with uncertainties which obey the position-momentum uncertainty relation and being minimal. Further on, such measurement we shall call ideal simultaneous measurement of the position and the momentum, or shortly, ideal measurement. In the phase space representation, matrix elements of the density matrix $\hat{\varrho}$ corresponding to a state ψ have the following form:

$$\langle Q'\,P'|\hat{\varrho}|\,Q\,P\rangle = 2\int dq\,dq'\,\psi^*(q+q')\,\psi(q-q')\exp\left\{-\frac{b}{2}(Q'-q+q')^2 - \right.$$

$$\left. -iP'(q-q') - \frac{b}{2}(Q-q-q')^2 + iP(q+q')\right\}. \qquad (2)$$

The domain of integrations extends over the whole range of the integration variables in all integrals. Note that these matrix elements depend, beside Q, P, Q' and P', also on the parameter b.

According to the probabilistic interpretation of the quantum mechanics, the diagonal matrix elements of the $\hat{\varrho}$ matrix give the probability density in Q and P, for the measurements in which the position and the momentum are simultaneously measured with uncertainties $\frac{1}{\sqrt{2b}}$ and $\sqrt{\frac{b}{2}}$, respectively. The off-diagonal matrix elements, in general, have no probabilistic interpretation (in the general case they are complex). Their role is to carry the part of the information about the state ψ which is not contained in the diagonal matrix elements. However, the phase space representation, which we here advocate, has a special feature which hitherto has (to our knowledge) passed unnoticed and unexploited. Namely, it can be shown that in this particular representation, the off-diagonal matrix elements carry no any new information about the state ψ which is not already contained in the diagonal matrix elements. Indeed, one can easily verify that in the phase space representation every off-diagonal matrix element of the $\hat{\varrho}$ matrix (corresponding to any vector ψ of the Hilbert space, without any further restriction on the $\hat{\varrho}$ matrix elements) can be expressed as a linear combination of the diagonal matrix elements in the following way:

$$\langle Q' P' | \hat{\varrho} | Q, P \rangle = F(Q, Q', P, P') \int \mathrm{d}Q_1 \, \mathrm{d}P_1 \, \mathrm{d}x \, \mathrm{d}y \, \langle Q_1 P_1 | \hat{\varrho} | Q_1 P_1 \rangle \cdot$$

$$\cdot \exp \left\{ \frac{b}{2} x (Q - Q') - \frac{1}{2b} y (P - P') + \frac{\mathrm{i}}{2} x (P + P' - 2P_1) + \right.$$

$$\left. + \frac{\mathrm{i}}{2} y (Q + Q' - 2Q_1) \right\} \tag{3}$$

where

$$F(Q, Q', P, P') = \frac{1}{4\pi^2} \exp \left\{ - \frac{b}{4} (Q - Q')^2 - \frac{1}{4b} (P - P')^2 + \right.$$

$$\left. + \frac{\mathrm{i}}{2} (Q + Q')(P - P') \right\}.$$

In the above integral the integration over Q_1 and P_1 should be performed first. Eq. (3) can be verified by straightforward calculation using for the $\hat{\varrho}$ matrix Eq. (2) Eq. (3) is new fundamental result, and due to its existence all the quantum mechanical relations and results can be expressed in terms of the diagonal matrix elements of the $\hat{\varrho}$ matrix (i. e., in terms of the probability density function) alone, so that we may forget about the Hilbert space. This is true as long as we are within the phase space representation, i. e., as long as we have no ambition to measure the position and the momentum of a particle exactly. But, of course, the situations in which the position or the momentum would be measured exactly (the existing quantum theory assumes that such measurements are possible, in principle at least) can not be treated within this representation (these situations would correspond to the values $b = +\infty$ and $b = 0$, and for these values of b the phase space representation has no sence), but within the coordinate or the momentum representations, and in these representations the relation analogous to Eq. (3) does not exist. The only possibility to avoid the Hilbert space is to invoke a new postulate which excludes the values $b = +\infty$ and $b = 0$. This new postulate, which shall be called *superquantum postulate* states that there are the smallest uncertainties l_0 and p_0 with which the position and the momentum, respectively, can be measured. The two universal constants l_0 and p_0 have dimensionalities of the length and the momentum, respectively, and they set the lower and the upper limits on the parameter b, $b_{max} = \frac{1}{l_0^2}$, $b_{min} = p_0^2$. Introducing the superquantum postulate we are now able to formulate a new nonrelativistic quantum mechanics of one spinless particle, entirely in terms of the probability density functions.

