On the Analogy Between Classical and Quantum Mechanics

P. A. M. DIRAC
St. John's College, Cambridge, England

THERE are two forms in which quantum mechanics may be expressed, based on Heisenberg's matrices and Schrödinger's wave functions respectively. The second of these is not connected very directly with classical mechanics. The first is in close analogy with classical mechanics, as it may be obtained from classical mechanics simply by making the variables of classical mechanics into non-commuting quantities satisfying the correct commutation relations. The development of this analogy has been greatly hampered by the mathematical methods available for working with non-commuting quantities being much weaker than those available for commuting quantities, owing to the fact that the only functions of non-commuting variables that one has been able to define are those expressible algebraically. The present paper will show how this difficulty can be avoided. In the case when the non-commuting quantities are observables, one can set up a theory of functions of them of almost the same degree of generality as the usual functions of commuting variables and one can use this theory to make closer the analogy between classical and quantum mechanics.

The non-commuting quantities of quantum mechanics are called observables when they are real (Hermitian or self-adjoint), and satisfy the condition of having sufficient eigenvectors to form a complete set, i.e., any of the vectors on which the non-commuting quantities operate can be expanded in terms of the eigenvectors. The latter condition enables one to define a general function of a single observable.[1] The method of this definition can be extended to provide functions of two non-commuting observables in the following way.

Consider two observables α and β. Let $f(ab)$ be any function of two real variables a and b which is defined whenever a is an eigenvalue of α and b is an eigenvalue of β. We can then give a meaning to $f(\alpha\beta)$. We first define the function $f(\alpha b)$ of the single observable α, involving b, an eigenvalue of β, as a parameter, by means of the equation

$$f(\alpha b)\,|\alpha'\rangle = f(\alpha' b)\,|\alpha'\rangle, \tag{1}$$

where $|\alpha'\rangle$ denotes an eigenvector of α belonging to the eigenvalue α'. We require Eq. (1) to hold for every eigenvector of α. It then fixes the result of $f(\alpha b)$ applied to a general vector $|X\rangle$, since this general vector can be expanded in terms the eigenvectors, and so it fixes the linear operator $f(\alpha b)$. We now define $f(\alpha\beta)$ by the equation

$$f(\alpha\beta)\,|\beta'\rangle = f(\alpha\beta')\,|\beta'\rangle, \tag{2}$$

where $|\beta'\rangle$ is any eigenvector of β belonging to the eigenvalue β', the right-hand side of (2) having a meaning from the fore-going definition of $f(\alpha b)$. Equation (2) holding for every eigenvector of β fixes the result of $f(\alpha\beta)$ applied to a general vector $|X\rangle$ and so fixes the linear operator $f(\alpha\beta)$.

In this way we can define a general function of two non-commuting observables α and β. However, *this definition is associated with an order for α and β*—we first define $f(\alpha b)$ and then use it to define $f(\alpha\beta)$. We could equally well use the reverse order, first defining $f(a\beta)$ and then using it to define $f(\alpha\beta)$. The resulting $f(\alpha\beta)$ would, in general, differ from the previous one. If α and β commute, the two $f(\alpha\beta)$'s are equal.

We may take a function $f(ab)$ consisting of a sum of terms, each of which is a function of a multiplied by a function of b, i.e.,

$$f(ab) = \sum_n u_n(a)v_n(b). \tag{3}$$

It is then easily seen that $f(\alpha\beta)$ defined by (1) and (2) is equal to the expression obtained by substituting α for a and β for b in the right-hand side of (3), the α-factor being always put to the left of the β factor, i.e.,

$$f(\alpha\beta) = \sum_n u_n(\alpha)v_n(\beta). \tag{4}$$

[1] See P. A. M. Dirac, *Principles of Quantum Mechanics*, second edition, §11.

Functions of non-commuting observables of this kind have been used by Jordan[2] for discussing contact transformations in quantum mechanics. They are called well-ordered functions. The method of Eqs. (1) and (2) thus provides a generalization of the concept of well-ordered functions, which does not require the use of the special algebraic form (4).

