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Development of the analogy between classical and quantum mechanics

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Abstract. A quantum-mechanical generalisation of Carathéodory's theorem in classical dynamics is established. Several related properties of classical canonical transformations are also generalised to the quantum case.

Keywords. Mechanics, classical; quantum mechanics; Carathéodory's theorem.

Introduction

It is well known that there are many analogies between the formal structure of classical Hamiltonian dynamics on the one hand, and the structure of quantum mechanics on the other. To each of the important conceptual elements in the former there exists a corresponding element in the latter. Thus, for example, we have the notions of Poisson Brackets (PB's), canonical transformations and the Hamiltonian form for the equations of motion in classical dynamics; and the analogous things in quantum mechanics are commutators of operators, unitary transformations, and the Heisenberg form for the equations of motion. Of course, the discussion of such parallels makes sense only in the case of quantum systems that possess classical analogues.

It is remarkable that the existence of these analogies does not stop at the level of the concepts mentioned above, but goes much further. Thus, several of the equations pertaining to classical transformation theory also turn out to possess quantum analogues: the equations in the two cases can be worked out so as to have exactly the same formal appearance, and differ only in the meanings attached to the various symbols. This was shown by Jordan and Dirac soon after the quantum mechanical transformation theory had been worked out (Jordan 1926; Dirac 1933). Leaving to the next section the tasks of establishing and explaining an adequate notation, the result of Jordan and Dirac may be briefly described as follows: If one considers a classical dynamical system described by canonical variable pairs q_r, p_r, a canonical transformation leads to new canonical pairs Q_r, P_r, given as functions of the old variables. In the case that the q's and Q's together constitute a maximal set of independent phase space variables, there exists a single real "generating function" $S(q;Q)$, determined upto an additive constant, in terms of which the canonical transformation is completely specified. The equations that do so are:

$$p_r = \frac{\partial S(q;\,Q)}{\partial q_r}\,, \quad P_r = -\,\frac{\partial S(q;\,Q)}{\partial Q_r} \tag{A}$$

Here, of course, all the quantities involved are classical real variables and functions. Jordan and Dirac demonstrated that for certain kinds of unitary transformations on the Hilbert space of a quantum mechanical system described by canonical position and momentum operator pairs, exactly the same equations as the above hold good; however, now the q's, p's, Q's and P's are all hermitian operators, and $S(q; Q)$ is also an operator which is determined by the unitary transformation. It is to be written in a particular "well-ordered" way, with dependences on q always appearing to the left of dependences on Q. The condition on the unitary transformation such that eq. (A) hold is just that the operators q and Q are all independent. One loses however, the reality property of S; in the quantum case, $S(q; Q)$ need not be a hermitian operator.

Going back to the classical case, it is known that a suitable generalisation of eq. (A) exists in the case of canonical transformations for which the q's and Q's do not form a maximal independent set of phase space variables (Whittaker 1927). One has to introduce additional variables which are just Lagrangian multipliers, and these appear explicitly in the formulae that replace eq. (A) above. Dirac has shown that this case too has a quantum analogue, with exactly similar looking equations being valid in both classical and quantum mechanics (Dirac 1945). In the quantum case one has to introduce the analogues of Lagrangian multipliers which however turn out to be operators; and the ordering prescription is to place them *in between* the q's and Q's.

There is in the classical case a very interesting property of canonical transformations that asserts the existence of a set of equations of the general form (A), whatever the transformation. It essentially says that if one is given any canonical transformation in phase space, one can always form a maximal independent set of phase space variables made up of equal numbers of old and new variables chosen in a special way. This result is due to Carathéodory (Carathéodory 1965). This property gives one a complete and satisfying description of *all* canonical transformations, even those for which eq. (A) or one of its commonly described three variants fails. Indeed, most treatments of canonical transformation theory stop with the consideration of four distinct types of generating functions $S^{(1)}(q; Q)$, $S^{(2)}(q; P)$, $S^{(3)}(p; Q)$ and $S^{(4)}(p; P)$; and if for a particular canonical transformation none of these types is suitable, then it is termed degenerate and is usually handled by the method of Lagrangian multipliers. Carathéodory's theorem tells us that as a matter of fact no canonical transformation is really degenerate in any general sense, since descriptions of it of the general form (A) always exist. We can go further and list the complete set of possible descriptions of a given canonical transformation and see explicitly how these different descriptions are related to each other.