The essential formulas of quantum mechanics can be expressed in terms of the probability density functions in the following way (in what follows the diagonal and the off-diagonal matrix elements of the density matrix $\hat{\varrho}$ will be designated by $2\pi D_i(Q, P)$ and $2\pi N_i(Q', P'; Q, P)$, respectively; the index i refers to the i-the state of the system). The three fundamental relations of quantum mechanics, namely, the time evolution of a state, the eigenvalue equation, and the absolute square of the scalar product, we shall first express in terms of the $\hat{\varrho}$ matrix in the phase space representation.

1. Time evolution law

$$\frac{\mathrm{d}}{\mathrm{d}t} D_i(Q, P; t) = \frac{-\mathrm{i}}{2\pi} \int [\langle Q, P|\hat{H}|Q', P'\rangle N_i(Q', P'; Q, P) -$$

$$-N_i(Q, P; Q', P') \langle Q', P'|\hat{H}|Q, P\rangle] \,\mathrm{d}Q' \,\mathrm{d}P'. \tag{4}$$

A similar expression can be written for $\frac{\mathrm{d}}{\mathrm{d}t} N_i$ but we shall not need it.

2. Eigenvalue equation for an operator $\hat{A}$

$$\frac{1}{2\pi} \int \langle Q, P|\hat{A}|Q', P'\rangle N_i(Q', P'; Q, P) \,\mathrm{d}Q' \,\mathrm{d}P' = \lambda_i D_i(Q, P). \tag{5}$$

Again, a similar expression can be written with N_i on the right side, but we shall not need it.

3. Absolute square of the scalar product of the state vector $|\psi_i>$ and $|\psi_j>$

$$\int N_i(Q', P'; Q, P) N_j(Q, P; Q', P') \,\mathrm{d}Q \,\mathrm{d}P \,\mathrm{d}Q' \,\mathrm{d}P'. \tag{6}$$

By using Eq. (3), we can express the three fundamental relations (4)—(6) entirely in terms of the probability density functions $D_i(Q, P)$ in the following way.

1'. Time evolution law

$$\frac{\partial D(Q, P, t)}{\partial t} = \frac{1}{2\pi^3} \mathrm{Im} \, [\int \mathrm{d}Q_1 \,\mathrm{d}P_1 \,\mathrm{d}x \,\mathrm{d}y \,\mathrm{d}Q_1' \,\mathrm{d}P_1' \, H(Q_1', P_1') \, D(Q_1, P_1) \cdot$$

$$\cdot \exp\{-b(Q - Q_1')^2 - \frac{1}{b}(P - P_1')^2 + bx(Q - Q_1') - \frac{1}{b} y (P - P_1') +$$

$$+ \mathrm{i}x(P_1' - P_1) + \mathrm{i}y(Q_1' - Q_1)\}] \tag{7}$$

where Im means the imaginary part of the expression.

2′. *Eigenvalue equation*

$$\lambda D(Q, P) = \frac{1}{4\pi^3} \int \mathrm{d}Q_1\, \mathrm{d}P_1\, \mathrm{d}Q_1'\, \mathrm{d}P_1'\, \mathrm{d}x\, \mathrm{d}y\, A(Q_1', P_1')\, D(Q_1, P_1) \cdot$$

$$\cdot \exp\left\{-b(Q - Q_1')^2 - \frac{1}{b}(P - P_1')^2 + b\,x(Q - Q_1') - \frac{1}{b}y(P - P_1') + \right.$$

$$\left. + \mathrm{i}y(Q_1' - Q_1) + \mathrm{i}x(P_1' - P_1)\right\}. \tag{8}$$

3′. *Absolute square of the scalar product*

$$|\langle\psi_1 | \psi_2\rangle|^2 = \frac{1}{2\pi} \int \mathrm{d}Q_1\, \mathrm{d}P_1\, \mathrm{d}Q_1'\, \mathrm{d}P_1'\, \mathrm{d}x\, \mathrm{d}y\, D_1(Q_1, P_1)\, D_2(Q_1', P_1') \cdot$$

$$\cdot \exp\left\{\frac{b}{2}x^2 + \frac{1}{2b}y^2 - \mathrm{i}x(P_1 - P_1') - \mathrm{i}y(Q_1 - Q_1')\right\}. \tag{9}$$

Note that in Eqs. (7) and (8) the integrations over Q_1' and P_1' should be performed first and, also, in Eq. (9), the integrations over Q_1, P_1 and Q_1', P_1' should be performed first.

