OPERATOR CALCULUS AND THE SOLUTION OF THE EQUATIONS OF QUANTUM DYNAMICS

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Abstract

A formal calculus is developed which includes the Born and Jordan matrix dynamics, and also the remarkable quantum condition of Schroedinger. A method for the calculation of the matrices which is in close analogy to the classical Hamilton-Jacobi method of solving dynamical problems is explained. These results have been obtained independently by E. Schroedinger [Ann. d. Physik. **79**, 734 (1926)].

The recent advances in quantum dynamics made by Heisenberg[1], Born and Jordan,[2] Dirac,[3] and most recently, by Schroedinger,[4] have lead to various mathematical formulations of the various physical hypotheses involved. In the present paper it is proposed to give a unified mathematical treatment, which, though it cannot pretend to be the final form of the theory, leads to methods of solution of the equations of Born and Jordan, and Dirac which are much simpler than those previously developed. Very little attempt to justify the mathematical steps by physical hypothesis will be made. The final achievement will be the inclusion of the results of Schroedinger in a single calculus with those of the other authors mentioned above. This would seem to be the strongest support which either of the two widely dissimilar theories have thus far received.

I. The Operator Calculus in the Classical Theory

Let q and f be numerical quantities[5] and qf their product. This product may be said to result from the action of the operator $[q\times]$ on f. For simplicity of notation we shall denote $[q\times]$ by the single symbol Q. This operator is not identical with q, e.g., the operation of multiplying by two is not identical with the integer 2. However, just as the result of multiplying the integer 1 by two is the integer 2, so in general the result of applying

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[1] Heisenberg, Zeits. f. Physik. **33**, 879 (1925).

[2] Born and Jordan, Zeits. f. Physik. **34**, 858 (1925).

[3] Dirac, Proc. Roy. Soc. A**109**, 642 (1925); A**110**, 561 (1926).

[4] Schroedinger, Ann. d. Physik. **79**, 361 (1926).

[5] Throughout this paper, the term numerical quantity will be used to distinguish between the quantities of the classical physical theories, and those appearing in the generalized calculus about to be developed. These latter quantities will be called, "operators," The numerical quantities will be denoted by lower case letters, while upper case will be used for the operators.

the operator Q to the integer 1 will be q; this may be expressed by the equation $Q1=q$.

To avoid lengthy explanations of the significance of equations it may be remarked that throughout Part I, the sense of any equation will become obvious if symbols such as Q,P or X are read as the "operation of multiplying by the numerical quantity q,p or x."

It is possible to define the addition and multiplication of operators. The equations

$$(Q+X)1=(X+Q)1=q+x$$
$$QX1=XQ1=qx$$

are sufficient for this. Similarly, the symbolism Q^n may be given a meaning, and from this a large class of functions of operators may be built up.

Beside the operation of multiplication, the operation of differentiation, d/dx, plays an important role in analytic theory. Its relations with the operators already defined must be investigated. Let $q=q(x)$; then the operator Q is a function of the operator $X: Q=Q(X)$. This definition is identical with the previous definition of a function of an operator, but will not as readily permit of generalization. The result of the operation of Q on an arbitrary function $f(x)$ is

$$Qf=qf$$

If we follow the operation Q by the operation d/dx, the result is

$$\frac{d}{dx}(Qf)=\frac{dq}{dx}f+q\frac{df}{dx}=\left[\frac{dq}{dx}\times\right]f+Q\frac{df}{dx}$$

Since f is entirely arbitrary, it may be omitted from the equations and the result, written in operator form, is

$$\frac{d}{dx}Q-Q\frac{d}{dx}=\left[\frac{dq}{dx}\times\right]=\frac{dQ}{dX} \tag{1}$$

The symbol dQ/dX which is defined by this equation is read "the operation of multiplying by dq/dx." This interpretation makes it unnecessary to prove that

$$\frac{d(QP)}{dX}=\frac{dQ}{dX}P+Q\frac{dP}{dX}$$

though such a proof could readily be constructed, and will be given when the present simple interpretation is abandoned in the next section.