The purpose of this paper is to extend the results of Jordan and Dirac by stating and proving a quantum-mechanical analogue to Carathéodory's theorem. We find that in addition to the existence of such an analogue, the detailed formulae for a canonical transformation in the classical case and a unitary transformation in the quantum case are again strikingly similar; this is perhaps to be expected. However, when one works out the equations that connect different possible descriptions of a given unitary transformation, one then finds a departure in form from the analogous equations valid for a canonical transformation. But this difference has an interesting interpretation and is reminiscent of the Feynman path integral formulation of quantum mechanics (Feynman 1948).

We present the material of this paper in the following order: In section 1 we set up a concise notation for dealing with the phase space of a classical dynamical system, with the help of which an elegant statement of Carathéodory's theorem and its consequences can be given. Section 2 contains the statement and proof of a quantum-mechanical version of Carathéodory's theorem. With the help of this result, we analyse in section 3 the details of the independent descriptions of a unitary transformation in quantum mechanics, and see how one can pass from one description to another. At this stage the characteristic differences between the classical and quantum formulae will become apparent. Finally, in the conclusion, we relate our results to those of Dirac, show how our results can be interpreted, and make some comments on the relationship between classical and quantum mechanics.

The level of mathematical rigour maintained in this paper does not pretend to be higher than the level maintained in the quoted papers of Dirac. In particular no attention is paid to questions of domains, and boundedness or unboundedness of operators. Since our purpose is to bring out the formal similarities between classical and quantum mechan'cs, this seems reasonable.

1. Resumé of classical results

We consider a classical dynamical system described by $2n$ canonical phase space coordinates $q_1, \ldots, q_n, p_1, \ldots, p_n$. Among functions of these variables, the PB is defined by

$$\{f(q,p), g(q,p)\} = \sum_{r=1}^{n} \left(\frac{\partial f}{\partial q_r}\frac{\partial g}{\partial p_r} - \frac{\partial f}{\partial p_r}\frac{\partial g}{\partial q_r}\right). \tag{1.1}$$

The values of the fundamental PB's are

$$\{q_r, q_s\} = \{p_r, p_s\} = 0, \ \{q_r, p_s\} = \delta_{rs} \tag{1.2}$$

For conciseness, we may sometimes write a single symbol ω_μ, $\mu = 1, 2, \ldots, 2n$, to stand for all the q's and p's: $\omega_1 = q_1$, $\omega_2 = p_1$, $\omega_3 = q_2$, $\omega_4 = p_2, \ldots$, $\omega_{2n-1} = q_n$, $\omega_{2n} = p_n$. Then with the help of an antisymmetric numerical matrix $\epsilon_{\mu\nu} \|$ whose only non-vanishing elements are

$$\begin{aligned} \epsilon_{12} &= \epsilon_{34} = \ldots = \epsilon_{2n-1,\,2n} = +1, \\ \epsilon_{21} &= \epsilon_{43} = \ldots = \epsilon_{2n,\,2n-1} = -1 \end{aligned} \tag{1.3}$$

equations 1.2 and 1.1 take the forms

$$\{\omega_\mu, \omega_\nu\} = \epsilon_{\mu\nu}, \ \{f(\omega), g(\omega)\} = \epsilon_{\mu\nu} \frac{\partial f(\omega)}{\partial \omega_\mu}\frac{\partial g(\omega)}{\partial \omega_\nu} \tag{1.4}$$

(A summation from 1 to $2n$ over repeated greek indices is understood, unless explicitly indicated otherwise).