The function $H(Q, P)$ in (7) is the classical Hamiltonian while the function $A(Q, P)$ in (8) is the classical function of Q and P corresponding to the operator A according to the Weyl's prescription[2)].

From the very derivation of the relations (7)—(9) it is clear that the eigenvalues λ_i are identical to the eigenvalues of the operator $\hat{A}$ in the ordinary quantum mechanics, and are independent of the parameter b. Also, the quantity (9), which is numerically equivalent to the corresponding absolute square of the scalar product in ordinary quantum mechanics, is independent of the parameter b. Thus, the spectra and the transition probabilities in this new theory are identical to the corresponding quantities of the ordinary quantum mechanics. What here depends on b it is the probability density function $D_i(Q, P)$, and this is quite natural since b is an external parameter dictated by the experimental arrangements we are using for the simultaneous measurement of the position and the momentum. If we whish to compare the probability density functions of the present theory with those of the ordinary quantum mechanics, we must look at the marginal distributions $D_i(Q)$ and $D_i(P)$ given by

$$D_i(Q) = \int D_i(Q, P)\, \mathrm{d}P$$

$$D_i(P) = \int D_i(Q, P)\, \mathrm{d}Q.$$

It can be easily shown that

$$D_i(Q) = \sqrt{\frac{b}{\pi}} \int \mathrm{d}q\, |\psi_i(q)|^2 \exp\{-b(q - Q)^2\}$$

$$D_i(P) = \sqrt{\frac{1}{b\pi}} \int \mathrm{d}p\, |\Phi_i(p)|^2 \exp\left\{-\frac{1}{b}(p - P)^2\right\}$$

where $\psi_i(q)$ and $\Phi_i(p)$ are the wave functions of the i-th state in the coordinate and the momentum representations, respectively. The function $D_i(Q)$ will not differ much from $|\psi_i(q)|^2$, if this latter does not change much in intervals which are of the order of $\frac{1}{\sqrt{b}}$. A similar conclusion follows for $D_i(P)$.

Note, also, that in the present theory the (deterministic) laws of the classical mechanics come out simply as the relations among the average values. Indeed, it is easy to show that the Ehrenfest theorem[3] follows simply from Eq. (7).

Additional comparison of our approach to quantum mechanics is provided by calculating average values. Using Eq. (3) one can calculate the average of a function of the position and momentum operators in the quantum state i

$$\langle \hat{A}(\hat{q}, \hat{p})\rangle_i = \mathrm{Tr}\,[\hat{\varrho}\,\hat{A}(\hat{q}, \hat{p})] =$$

$$= \frac{1}{4\pi^3} \int \mathrm{d}Q\,\mathrm{d}P\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}Q_1'\,\mathrm{d}P_1'\,\mathrm{d}Q_1\,\mathrm{d}P_1\,A(Q_1', P_1')\,D_i(Q_1, P_1)\,\cdot$$

$$\cdot \exp\{-b(Q - Q_1')^2 - \frac{1}{b}(P - P_1')^2 + b\,x(Q - Q_1') - \frac{1}{b}y(P - P_1') +$$

$$+ \mathrm{i}y(Q_1' - Q_1) + \mathrm{i}x(P_1' - P_1)\}. \tag{10}$$

In the case $\hat{A}(\hat{q}, \hat{p}) = \hat{q}$ we have

$$\langle \hat{q}\rangle_i = \int Q\,D_i(Q, P)\,\mathrm{d}Q\,\mathrm{d}P \tag{11}$$

and for $\hat{A}(\hat{q}, \hat{p}) = \hat{p}$

$$\langle \hat{p}\rangle_i = \int P\,D_i(Q, P)\,\mathrm{d}Q\,\mathrm{d}P. \tag{12}$$

The results (11) and (12) are valid under the condition of differentiability and absolute integrability of $D_i(Q, P)$. Of course, the results (11) and (12) are expected results showing the consistency of our approach.