If the $2n$ quantities q_i and p_i satisfy the equations

$$\frac{dp_i}{dt}=-\frac{\partial H}{\partial q_i} \qquad \frac{dq_i}{dt}=\frac{\partial H}{\partial p_i} \tag{2}$$

it is fairly obvious that the corresponding operator equations are

$$\frac{dP_i}{dT} = -\frac{\partial H(PQ)}{\partial Q_i} \qquad \frac{dQ_i}{dT} = \frac{\partial H(PQ)}{\partial P_i} \tag{3}$$

Expressed in words, the first equation reads "the operation of multiplying by dp_i/dt is equivalent to the operation of multiplying by $-\partial H/\partial q_i$."

In translating ordinary equations into operator notation, nothing new is introduced. The translation involves merely a change of mental focus. Instead of concentrating the attention on the numerical quantities, it is directed to the operations of combining them. Since the great problem of the quantum theory seems to be to find new methods of computation, new operations of combining numerical quantities, it may be supposed that this change of view-point will be of value in the development of the theory. This value may be purely heuristic, and it may be possible to reduce the equations finally obtained to ordinary differential equations, or at least, to equations involving only the ordinary mathematical operations with which we are already familiar. It is also conceivable, though not probable, that this will not be possible. If this should be the case, it will not mean that the fundamental entities of the mathematical theory will be other than ordinary numbers. The operators (we shall see later that matrices may be regarded as operators) will be secondary entities in the same sense that the operations of multiplication and addition are secondary to the numbers of arithmetic.

We might now proceed to consider operations of a more general class than those considered above. It seems preferable, however, to give a short discussion of the methods of solving the operator equations which have already been defined. The simplest way, but the least instructive, would be to translate them directly into ordinary equations and solve these. In order to illustrate the new point of view, the equation

$$\frac{d^2Q}{dT^2} + \omega^2 Q = 0 \tag{4}$$

will be solved by a less direct method. From Eq. (1) it follows that this equation may also be written

$$\frac{d^2}{dt^2}Q - 2\frac{d}{dt}Q\frac{d}{dt} + Q\frac{d^2}{dt^2} + \omega^2 Q = 0 \tag{4a}$$

The problem is to find a function $q(t)$ such that

$$\frac{d^2}{dt^2}(qf) - 2\frac{d}{dt}\left(q\frac{df}{dt}\right) + q\frac{d^2f}{dt^2} + \omega^2 qf = 0 \tag{4b}$$

for any choice of the function $f(t)$. If the operations indicated in (4b) are carried out, it reduces to

$$f\left(\frac{d^2q}{dt^2}+\omega^2 q\right)=0 \tag{5}$$

which, since f is certainly not always zero, reduces in turn to

$$\frac{d^2q}{dt^2}+\omega^2 q=0 \tag{6}$$

which is the result which would have been obtained if the more direct method of solution had been used.

There is yet anothei problem related to the previous one, as will presently be apparent. In the Eq. (4a), the operator d/dt may be replaced by the operator $\vartheta=\vartheta[q,(d/dq)]$. The problem is then to find the operator ϑ such that

$$\vartheta^2 q\phi-2\vartheta q\vartheta\phi+q\vartheta^2\phi+\omega^2 q\phi=0 \tag{7}$$

is an identity in $\phi(q)$. Without entering into the general theory, we try

$$\vartheta=\frac{\sigma S}{\sigma q}\frac{d}{dq}$$

where S is a function of q which is to be determined so that Eq. (7) is satisfied. If this value of ϑ is substituted into (7) it becomes on simplification

$$\phi\cdot\left\{\frac{dS}{dq}\frac{d^2S}{dq^2}+\omega^2 q\right\}=0. \tag{8}$$

which is satisfied for all ϕ provided that

$$\frac{1}{2}\left(\frac{dS}{dq}\right)^2+\omega^2 q=W=\text{const.} \tag{8a}$$

This is none other than the Hamilton-Jacobi equation corresponding to Eq. (4), and it is known that the solution of the original problem connected with (4) can be reduced to the solution of

$$\frac{dq}{dt}=\frac{dS}{dq}$$

when S has been determined. The operator calculus thus leads to a new conception of the Hamilton-Jacobi theory of the solution of the equations of dynamics.

