[London]

The Relation between Classical and Quantum Mechanics

L. M. S. 16-2-33.

The laws of Newtonian mechanics and Maxwellian electrodynamics have been found to be inadequate for the building up of a theory of atomic phenomena.

This is shown up very clearly by the appearance of a new universal constant, Planck's constant of action h, which plays an important part in the description of experimental results about the atom.

There is no natural place for fitting in such a universal constant, with the dimensions of action, into the old schemes of mechanics.

A new scheme of mechanics has been set up in recent times, called Q.M., based on the work of Heisenberg and Schrödinger in 1925-6.

The new mechanics has been found to be remarkably well fitted for describing atomic phenomena.

The new mechanics differs in fundamental ~~respects~~ ways from the old one.

It requires the introduction of new physical concepts which are unknown in classical mechanics, and it involves h, which plays an important rôle.

Inspite of the fundamental difference in physical ideas, there is a great formal resemblance between them.

There is a correspondence between the equations of one and those of the other.

The classical theory appears as the limit of the quantum theory as $h \to 0$.

h appears in the quantum equations often in such a peculiar way that the passage to the limit $h \to 0$ is not a trivial process.

It thus becomes of interest to trace in detail the connection between the various equations and methods of classical mechanics and their quantum analogues.

In classical mechanics there are two general methods of dealing with a dynamical system — the Lagrangian method and the Hamiltonian method.

It is quite an easy matter to pass from one to the other, but all the same the two methods do involve two rather different sets of ideas.

Each of these methods has its analogue in the Q.T.

The two quantum methods tend to emphasize the wave and the corpuscular properties of matter respectively.

i.e. for understanding the connection between the Hamiltonian methods in class and Q.M. it is best to consider the atomic system from the corpuscular point of view

and — — — — — Lagrangian methods — — — — — wave point of view.

I should like to deal with both these methods in this lecture, taking first the Hamiltonian, which is the better known in Q.M.

The classical Hamiltonian method is based on the notion of canonical coords and momenta.

In the corresp. Q.T we keep to the corpuscular picture and we still have canonical coords and momenta describing the motions of the particle.

In the Q.T. though, the coords and momenta are to be considered, not as numbers, but as quantities of a kind which do not obey the commutative law of multiplication.

They may be supposed to be matrices, or linear operators, or else just abstract quantities subject to certain algebraic laws. They may be generalized "matrices" with a continuously infinite no of rows and columns, so that the law of multiplication involves an integration process instead of summation

Instead of the commut. law of multiplication we have these equations, known as the quantum conditions

$$q_r q_s - q_s q_r = 0 \qquad p_r p_s - p_s p_r = 0 \qquad q_r p_s - p_s q_r = i\hbar\delta_{rs} \qquad \hbar = h/2\pi$$

With the help of these equations we can evaluate $fg - gf$ where f and g are any two algebraic fns of the p's & q's

Any algebraic expression equation in classical mechanics can now be take over into Q.M. e.g. $m_x = y p_z - z p_y$

There is, of course, the difficulty that the classical expression of eqn may involve a term consisting of a product of factors whose quantum analogues do not commute, and one may then not know in what order to put the quantum factors.

In practice, however, one has never found any difficulty in guessing what this order should be.

The next question is how to take over the differential operations that occur in the classical theory.

There is no trouble with a total differential coeff, such as $\frac{d\alpha}{dt}$.

If α is a matrix or operator involving a parameter t, we can define $\frac{d\alpha}{dt}$ as $\lim_{\delta t \to 0} \frac{\alpha(t+\delta t) - \alpha(t)}{\delta t}$.

There is trouble, though, when one comes to partial derivatives, $\frac{\partial}{\partial \alpha}$.

Attempts have been made by Born, H. and J. to give a meaning to partial differentiation w. r. to quantum variables, but they are successful only in special cases.

One can see the difficulty by taking the example $f(\alpha\beta) = \alpha\beta - \beta\alpha$.

In general f does not vanish, and then there does not seem to be any way of giving a meaning to $\frac{\partial f}{\partial \alpha}$ or $\frac{\partial f}{\partial \beta}$.

There is thus no general process of partial differentiation applicable to quantum variables.

There does exist, however, a process which plays the part of partial diff^{n} and is sufficiently general for the purposes of dynamics.

This is the process of forming the P.B of two dynamical variables

P.B. in classical theory is $[\alpha,\beta] = \sum_r \left\{ \frac{\partial\alpha}{\partial q_r}\frac{\partial\beta}{\partial p_r} - \frac{\partial\alpha}{\partial p_r}\frac{\partial\beta}{\partial q_r} \right\}$

in in Q. — — $[\alpha,\beta] = \frac{\alpha\beta - \beta\alpha}{i\hbar}$

It is easily ~~seen~~ seen that there is a strong analogy between the classical and quantum P.B's,

e.g multiplication law $[\alpha_1\alpha_2, \beta] = \alpha_1[\alpha_2,\beta] + [\alpha_1,\beta]\alpha_2$ is same for both.

The reason for the above definition of the Q. PB is this analogy, together with the fact that it makes

The quantum conditions ~~now~~ become $[q_r, p_s] = \delta_{rs}$, etc

which just correspond to the classical conditions for canonical variables.

General classical eqn of motion is $\dot{\alpha} = [\alpha, H]$,

which can be taken over directly into the Q.T.