In the case of the customary Hamiltonian of the one particle quantum system in one dimension, $H(\hat{q}, \hat{p}) = \frac{1}{2m}\hat{p}^2 + \hat{V}(\hat{q})$, and if $\hat{V}(\hat{q})$ can be expanded in the power series, than Eq. (7) takes the form:

$$\frac{\partial D(Q, P, t)}{\partial t} = 2\,\mathrm{Im}\left[\frac{1}{2m}\left(-\frac{\mathrm{i}}{2}\frac{\partial}{\partial Q} + \frac{b}{2}\frac{\partial}{\partial P} + P\right)^2 + \right.$$

$$\left. + V\left(\frac{\mathrm{i}}{2}\frac{\partial}{\partial P} + \frac{1}{2b}\frac{\partial}{\partial Q} + Q\right)\right] D(Q, P, t) \tag{7'}$$

and Eq. (8) for $A(\hat{q}, \hat{p}) = H(\hat{q}, \hat{p})$ takes the form

$$E_t D_t(Q, P) = \left[\frac{1}{2m}\left(-\frac{i}{2}\frac{\partial}{\partial Q} + \frac{b}{2}\frac{\partial}{\partial P} + P\right)^2 + \right.$$
$$\left. + V\left(\frac{i}{2}\frac{\partial}{\partial P} + \frac{i}{2b}\frac{\partial}{\partial Q} + Q\right)\right] D_t(Q, P). \tag{8'}$$

In this case, Eqs. (7′) and (8′) reduce to partial differential equations.

For the stationary state, l. h. s. of (7′) equals zero, so, the stationary states of the one particle quantum system is determined by two equations:

$$\mathrm{Im}\left[\frac{1}{2m}\left(-\frac{i}{2}\frac{\partial}{\partial Q} + \frac{b}{2}\frac{\partial}{\partial P} + P\right)^2 + V\left(\frac{i}{2}\frac{\partial}{\partial P} + \frac{1}{2b}\frac{\partial}{\partial Q} + Q\right)\right] D(Q, P) = 0$$

$$\mathrm{Re}\left[\frac{1}{2m}\left(-\frac{i}{2}\frac{\partial}{\partial Q} + \frac{b}{2}\frac{\partial}{\partial P} + P\right)^2 + V\left(\frac{i}{2}\frac{\partial}{\partial P} + \frac{1}{2b}\frac{\partial}{\partial Q} + Q\right)\right] D(Q, P) =$$
$$= E\, D(Q, P). \tag{13}$$

At the end let us give a short comment concerning the constants l_0 and p_0. On the general grounds, one expects these constants to be very small, and at the present moment one can hardly envisage an experiment which would be able to test their existence and to fix their values. A natural candidate for l_0 could be Planck's length, but for p_0 there is no such natural candidate among the existing fundamental constants. One intriguing, albeit bizzar, possibility is to take for p_0 the inverse of the radius R_0 of the universe, if one takes seriously the present day belief that the universe is close and finite. But this would mean that p_0 actually is not a constant if the universe is expanding (or oscillating). The nonconstancy of p_0, however, would not have serious consequences on the properties of the atomic phenomena (and the subatomic, if the present theory can be generalized to comprise these phenomena) as long as R_0 is much greater then atomic radius.

The relation of our approach to Wigner's function approach[4] and to R. J. Glauber's coherent states approach[5] will be discussed in the next paper.

References

1) J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton, Princeton University Press, 1955);
2) H. Weyl, Z. Phys. **46** (1927) 1;
3) A. Messiah, *Mecanique Quantique,* Tom I, Dunod, Paris 1960;
4) M. Hillery, R. F. O' Connel, M. O. Scully and E. P. Wigner, Phys. Reports **106** (1984) 123;
5) R. J. Glauber, Phys. Rev. **731** (1963) 2766.

O MOGUĆNOSTI FORMULACIJE KVANTNE MEHANIKE POMOĆU FUNKCIJA GUSTINE VJEROVATNOĆE U FAZNOM PROSTORU

NURUDIN BIJEDIĆ i DRAGAN LALOVIĆ

Institut »Boris Kidrič«, Vinča, 11001 Beograd

UDK 530.145

Originalni znanstveni rad

Pokazano je da se svi bitni rezultati nerelativističke kvantne mehanike za jednu česticu bez spina mogu izraziti pomoću funkcija gustine vjerovatnoće u faznom prostoru. Ovo se postiže reprezentovanjem matrice gustine $\hat{\varrho}$ u reprezentaciji minimalnih talasnih paketa i uz korišćenje specijalne osobine te reprezentacije, koja je do sada ostala nezapažena i neiskorišćena.