II. The Generalization of the Operator Calculus

The definition of an operator will now be generalized; the notation Qf will henceforth be interpreted to represent the result of any general way of combining the numerical quantities q and f, subject only to the restriction that $Q(f+g)=Qf+Qg$. In more usual language, Qf is a function of q and f, and perhaps also of their derivatives with respect to any independent variable of which they may be functions. Since f is entirely arbitrary, it may again be suppressed in the equations to be derived, making them operator equations in the sense already explained.

In the previous section, because of the interpretation given Q as the simple operation of multiplication by q, the multiplication of operators obeyed the commutative law $QP=PQ$. In a more general calculus, this law will not in general be valid; for Q might be $[q\times]$, while P might be d/dq, and these operations are certainly not commutative.

The operator d/dx loses its utility in the generalized calculus (though not its existence nor its significance). It is possible to define another operator by the relation

$$D_x X - X D_x = [1\times] \tag{9}$$

which will replace it. The solution of equations of this type for D_X in terms of X must be considered as one of the fundamental problems of operator theory. We assume the existence of a solution in all cases, though this must be proven.

If Q is a function of X, in the sense that its operation is the equivalent of a series of operations involving the operation X one or more times, the operation defined by

$$\frac{dQ}{dX} = D_x Q - Q D_x \tag{10}$$

will play a part in the solution of operator equations which is entirely analogous to that played by dq/dx in the solution of ordinary equations.[6] The laws of operation of d/dX are:

$$\begin{aligned} \frac{d}{dX}(Q+P) &= \frac{dQ}{dX} + \frac{dP}{dX} \\ \frac{d}{dX}(QP) &= \frac{dQ}{dX}P + Q\frac{dP}{dX} \end{aligned} \tag{11}$$

The proof of the first is obvious. The second also follows from the definition:

$$\frac{d}{dX}(QP) = D_x QP - QPD_x$$

[6] Cf. the references to Born and Jordan, and Dirac already cited. Also S. Pincherle, Funktionaloperationen und -gleichungen Enc, Math. Wiss. II A 11, or Équations et opérations fonctionelles, Enc. sciences math., II vol. 5, fasc. 1.

$$\begin{aligned}&= D_xQP-QD_xP+QD_xP-QPD_x\\&= (D_xQ-QD_x)P+Q(D_xP+PD_x)\\&= \frac{dQ}{dX}P+Q\frac{dP}{dX}\end{aligned}$$

In this last equation, the order in which Q and P are written must be preserved. From this remark it follows that there will be no rule analogous to the rule for the differentiation of a function of a numerical quantity.

If we are concerned with functions of more than one variable, say $Q_1 \cdots Q_n$, the operations analogous to partial differentiation are defined by the relations

$$D_jQ_i-Q_iD_j=[\delta_{ij}\times] \tag{12}$$

where the numbers δ_{ij} are zero when $i\neq j$, and unity when $i=j$. The compound operators $\partial/\partial Q_j$ defined by

$$\frac{\partial F}{\partial Q_j}=D_jF-FD_j \tag{13}$$

are then quite analogous to the operations denoted by the same symbol in Part I. It must again be remarked that the non-commutativity of multiplication prevents the expression of the total derivative in terms of the partials.

Before proceeding to a discussion of the quantum theory, the significance of the modified operation of multiplication must be considered. The validity of $2\times 2=4$ can certainly not be called into question. The generalized multiplication is perhaps more closely analogous to vector than to arithmetic multiplication. The operators are compound, built up from the elementary arithmetic operations of multiplication and addition in an undetermined manner. In the terminology which has been developed above, they are functions of the arithmetic operations. The problem of the quantum theory is to determine these functions of the simple operations so that the solution of the Hamiltonian equations represents the observed phenomena.