The method may readily be extended to provide a definition for a function $f(\alpha\beta\gamma\delta\cdots\zeta)$ of any number of non-commuting observables $\alpha, \beta, \gamma, \delta, \cdots\zeta$, where $f(abcd\cdots z)$ is a function of the real variables $a, b, c, d, \cdots z$ which is defined for $a, b, c, d, \cdots z$ eigenvalues of $\alpha, \beta, \gamma, \delta, \cdots\zeta$ respectively. We first define $f(\alpha bcd\cdots z)$ by

$$f(\alpha bcd\cdots z)\,|\,\alpha'\rangle = f(\alpha' bcd\cdots z)\,|\,\alpha'\rangle, \qquad (5)$$

then use this to define $f(\alpha\beta cd\cdots z)$ by

$$f(\alpha\beta cd\cdots z)\,|\,\beta'\rangle = f(\alpha\beta' cd\cdots z)\,|\,\beta'\rangle, \qquad (6)$$

and then use this to define $f(\alpha\beta\gamma d\cdots z)$ by

$$f(\alpha\beta\gamma d\cdots z)\,|\,\gamma'\rangle = f(\alpha\beta\gamma' d\cdots z)\,|\,\gamma'\rangle, \qquad (7)$$

and so on. We finish with a definition of $f(\alpha\beta\gamma\delta\cdots\zeta)$ associated with a certain order $\alpha, \beta, \gamma, \delta, \cdots\zeta$ of the observables concerned. It is easily seen that if some of the observables occupying consecutive positions in the order commute, one can change the order of these observables among themselves without affecting the function.

The observables that one uses in practice in Heisenberg's form of quantum mechanics are the values of dynamical variables at particular times. They fall into a natural linear order, namely the order of the times to which they refer. Our theory now enables us to set up general functions of them, based on this order. The functions must not involve two observables referring to exactly the same time, unless they commute. Apart from this limitation, the power of forming functions that we now have is just as general as in the classical theory.

If we are working with a relativistic theory, our observables will each refer to a certain point in space-time and they will no longer have a unique time order. However, observables referring to points in space-time lying outside each other's light-cones always commute with one another, so that the order of such observables in constructing functions does not matter. We may thus order our observables according to their times in some particular Lorentz frame, and functions defined relative to this order will be the same as those defined relative to the order of their times in a different Lorentz frame. The only limitation we now have is that the functions must not involve two non-commuting observables referring to exactly the same point in space-time.

In working with functions of non-commuting observables, care must be taken not to use ordinary algebraic procedures when they are not permissible for these functions. For example, if one is given an equation between observables, $A=B$, this does not in general allow one to substitute B for A in functions of A and other observables, since, if A and B contain observables referring to different times, such a substitution may spoil the order of the observables in the function.

APPLICATION TO PROBABILITIES

Take the function $f(abc\cdots)$ which is equal to unity when $a=\alpha', b=\beta', c=\gamma', \cdots$, ($\alpha', \beta', \gamma', \cdots$ being eigenvalues of the observables $\alpha, \beta, \gamma, \cdots$,) and which vanishes otherwise, and form the function $f(\alpha\beta\gamma\cdots)$. Let us evaluate the average of this function for the dynamical system in a certain state. If the state corresponds to the normalized vector $|X\rangle$ (a fixed vector in the Heisenberg scheme of quantum mechanics), and $\langle X|$ is the conjugate imaginary vector, then this average may be written as a scalar product

$$\langle X\,|\,f(\alpha\beta\gamma\cdots)\,|\,X\rangle. \qquad (8)$$

According to ordinary ideas of probability, expression (8) would be just the probability of α having the value α', β having the value β', γ having the value γ', and so on, for the state concerned. However, the number (8) is in general complex. Thus the theory allows one formally to give a value for the probability of non-commuting observables having specified numerical values, but this probability is in general a complex number, so it does not have an immediate physical application. All the same, if the probability is close to zero it can be interpreted as meaning that the observables $\alpha, \beta, \gamma, \cdots$ are unlikely to have the values $\alpha', \beta', \gamma', \cdots$, so there

[2] P. Jordan, Zeits. f. Physik **38**, 513 (1926).

is a limited application for it. If some of the observables α, β, γ, $\cdots$ have continuous ranges of eigenvalues, we should take $f(abc\cdots)$ to equal unity when the corresponding variables lie in small ranges, instead of when they have precise values, and so get the probability of those observables lying in small ranges.

