

On a type of canonical transformation

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1. A well known theorem in classical dynamics tells us that if Q , P , and $\left(\frac{\partial W}{\partial t}\right)_{q, Q}$ are written as functions of q , p and t by means of the equations

$$P = \left(\frac{\partial W}{\partial Q}\right)_{q, t} \quad p = - \left(\frac{\partial W}{\partial q}\right)_{Q, t}$$

where $W(q, Q, t)$ is an arbitrary function, and if two functions $F(Q, P, t)$ and $f(q, p, t)$ are related by

$$f(q, p, t) \equiv F\{Q(q, p, t), P(q, p, t), t\} + \left(\frac{\partial W}{\partial t}\right)_{q, Q}(q, p, t) \quad (1)$$

then q and p are conjugate with respect to $f(q, p, t)$ if Q and P are conjugate with respect to $F(Q, P, t)$.

2. By extending the transformation theorem of E. T. Whittaker,¹ studied in detail by W. O. Kermack and W. H. McCrea,² we will derive in this section, a theorem which has some formal analogy with that of section 1.

We will write p for $\frac{1}{\alpha} \frac{\partial}{\partial q}$ and P for $\frac{1}{\alpha} \frac{\partial}{\partial Q}$. Let $W(q, Q, t)$ be a function such that, with the aid of rules given by Kermack and McCrea³ (or otherwise), we can specify operators $Q(q, p, t)$, $P(q, p, t)$ and $\frac{\partial W}{\partial t}(q, p, t)$, satisfying the equations

$$(Q - Q) e^{-\alpha W} = 0 \dots (2), \quad (P + P) e^{-\alpha W} = 0 \dots (3), \quad \left(\frac{\partial W}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial t}\right) e^{-\alpha W} = 0$$

¹ These *Proceedings* (2), 2, 1931, pp. 189-204.

² *Ibidem*, 205-239.

³ *l.c.* 206-7.

From a given function $\phi(Q, t)$ we will define a function $\psi(q, t)$ by

$$\psi(q, t) = h^{-\frac{1}{2}} \int e^{-\alpha W} \phi(Q, t) dQ \tag{5}$$

where h is any constant, α is $2\pi i/h$, and the integration is along a specified path. A theorem of Kermack and McCrea¹ shows that if $F(Q, P, t)$ consists of a series of terms of the form $g(t) Q^a P^b Q^c P^d \dots$, and if f is $F(Q, P, t)$, then

$$f \psi = h^{-\frac{1}{2}} \int e^{-\alpha W} \{F \phi\} dQ \tag{6}$$

provided that on carrying out certain requisite integrations by parts the integrated terms vanish. There are, especially in a many dimensional generalisation, important cases in which f and F , though satisfying (6), cannot be expanded in a series of positive powers; but we may still write f formally as $F(Q, P, t)$, by using suitable definitions to specify the meanings of differential processes which, in simple algebra, have no meanings.

By (4) we have

$$\begin{aligned} \left(\frac{\partial W}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial t}\right) \psi &= h^{-\frac{1}{2}} \int \left\{ \phi \left(\frac{\partial W}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial t}\right) e^{-\alpha W} + e^{-\alpha W} \frac{1}{\alpha} \frac{\partial \phi}{\partial t} \right\} dQ \\ &= h^{-\frac{1}{2}} \int e^{-\alpha W} \left\{ \frac{1}{\alpha} \frac{\partial}{\partial t} \phi \right\} dQ. \end{aligned} \tag{7}$$

Adding (6) to (7) shows that f and F in (6) may be replaced by

$$\left. \begin{aligned} f\left(q, p, t, \frac{1}{\alpha} \frac{\partial}{\partial t}\right) &= F(Q, P, t) + \frac{\partial W}{\partial t}(q, p, t) + \frac{1}{\alpha} \frac{\partial}{\partial t} \\ \text{and } F\left(Q, P, t, \frac{1}{\alpha} \frac{\partial}{\partial t}\right) &= F(Q, P, t) + \frac{1}{\alpha} \frac{\partial}{\partial t} \end{aligned} \right\} \tag{8}$$

The relationship between the operators f and F may be compared with the relation (1) of Hamiltonian dynamics.²

By the same argument f and F in (6) may be replaced by

$$f = F\left(Q, P, t, \frac{\partial W}{\partial t} + \frac{1}{\alpha} \frac{\partial}{\partial t}\right); \quad F = F\left(Q, P, t, \frac{1}{\alpha} \frac{\partial}{\partial t}\right).$$

¹ *loc. cit.*

² The author is indebted to Dr A. Erdélyi for assistance in the mathematical presentation of the paper.

In wave mechanics the significance of such an equation as (6) when satisfied by two of our operators, say f and \mathbf{F} , is not confined to the fact, which immediately follows from it, that $f\psi = 0$ if $\mathbf{F}\phi = 0$.

3. We consider now some further properties of these transformations, in simple but important cases. Let us take \hbar and t real (having wave mechanics in mind), and consider the case $W = q_1(q, t) + q_2(q, t)Q$, where q_1 is real for values of q which make q_2 real. The operators satisfying (2), (3), (4) are easily specified; and (5), if we take the path of integration as $-\infty$ to ∞ , is

$$e^{\alpha q_1} \psi = \hbar^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\alpha q_2 Q} \phi \, dQ \tag{9}$$

whence we have by Fourier's reciprocal theorem

$$\phi = \hbar^{-\frac{1}{2}} \int e^{\alpha W} \psi \left(\frac{\partial q_2}{\partial q} \right) dq.$$

Let $f\left(q, p, t, \frac{1}{\alpha} \frac{\partial}{\partial t}\right)$ and $\mathbf{F}\left(Q, P, t, \frac{1}{\alpha} \frac{\partial}{\partial t}\right)$ be a pair of operators satisfying (6); then (9) holds when ϕ and ψ are replaced by $\mathbf{F}\phi$ and $f\psi$. Hence, by the generalised theorem of Plancherel,

$$\int_{-\infty}^{\infty} \phi_n^* \phi_m \, dQ = \int \psi_n^* \psi_m \frac{\partial q_2}{\partial q} \, dq \tag{10}$$

and
$$\int_{-\infty}^{\infty} \phi_n^* \mathbf{F}\phi_m \, dQ = \int \psi_n^* f\psi_m \frac{\partial q_2}{\partial q} \, dq \tag{11}$$

where ϕ_n and ϕ_m are arbitrary functions from which ψ_n and ψ_m are defined by (5) and ϕ^* is conjugate complex to ϕ . In these equations we could, of course, have written dq_2 instead of $\frac{\partial q_2}{\partial q} dq$, and the integration would then have been from $-\infty$ to ∞ . In the actual expressions the path is the corresponding range of q . The simplest of such W 's is $W = qQ$ which transforms a "wave function in coordinate space" to a "wave function in momentum space"; we may note that in a generalisation to three Q 's, say Cartesian coordinates X, Y, Z , it can be shown that if \mathbf{F} contains a term R^{-1} the corresponding term in f is an integral operator of simple

type; it is discussed by Copson.¹ (10) is chiefly of interest when we are concerned with an infinite set of ϕ 's. As an example of (11) we may take ϕ_n and ϕ_m to be the same arbitrary function in which we vary a parameter, perhaps to determine the minimum value of the integral. The equation then expresses a correspondence between two variational calculations, in coordinates Q and q .

¹ *Proc. Roy. Soc., Edinburgh*, A, 61, Part 3.

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