A special example, having no direct application to the present subject will serve to make this clear. The velocities of two bodies relative to an observer on a third are readily measured. So is the velocity of one of them relative to the other. According to pre-relativity kinematics, the three velocities are related (provided they all have the same direction) by the formula

$$v_{13}=v_{12}+v_{23} \tag{14}$$

where v_{12} is the velocity of the body 1 relative to the body 2, etc. The sign $+$ represents the ordinary arithmetic operation of addition. This formula, however, is found to be too simple to represent the observational data accurately, and is replaced by a more elaborate one:

$$v_{13} = \frac{v_{12} + v_{23}}{1 + \dfrac{v_{12} \cdot v_{23}}{c^2}}$$

This is the usual way of stating the modification which kinematics has undergone. An exponent of the operator calculus might prefer to state it in another way, saying that the Eq. (14) has not been altered, but that the sign $+$ no longer represents the arithmetic operation of addition. Fundamentally, neither statement is preferable to the other. Neither results in simpler numerical computations than the other, and both would lead to the same numbers v_{13}.

The operator calculus developed above is merely a logical application of the same ideas to the operation of multiplication. A special case of it might have been developed by changing the significance of the sign $\times$. Such a calculus, having a definite geometrical interpretation, is vector analysis. By associating with each numerical quantity its own operation of multiplication, however, we have obtained a more general calculus.

III. Quantum Dynamics

The equations of the new mechanics have been developed by Born and Jordan on a frankly empirical basis. Their discovery was not entirely a matter of chance, however, but was accomplished by the aid of a principle which has been most clearly stated by Dirac: in seeking for the new equations, the classical equations are to be retained formally without alteration. Only the operations by which the quantities involved are combined are to be altered. In order to obtain the necessary freedom to alter the operation of multiplication, the "quantities involved" were first interpreted as matrices. Then it was shown by Born and Wiener[7] that the matrices were closely related to a special form of operator, and that the operator calculus furnished a means of calculating the matrices. The present paper is the application of a general operator calculus to the same problem. The significance of the operators is suggested by the remarks at the end of the last section. It does not seem worth the trouble to pursue any more detailed speculations at this time.

Let P_j and Q_j be the operators which correspond to the classical $[p_j\times]$ and $[q_j\times]$, where p_j and q_j are the momenta and coordinates of a dynamical system. The first relation existing between the classical analogues to P_j and Q_j is the commutation law of multiplication. Accord-

[7] Born and Wiener, Zeits. f. Physik. **36,** 174 (1926).

ing to the results of Heisenberg, the corresponding relations in the new mechanics are

$$
\begin{aligned}
&P_iQ_j - Q_jP_i = \left[\frac{h}{2\pi i}\delta_{ij}\times\right] \\
&Q_iQ_j - Q_jQ_i = 0 \\
&P_iP_j - P_jP_i = 0
\end{aligned}
\qquad \text{(I)}
$$

which also take the place of the quantum conditions.

These operators are related by the following Hamiltonian equations:

$$
\begin{aligned}
\frac{dP_i}{dT} &= \frac{d}{dt}P_i - P_i\frac{d}{dt} = -\frac{\partial H(PQ)}{\partial Q_i} \\
\frac{dQ_i}{dT} &= \frac{d}{dt}Q_i - Q_i\frac{d}{dt} = \frac{\partial H(PQ)}{\partial Q_i}
\end{aligned}
\qquad \text{(II)}
$$

These two sets of equations are apparently sufficient to determine the operators in terms of t and d/dt, except for a certain arbitrariness which will be removed later by another postulate.

In the operator calculus of the classical theory, there is a relation between the operators and the numerical quantities, as was pointed out in the first part of this paper. It is $Q1 = q$. In the same way, it is possible to define a numerical quantity related to each operator of the new theory by a relation which has already been used by Born and Wiener:

$$
\begin{aligned}
&\frac{1}{\psi}P_j\psi = p_j \\
&\frac{1}{\psi}Q_j\psi = q_j
\end{aligned}
\qquad \text{(III)}
$$

and in general

$$\frac{1}{\psi}F\psi = f$$

where F is any function of P_j and Q_j. The numerical quantity ψ in the Born and Wiener calculus has the value exp $[2\pi iWt/h]$, where W is the energy in the nth quantum state. In the present calculus it will be defined by the relation.

$$\frac{1}{\psi_n}H(P_jQ_j)\psi_n = W_n \qquad (15)$$

It will be seen that this is the equation published by Schroedinger in another form, and which in addition to defining ψ_n, serves to distinguish a certain discrete sequence of values of W from all others.