We are now able to set up a formal probability for non-commuting observables to have specified values, subject to the limitation that there must not be two non-commuting observables referring to exactly the same time. This probability would give correctly the average value of any function of the observables by means of the formula

$$\text{average } f(\alpha\beta\gamma\cdots) = \text{sum or integral of } f(abc\cdots)P(abc\cdots), \quad (9)$$

P being the probability, provided the function is defined in accordance with our general definition, Eqs. (5)–(7). It would not, in general, give the correct average value for a function defined differently, for example, for a function defined by an algebraic formula in which the non-commuting observables are not properly ordered.

The possibility of setting up in quantum mechanics a probability for non-commuting observables to have specified values has been previously considered by J. E. Moyal.[3] Moyal obtained a probability for a coordinate q and a momentum p to have specified values at any time, which probability would give by Eq. (9) the correct average value for any quantity of the form $e^{i(aq+bp)}$, where a and b are real numbers. Moyal's probability is always real, though not always positive, and is thus one step more physical than the probability of the present paper, but its region of applicability is rather restricted, as it does not seem to be connected with a general theory of functions like the present one.

We can use the formal probability to set up a quantum picture rather close to the classical picture in which the coordinates q of a dynamical system have definite values at any time. We take a number of times t_1, t_2, t_3, $\cdots$ following closely one after another and set up the formal probability for the q's at each of these times lying within specified small ranges, this being permissible since the q's at any time all commute. We then get a formal probability for the trajectory of the system in quantum mechanics lying within certain limits. This enables us to speak of some trajectories being improbable and others being likely.

An analytical expression for this formal probability in terms of the transformation functions may be obtained in the following way. Denote by q_1 the q's at time t_1, by q_2 the q's at time t_2, and so on, and assume that the q's at any time form a complete set of commuting observables. Then there exists a representation whose basic vectors are $|q_1'\rangle$, $\langle q_1'|$, labelled by values for the q_1's, a second representation whose basic vectors are $|q_2'\rangle$, $\langle q_2'|$, labelled by values for the q_2's, and so on. Let us restrict ourselves to three times t_1, t_2, t_3 to save writing, so that we have only three sets of q's, namely q_1, q_2 and q_3. A general function of these q's is then defined, corresponding to (5)–(7), by

$$\begin{aligned} f(q_1q_2'q_3')\,|q_1'\rangle &= f(q_1'q_2'q_3')\,|q_1'\rangle, \\ f(q_1q_2q_3')\,|q_2'\rangle &= f(q_1q_2'q_3')\,|q_2'\rangle, \\ f(q_1q_2q_3)\,|q_3'\rangle &= f(q_1q_2q_3')\,|q_3'\rangle. \end{aligned}$$

Thus for any vector $|X\rangle$,

$$\begin{aligned} &f(q_1q_2q_3)\,|X\rangle \\ &= \int f(q_1q_2q_3)\,|q_3'\rangle dq_3'\langle q_3'|X\rangle \\ &= \int f(q_1q_2q_3')\,|q_3'\rangle dq_3'\langle q_3'|X\rangle \\ &= \int\int f(q_1q_2q_3')\,|q_2'\rangle \\ &\qquad \times dq_2'\langle q_2'|q_3'\rangle dq_3'\langle q_3'|X\rangle \\ &= \int\int f(q_1q_2'q_3')\,|q_2'\rangle \\ &\qquad \times dq_2'\langle q_2'|q_3'\rangle dq_3'\langle q_3'|X\rangle \\ &= \int\int\int f(q_1q_2'q_3')\,|q_1'\rangle dq_1'\langle q_1'|q_2'\rangle \\ &\qquad \times dq_2'\langle q_2'|q_3'\rangle dq_3'\langle q_3'|X\rangle \\ &= \int\int\int f(q_1'q_2'q_3')\,|q_1'\rangle dq_1'\langle q_1'|q_2'\rangle \\ &\qquad \times dq_2'\langle q_2'|q_3'\rangle dq_3'\langle q_3'|X\rangle. \end{aligned} \quad (10)$$

If $|X\rangle$ is normalized, the average value of $f(q_1q_2q_3)$ for the state corresponding to it is

$$\langle X|f(q_1q_2q_3)|X\rangle = \int\int\int f(q_1'q_2'q_3')\langle X|q_1'\rangle \times dq_1'\langle q_1'|q_2'\rangle dq_2'\langle q_2'|q_3'\rangle dq_3'\langle q_3'|X\rangle.$$

[3] This work is not yet published. I am indebted to J. E. Moyal for letting me see the manuscript.