All the eqns of Hamiltonian dynamics can be taken over into the Q.T. on this basis.

One gets a satisfactory basis for the notions of real and pure imaginary quantum variables by assuming that when α and β are real, $\alpha\beta + \beta\alpha$ is real and $\alpha\beta - \beta\alpha$ is pure imaginary, so that the P.B $\frac{\alpha\beta - \beta\alpha}{i\hbar}$ is real.

In the classical theory one may perform a contact transfn.

This consists in introducing new variables P_r, Q_r, which are also canonical, i.e., $[Q_r, P_s] = \delta_{rs}$ etc.

One can do the same thing in the Q.T.

In the Q.T. we can express the new variables explicitly in terms of the old ones by equations of the type

1) $$P_r = T p_r T^{-1} \qquad Q_r = T q_r T^{-1}$$

We may take T to be any fn of the p's and q's that has a reciprocal, and the P's and Q's defined in this way will be canonical. They will satisfy just the same algebraic relations as the p, q. $f(PQ) = T f(pq) T^{-1}$

For the P's and Q's to be real, T must satisfy the unitary condition $T\bar{T} = 1$ conj. hermitian

There do not exist any classical eqns corresponding to eqns 1)

The classical eqns for a contact transf. may be put in the form

2) $$p_r = \frac{\partial S}{\partial q_r} \qquad P_r = -\frac{\partial S}{\partial Q_r}$$

and there is no obvious relation between 1) and 2)

This makes the study of the relation between classical and quantum contact transfns interesting, and this study will also enable us to pass over to a discussion of the Lagrangians.

We shall examine how 1) goes over into 2) in the limit $h \to 0$.

The first thing to notice about 1) is that if we regard it as an equation between matrices, there need be no (1,1) correspondence between the rows and columns of the P, Q's and those of the p's q's.

We may use letters m n .. to label the rows and columns of P + Q, and an entirely different set α, β.. to label the rows and columns of the p, q's

$$P_{mn} = T_{m\alpha}\, p_{\alpha\beta}\, T^{-1}_{\beta n}$$

T is a mixed matrix $T_{m\alpha}$, and T^{-1} is another mixed matrix satisfying $T_{m\alpha} T^{-1}_{\alpha n} = \delta_{mn}$.

Unitary condition is $T_{m\alpha} \bar{T}_{\alpha n} = \delta_{mn}$ $\quad \bar{T}_{\alpha n} = T^{-1}_{\alpha n}$

We nowhere require a connection between the m n and the α, β

We thus have a transfn between two sets of matrices with no connection between their labels for rows and columns.

We may now regard eqns 1) in a different way, namely as giving the connection between two sets of matrices which both represent the same dynamical variables.

This corresponds to the fact that if we have equations for the rotation of a set of vectors in any space, we may regard them instead as giving the connection between the coords of the same set of vectors referred to two different coord systems.

3) We have the eqns $x^{\times} = T x T^{-1}$ or $x^{\times}_{mn} = T_{m\alpha}\, x_{\alpha\beta}\, T^{-1}_{\beta n}$

If we are to compare this transfn with the classical transfn from pq to PQ, ~~and~~ we ~~now~~ must regard $x^{\times}_{mn}$ and $x_{\alpha\beta}$ as two matrices represent^g the ~~same dyn variables~~ thing, the $x_{\alpha\beta}$ matrix being in a matrix representation which is in some way fixed by the dyn variables $q_r\, p_r$, and the $x^{\times}_{mn}$ representation being correspondingly fixed by Q_r, P_r.

One can have a matrix representation fixed by a set of canonical dyn. variables q_r, p_r by requiring that the q's shall be diagonal and the p's shall become the operators $-i\hbar\frac{\partial}{\partial q}$

$$\left[\, q\left(-i\hbar\frac{\partial}{\partial q}\right) - \left(i\hbar\frac{\partial}{\partial q}\right)q = i\hbar \,\right]$$

The rows and columns of these matrices ~~of~~ may be labelled by the values of the diag. elements of the q's which occur in them. These values we call q', q'' etc.

Similarly for the Q_r, P_r.

We can now use $q'q''$ instead of α, β and $Q'Q''$ instead of mn, and $(Q'|q')$ $(q'|Q')$ instead of $T_{m\alpha}$, $T^{-1}_{\alpha n}$

Thus eqn 3) may be written $$(Q'|x|Q'') = \iint (Q'|q')\,dq'\,(q'|x|q'')\,dq''\,(q''|Q'')$$

Transfn is specified by $(q'|Q')$ or $(Q'|q')$, which we call the transfn fn.

~~It may now be shown that~~ Hence $(q'|Q')$ corresponds to the classical fn $e^{iS/\hbar}$ with the S of 2)

To make the comparison with the Q. contact transfn and the classical transfn in the form 2), we must introduce the mixed repn $(q'|\;|Q')$, corresponding to the fact that in the classical theory we express everything as a fn of q and Q

It can then easily be proved that $\quad (q'|f(qQ)|Q') = f(q'Q')\,(q'|Q')$ $\quad$ provided f is well ordered.

and that
$$(q'|p_r|Q') = -i\hbar\frac{\partial}{\partial q_r'}(q'|Q')$$
$$(q'|P_r|Q') = i\hbar\frac{\partial}{\partial Q_r'}(q'|Q')$$

These results correspond to 2) if we take $(q|Q) = e^{iS/\hbar}$ [illegible]