IV. The Solution of the Equations

The first step in the solution of the operator equations of the last section is to find an operator $\vartheta(q,\partial/\partial q)$ such that the equations are identities when ϑ is substituted for d/dt, and the operator Q_j is assumed to be $[q_j\times]$.

Let F be any function of the operators P_j and Q_j. Then it may be shown that the conditions (I) are entirely equivalent to

$$\begin{aligned} P_jF - FP_j &= \frac{h}{2\pi i}\frac{\partial F}{\partial Q_j} \\ Q_jF - FQ_j &= \frac{h}{2\pi i}\frac{\partial F}{\partial P_j} \end{aligned} \qquad \text{(Ia)}$$

The proof is easily constructed using the method of induction.[8] Hence Eq. (II) may be written

$$\begin{aligned} \frac{d}{dt}P_j - P_j\frac{d}{dt} &= \frac{2\pi i}{h}(HP_j - P_jH) \\ \frac{d}{dt}Q_j - Q_j\frac{d}{dt} &= \frac{2\pi i}{h}(HQ_j - Q_jH) \end{aligned} \qquad \text{(IIa)}$$

It is to be noted that this is a direct consequence of Eq. (I) and therefore has no analogon in the classical theory.

From the form of (IIa) it is seen that the operator ϑ for which we are seeking will be

$$\vartheta = \frac{2\pi i}{h}H(PQ)$$

The first part of the problem is thus reduced to finding P_j such that it satisfies the Eq. (I) when $Q_j = [q_j\times]$. The solution of this problem is not difficult; if $P_j = (h/2\pi i)(\partial/\partial q_j)$ be substituted into (I) and both sides of the equations allowed to act on an arbitrary function of q_i, we get

$$\frac{h}{2\pi i}\frac{\partial}{\partial q_j}(q_i f) - \frac{h}{2\pi i}q_i\frac{\partial f}{\partial q_j} = \frac{h}{2\pi i}\delta_{ij}f$$

Remembering the rule for the differentiation of a product, it is readily seen that the equations are identities in f. Hence the first part of the problem is competely solved:

$$\vartheta = \frac{2\pi i}{h}H\left(\frac{h}{2\pi i}\frac{\partial}{\partial q_j},\ q_j\right) \qquad (16)$$

[8] Born, Heisenberg, and Jordan, Zeits. f. Physik. **35**, 557 (1926).

Eq. (15) becomes on substituting this value of ϑ:

$$\frac{1}{\psi} H\left(\frac{h}{2\pi i}\frac{\partial}{\partial q_j}, q_j\right)\psi = W \tag{17}$$

which may also be written

$$\frac{1}{\psi}\vartheta\psi = \frac{2\pi i W}{h} \tag{18}$$

In the case of Keplerian motion, where

$$H(PQ) = \frac{1}{2\mu}[P_x^2+P_y^2+P_z^2] - \frac{e^2}{R}$$

Eq. (17) becomes

$$-\frac{h^2}{8\pi^2\mu}\frac{1}{\psi}\nabla^2\psi - \left(\frac{e^2}{r}+W\right) = 0 \tag{17a}$$

which is the equation derived by Schroedinger from entirely different considerations. It is a linear differential equation of the second order, and from the theory of such equations it is known that when W takes on a certain sequence of values called the characteristic values of the equation, the corresponding solutions for ψ are especially simple. Schroedinger has shown that the characteristic values of (17a) are

$$W_n = -\frac{2\pi^2\mu e^4}{h^2 n^2}, \quad n = 1, 2, 3, \cdots. \tag{19}$$

which are the Bohr energy levels for the hydrogen atom.

The solution of the problem may now be completed by making use of a certain property of the solutions of (17) or (18) which correspond to the characteristic values of W_n. Call these solutions ψ_n. Then it is possible to choose them so that they have no singularities in the finite part of the q_j manifold, and vanish on its infinite boundary. Any function subject to certain immaterial restrictions can be expanded as an infinite series in ψ_n. Let us expand the function

$$q_j\psi_n(q) = \sum_k Q_j(nk)\psi_k(q) \tag{20}$$

or

$$q_j = \sum_k Q_j(nk)\frac{\psi_k}{\psi_n}$$

If this expression for q_j be substituted into $Q_j = [q_j\times]$ and thence into the equations (II), they will still be identically satisfied by the operator ϑ.