Taking f to equal unity for the q_1's in the ranges q_1' to $q_1'+dq_1'$, the q_2's in the ranges q_2' to $q_2'+dq_2'$ and the q_3's in the ranges q_3' to $q_3'+dq_3'$, and zero otherwise, we get

$$\langle X|f|X\rangle=\langle X|q_1'\rangle dq_1'\langle q_1'|q_2'\rangle \times dq_2'\langle q_2'|q_3'\rangle dq_3'\langle q_3'|X\rangle. \quad (11)$$

This is the probability of the q_1's, q_2's, q_3's lying in the ranges q_1' to $q_1'+dq_1'$, q_2' to $q_2'+dq_2'$, q_3' to $q_3'+dq_3'$, respectively. The extension of this result to the case of more than three times is obvious. The extension to the case when the q's do not form a complete set of commuting observables (owing, say, to the presence of spin variables), is also obvious, as one has only to insert the necessary extra variables in the transformation functions and sum or integrate over them.

The theory provides us with a rather more definite picture of the motion of a particle in quantum mechanics than we had previously. For example in a relativistic theory, if the time intervals are very short, the transformation functions $\langle q_r'|q_{r+1}'\rangle$ are very small unless the difference between q_r' and q_{r+1}' corresponds to the particle having moved with the velocity of light during the time interval t_r to t_{r+1}. Thus we see that the probability is very small for the particle to move in any way except along a sequence of straight paths with the velocity of light all the time. A closer investigation shows that the duration of these straight paths is likely to be of the order of magnitude of the period of oscillation of the de Broglie waves associated with the particle. These results hold both for a particle with a spin like an electron and for a non-spinning Klein-Gordon particle.

APPLICATION TO CONTACT TRANSFORMATIONS

The similarity between classical and quantum contact transformations has already been shown by Jordan and by the author.[4] The present methods enable one to establish this similarity on a more general basis.

Consider two sets of coordinates, q's and Q's say, for a system in quantum mechanics describable in terms of coordinates and conjugate momenta (i.e., no spins), and suppose the q's refer to one time and the Q's to a later time. We can now set up general functions of the q's and Q's. The question arises whether every dynamical variable can be expressed as such a function or not.

From the method that led to Eq. (10) we find that any function $f(qQ)$ of the q's and Q's is represented in the mixed $q-Q$ representation by

$$\langle q'|f(qQ)|Q'\rangle=f(q'Q')\langle q'|Q'\rangle. \quad (12)$$

If a dynamical variable α can be expressed as a function of the q's and Q's, its representative $\langle q'|\alpha|Q'\rangle$ must be of the form of the right-hand side of (12). Now for a general dynamical variable $\langle q'|\alpha|Q'\rangle$ is an arbitrary function of the q''s and Q''s, and the condition that it shall always be expressible in the form of the right-hand side of (12) is that $\langle q'|Q'\rangle$ shall not vanish for any values of the q''s and Q''s in the domains of these variables. This is then the condition that every dynamical variable can be expressed as a function of the q's and Q's.

Assuming this condition is fulfilled, define the function $S(q'Q')$ by

$$\langle q'|Q'\rangle=\exp(iS(q'Q')/\hbar).$$

Then

$$\langle q'|p_r|Q'\rangle=-i\hbar\frac{\partial}{\partial q_r'}\langle q'|Q'\rangle=\frac{\partial S(q'Q')}{\partial q_r'}\langle q'|Q'\rangle$$

$$=\left\langle q'\left|\frac{\partial S(qQ)}{\partial q_r}\right|Q'\right\rangle$$

from (12). Thus

$$p_r=\frac{\partial S(qQ)}{\partial q_r}. \quad (13)$$

Similarly

$$\langle q'|P_r|Q'\rangle=i\hbar\frac{\partial}{\partial Q_r'}\langle q'|Q'\rangle=-\frac{\partial S(q'Q')}{\partial Q_r'}\langle q'|Q'\rangle$$

$$=-\left\langle q'\left|\frac{\partial S(qQ)}{\partial Q_r}\right|Q'\right\rangle,$$

so that

$$P_r=-\frac{\partial S(qQ)}{\partial Q_r}. \quad (14)$$

Equations (13) and (14) are of the same form as the classical equations of a contact transformation in the case when every dynamical variable can be expressed as a function of the q's and Q's. However $S(q'Q')$ is not in general a real

[4] P. Jordan, see reference 2; P. A. M. Dirac, reference 1, §30.

function of the q''s and Q''s, so the analogy is not perfect.

In the case when $\langle q'|Q'\rangle$ vanishes for some values of the q''s and Q''s, we can choose a function $F(q'Q')$ which vanishes everywhere except where $\langle q'|Q'\rangle$ vanishes, and then

$$F(q'Q')\langle q'|Q'\rangle=0$$

everywhere. Equation (12) now shows that

$$F(qQ)=0$$

so that we have a connection between the q's and the Q's. There may be several independent connections like this, say

$$F_1(qQ)=0,\ F_2(qQ)=0,\ \cdots F_u(qQ)=0. \quad (15)$$

If the functions $F_n(q'Q')$, $(n=1, 2, \cdots u)$ are all algebraic functions of the q''s, Q''s, we can again set up an analogy with classical contact transformations. $\langle q'|Q'\rangle$ must now be of the form

$$\langle q'|Q'\rangle=X(q'Q')\delta(F_1)\delta(F_2)\cdots\delta(F_u).$$

Defining $S(q'Q')$ now by

$$X(q'Q')=\exp(iS(q'Q')/\hbar),$$

we have

$$\langle q'|p_r|Q'\rangle=-i\hbar\frac{\partial}{\partial q_r'}\langle q'|Q'\rangle$$
$$=\frac{\partial S}{\partial q_r'}\langle q'|Q'\rangle-i\hbar X\sum_n\delta(F_1)$$
$$\times\delta(F_2)\cdots\delta(F_{n-1})\delta'(F_n)$$
$$\times\delta(F_{n+1})\cdots\delta(F_u)\frac{\partial F_n}{\partial q_r'}.$$

Let λ_n be the dynamical variable whose representative is

$$\langle q'|\lambda_n|Q'\rangle=-i\hbar X\delta(F_1)\delta(F_2)\cdots$$
$$\times\delta(F_{n-1})\delta'(F_n)\delta(F_{n+1})\cdots\delta(F_u).$$

Then we have

$$p_r=\frac{\partial S(qQ)}{\partial q_r}+\sum_n\left\{\lambda_n\frac{\partial F_n(qQ)}{\partial q_r}\right\}, \quad (16)$$

where $\{\lambda_n\partial F_n(qQ)/\partial q_r\}$ denotes, not the product of λ_n on the left with $\partial F_n(qQ)/\partial q_r$ on the right, but a function of the non-commuting observables, the q's, λ_n, and the Q's in that order, i.e., with λ_n in the middle. Similarly

$$P_r=-\frac{\partial S(qQ)}{\partial Q_r}-\sum_n\left\{\lambda_n\frac{\partial F_n(qQ)}{\partial Q_r}\right\}. \quad (17)$$

Equations (16) and (17) are of the same form as the classical equations of a contact transformation in the case when the q's and Q's are connected by the Eqs. (15). Equations (16) and (17) involve the dynamical variables λ_n, which are not expressible in terms of the q's and Q's, and which in the quantum theory must occur in the middle position between the q's and Q's.

SUMMARY

A method is given for defining general functions of non-commuting observables in quantum mechanics, with a certain limitation. The method is developed to provide a formal probability for non-commuting observables to have numerical values. This probability turns out to be in general a complex number, but all the same it has some physical meaning, since when it is close to zero one can say that the numerical values are unlikely.

The method enables one to discuss trajectories for the motion of a particle in quantum mechanics and thus makes quantum mechanics more closely resemble classical mechanics. The method also enables one to set up the analogy between classical and quantum contact transformations on a more general basis.