The problem is now that of passing from the operator ϑ to the operator d/dt. Evidently the reasoning of the first part of this section is still valid, and from (IIa) we deduce that

$$H(P_iQ_i) = \frac{h}{2\pi i}\frac{d}{dt} \tag{21}$$

so that (15) becomes

$$\frac{1}{\psi_n}\frac{h}{2\pi i}\frac{d\psi n}{dt} = W_n \tag{15a}$$

or

$$\psi_n = e\frac{2\pi i}{h}W_nt$$

It will be logical, from our empirical point of view, to admit only those values of W_n in (15a) which are the characteristic values for (17).

But now we are no longer free to assume that $Q_i = [q_i\times]$. It will become apparent in the following that Q_i is now an operator defined by the Born and Jordan-Dirac matrices, provided that one further assumption is made. Thus far the functions ψ_n have been indeterminate to the extent of an arbitrary factor A_n which might be a function of the particular one of the sequence W_n to which the solution corresponds. It will now be shown that the coefficients $Q(nk)$ defined above possess the properties of the matrices. To do this, we return to the functions ψ_n defined by (17) and expand $q^2\psi_n$ in terms of them:

$$q^2\psi_n = \sum_k Q(nk)q\psi_k = \sum_{kl} Q(nk)Q(kl)\psi_l \tag{22}$$

which yields the law of the multiplication of matrices.
Also

$$(\vartheta q - q\vartheta)\psi_n = \sum_k Q(nk)q\psi_k - q\vartheta\psi_n = \sum_k \frac{2\pi i}{h}(W_k - W_n)Q(nk)\psi_k$$

so that the operator $\vartheta Q - Q\vartheta$ may be represented by the matrix $2\pi i/h$ $(W_k - W_n)Q(nk)$ and therefore the operator ϑ by the matrix

$$\frac{2\pi i}{h} W_n \delta_{nk} \tag{23}$$

It must also be shown how the result of the action of the operators previously defined on an arbitrary function can be calculated from a knowledge of the matrices. Let $f = \Sigma_n F_n \psi_n$ be an arbitrary function, subject only to the restriction that it may be expanded in such a series. Then

$$Qf = qf = \sum_n F_n q\psi_n = \sum_{nk} F_n Q(nk)\psi_k$$

and

$$Pf = \frac{h}{2\pi i}\frac{\partial f}{\partial q} = \frac{h}{2\pi i}\sum_n F_n \frac{\partial \psi_n}{\partial q} = \sum_{nk} F_n P(nk)\psi_k$$

provided that

$$\frac{h}{2\pi i}\frac{\partial\psi_n}{\partial q} = \sum_k P(nk)\psi_k \tag{24}$$

The matrices of the earlier calculus were defined to have one property which those obtained in this way do not in general possess: they were defined to be Hermitian, which is to say that $X(nm)$ is the conjugate complex quantity to $X(mn)$. Since in the preceding, $Q(nm)$ is a real quantity, while $P(nm)$ is a pure imaginary, they should satisfy the conditions

$$\begin{aligned} Q(nm) &= Q(mn) \\ P(nm) &= -P(mn) \end{aligned} \tag{25}$$

in order to be identical with the earlier matrices. It will shortly be shown that this condition serves to determine the functions ψ_n uniquely. The physical significance of this condition will probably become evident only when the theory has been placed on a more physical basis than the present, and at the moment it need not be discussed further than to say that it must be related in some way with the equality of the probability of emission and absorption (Stefan's Law).

In order to show how the condition (25) serves to determine the constants A_n, it is necessary to consider the process of expanding a function in a series of the form $\Sigma F_n\psi_n$. Without serious loss of generality, we may limit ourselves to the case of a single mass moving under the action of a force which possesses the potential $V(xyz)$. Then

$$H = \frac{1}{2\mu}(P_x^2+P_y^2+P_z^2)+V(X\ \ Y\ \ Z)$$

and Eq. (17) becomes

$$-\frac{h^2}{8\pi^2\mu}\nabla^2\psi+[V(xyz)-W]\psi=0 \tag{26}$$

If the potential V vanish on the infinite sphere, and W have one of the characteristic values of the equation, it may be shown that there are solutions of this equation which vanish exponentially on the infinite sphere. Let ψ_n be a sequence of such solutions, each corresponding to a certain value of W_n. By Green's theorem we have

$$\iiint_{-\infty}^{+\infty} (\psi_n\nabla^2\psi_m-\psi_m\nabla^2\psi_n)dv = \iint_{\infty}\left(\psi_n\frac{\partial\psi_m}{\partial\nu}-\psi_m\frac{\partial\psi_n}{\partial\nu}\right)dS$$

The right side of this vanishes from what has just been said, and on substituting the value of $\nabla^2\psi$ from Eq. (26) it reduces to

$$(W_m - W_n) \int\int\int_{-\infty}^{\infty} \psi_m \psi_n dv = 0$$

whence it may be concluded that

$$\begin{aligned} \int\int\int_{-\infty}^{+\infty} \psi_m \psi_n dv &= 0 \quad n \neq m \\ &= C_n \quad n = m \end{aligned} \tag{27}$$

This gives the formal method of expanding a function in a series of ψ_n. For, if

$$f(xyz) = \sum_n F_n \psi_n$$

then by (27),

$$\int\int\int_{-\infty}^{+\infty} f\psi_m dv = C_m F_m$$

The matrices can now be calculated from (22) and (23), and it is found that

$$C_m Q(nm) = \int\int\int_{-\infty}^{+\infty} q\psi_m \psi_n dv = C_n Q(mn)$$

where q represents either x, y or z.

$$C_m P(mn) = \int\int\int_{-\infty}^{+\infty} \frac{h}{2\pi i} \frac{\partial \psi_n}{\partial q} \psi_m dv = -\int\int\int_{-\infty}^{+\infty} \frac{h}{2\pi i} \psi_n \frac{\partial \psi_m}{\partial q} dv = -C_n P(mn)$$

The condition (25) will then be satisfied if and only if

$$C_m = C_n$$

which can always be attained if we replace the functions ψ_n by the functions $\psi_n/\sqrt{C_n}$ which are also solutions of (26).

The method of obtaining the matrices which has just been outlined differs very little from Lanczos' interpretation of the matrix calculus[9] which is thus also included in the present calculus.

Before solving a special example with these methods, some discussion of the possible physical significance of the functions ψ_n may not be out of place. If the independent variable in (26) be changed by the substitution $S = h/2\pi i \log \psi$ it becomes

$$\frac{1}{2\mu} \frac{h}{2\pi i} \nabla^2 S + \frac{1}{2\mu} \left\{ \left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2 \right\} + V(xyz) = W$$

[9] Lanczos, Zeits. f. Physik. **35**, 812 (1926). In a preliminary paper, (Proc. Natl. Acad. **12**, 473 (1926) the present author has given the solution of the simple oscillator on Lanczos theory, as modified by some of the results of the present paper. These are used without explanation in that place.

and this reduces to the classical Hamilton-Jacobi equation when h approaches zero. The presumption is that the function S thus defined has no other significance than the classical Hamilton-Jacobi function.

V. Solution of the Equations for the Simple Oscillator

In the case of the simple harmonic oscillator, the Hamiltonian function has the form

$$H=\frac{1}{2\mu}P^2+\frac{1}{2}\mu\omega^2X^2$$

whence

$$\frac{h}{2\pi i}\vartheta=-\frac{h^2}{8\pi^2\mu}\frac{d^2}{dx^2}+\frac{1}{2}\mu\omega^2x^2$$

and Eq. (26) is

$$-\frac{h^2}{8\pi^2\mu}\frac{d^2\psi}{dx^2}+\left\{\frac{1}{2}\mu\omega^2x^2-W\right\}\psi=0 \tag{28}$$

The solution of this equation has been discussed by P. S. Epstein.[10] If we write $x=(h/4\pi\mu\omega)^{\frac{1}{2}}\cdot u$, it becomes

$$\frac{d^2\psi}{du^2}-\left\{\frac{u^2}{4}-\frac{2\pi W}{h\omega}\right\}\psi=0 \tag{29}$$

This equation possesses solutions of the forms $f(u)\exp(-u^2/4)$ and $F(u)\exp(+u^2/4)$ where the functions f and F satisfy

$$\begin{aligned}\frac{d^2f}{du^2}-u\frac{df}{du}+\left\{\frac{2\pi W}{h}-\right\}\frac{1}{2}f=0\\ \frac{d^2F}{du^2}+u\frac{dF}{du}-\left\{\frac{2\pi W}{h}-\frac{1}{2}\right\}f=0.\end{aligned} \tag{30}$$

The solution of these equations leads in general to infinite series in u, but if W has such a value that $(2\pi W/n-\frac{1}{2})$ is a positive integer, then both f and F are finite polynomials. Hence the sequence of characteristic values is

$$W=\left(n+\frac{1}{2}\right)\frac{h\omega}{2\pi}\cdot$$

[10] P. S. Epstein, Dissertation: Ueber die Beugung an einem ebenem Schirm, etc., Munich, 1914.

The corresponding solutions of (30) are polynomials given by the recursion formulae

$$f_{n-2}-uf_{n-1}+nf_n=0$$
$$F_{n-2}+uF_{n-1}-nF_n=0 \tag{31}$$

where the arbitrary constants are to be determined by the conditions

$$f_0=F_0=1 \qquad f_1=F_1=u$$

As has been shown in the previous section, if we wish to obtain the Born-Jordan matrices, the functions ψ_n must be chosen so that they satisfy the conditions.

$$\int_{-\infty}^{+\infty} \psi_n \psi_m dx = 0 \qquad m \neq n$$
$$= 1 \qquad m = n$$

The first of these is satisfied by all solutions of (28) which vanish for $x = \pm\infty$ and the second can be satisfied by a proper choice of the arbitrary constant with which each solution may be multiplied. The solution

$$\psi_n(x) = \sqrt{n!}\sqrt[4]{\frac{2\mu\omega}{h}}\, f_n(u)\ exp.\left[-\frac{u^2}{4}\right] \tag{32}$$

satisfies both conditions.

The matrix for X is to be obtained by expanding $x\psi_n$ in terms of ψ_k. This may be accomplished by the general method given in the previous section, but it may be done in a simpler manner by using the recursion formula (31) for f_n:

$$x\psi_n(x) = \sqrt{\frac{h}{4\pi\mu\omega}}\left\{\sqrt{n}\,\psi_{n-1} + \sqrt{n+1}\,\psi_{n+1}\right\}$$
$$= \sum_k X(nk)\psi_k$$

whence

$$X(nk) = 0 \qquad\qquad k \neq n \pm 1$$

$$X(n,\ n-1) = \sqrt{\frac{hn}{4\pi\mu\omega}} \qquad X(n,\ n+1) = \sqrt{\frac{h(n+1)}{4\pi\mu\omega}}$$

This is precisely the matrix which Born and Jordan give as the solution of this problem.

The matrix P can most readily be obtained from the relation

$$P(nk) = \mu\frac{2\pi i}{h}(W_k - W_n)X(nk)$$

which gives

$$P(nk)=0 \qquad k\neq n\pm 1$$
$$P(n,\ n-1)=i\mu\omega X(n,\ n-1)$$
$$P(n,\ n+1)=-i\mu\omega X(n,\ n+1)$$

Conclusion

1. It has been shown that the classical equations of dynamics can be written in operator form.

2. The operator calculus of the classical theory has been generalized and applied to the solution of the equations of quantum dynamics. The remarkable results of Schroedinger have been included in the same calculus as those of Born and Jordan, and a method of calculating the matrices of the last named authors has been developed.

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Note added with proof, September 2, 1926.—In an article dated March 18, 1926 [Ann. d. Physik, **79** 734, (1926)], but which did not reach this Institute until after the above was in course of publication, Schroedinger has published all the essential results contained in the above paper. Since Schroedinger's presentation is based on his wave-mechanics, while this is based on the matrix-mechanics, it seems not without interest to publish this even now. The author agrees, however, that the wave-mechanics is more fundamental than the matrix mechanics, and holds out more hope for an eventual physical interpretation of the results obtained. The conclusion of this paper may be stated, with Schroedinger, to be "that the wave-mechanics and the matrix-mechanics are mathematically identical".