We are interested in subsets of n variables picked out from the $2n$ quantities ω_μ in a particular way. Let $x = \{x_\mu\}$ denote such a subset. It is to be formed by including one variable from each canonical pair (q_r, p_r), $r = 1, 2, \ldots, n$ and dropping the other. Thus we have, for each value of r from 1 to n, either

$$x_{2r-1} = q_r, x_{2r} = 0. \tag{1.5}$$

or

$$x_{2r-1} = 0, \quad x_{2r} = p_r \tag{1.6}$$

Clearly there are precisely 2^n such subsets. These subsets of the phase space coordinates are just the maximal subsets one can form consisting of variables in involution with one another; two dynamical variables $f(\omega)$ and $g(\omega)$ are said to be in involution if their PB vanishes. Given such a special subset x with elements x_μ (half of these elements are zeros), we shall denote the complementary set of variables, namely, those left out of x, by $\tilde{x}$, and its elements by $\tilde{x}_\mu$. Along with each x, $\tilde{x}$ is also one of the 2^n special subsets defined above, and we always have

$$x_\mu + \tilde{x}_\mu = \omega_\mu, \mu = 1, 2, \ldots, 2\,n \tag{1.7}$$

In this paper we shall for simplicity deal with time-independent canonical transformations in the classical case, and time-independent unitary transformations in the quantum case. (Generalisation of our results to the time-dependent case is straightforward). A classical canonical transformation consists in giving $2\,n$ independent phase space functions $Q_r(q, p)$, $P_r(q, p)$, $r = 1, 2, \ldots, n$, which obey the fundamental PB relations

$$\{Q_r, Q_s\} = \{P_r, P_s\} = 0, \quad \{Q_r, P_s\} = \delta_{rs} \tag{1.8}$$

All these PB's are to be evaluated using eq. 1.1. It is very well known that if any such transformation is given, one always has

$$\sum_{r=1}^{n} (p_r \mathrm{d}q_r - P_r \mathrm{d}Q_r) = \mathrm{d}W \tag{1.9}$$

where W is some function on phase space; in fact the condition that the left hand side of eq. 1.9 be a perfect differential is the necessary and sufficient condition that the transformation $q, p \rightarrow Q, P$ be canonical. If for a given transformation, the $2n$ variables q_r, Q_r form an independent set, one can imagine the function W expressed as a function of them; writing $W = S(q; Q)$, one immediately obtains eq. (A) of the introduction characterising such canonical transformations. The other three commonly treated types of generating functions correspond to the variable sets (q, P), (p, Q), (p, P) forming maximal independent sets (Kilmister, 1964). One deals with each of these by suitably altering the left hand side of eq. 1.9. However, it is easy to write down canonical transformations for which none of these four possibilities exists.

We now state Carathéodory's theorem. Let a canonical transformation $q_r, p_r \rightarrow Q_r, P_r$ be given, and let x be any special subset of the q's and p's chosen in the manner described earlier. Then the theorem says that there will always be at east one special subset X formed from the new variables Q, P such that the $2n$, quantities x_μ, X_μ form a maximal independent set. With the given canonical transformation we can then associate several such complete sets of variables (x, X), there being *at least one* for each of the 2^n possible choices of x; and with the help of each such complete set we get one explicit description of the transformation. With the use of the matrix $\| \epsilon^{\mu\nu} \|$ which is inverse to $\| \epsilon_{\mu\nu} \|$, we can easily manipulate eq. 1.9 so as to read

$$\epsilon^{\mu\nu} (\tilde{x}_\mu \mathrm{d}x_\nu - \tilde{X}_\mu \mathrm{d}X_\nu) = \text{perfect differential}$$
$$= \mathrm{d}S(x; X) \tag{1.10}$$

The generating function $S(x; X)$ is unique up to an additive constant, and has been written in terms of the independent set (x, X). The generalisation of eq. (A) of the introduction clearly reads

$$\tilde{x}_\lambda = - \epsilon_{\lambda\mu} \frac{\partial S(x; X)}{\partial x_\mu}, \quad \tilde{X}_\lambda = \epsilon_{\lambda\mu} \frac{\partial S(x; X)}{\partial X_\mu} \tag{1.11}$$

and the function $S(x; X)$ will obey the condition that the first half of the above transformation equations allow the X's to be solved for in terms of x, $\tilde{x}$. (One must restrict λ in eq. 1.11 to those values that correspond to non-zero components of $\tilde{x}$ and $\tilde{X}$). Let now (x, X) and (y, Y) be two complete sets of co-ordinates associated with a given canonical transformation, and write $S(x; X)$, $S'(y; Y)$ for the generating functions in the two cases. The final equation we are interested in is the one that relates these two generating functions. Apart from an additive constant, one easily finds the relation to be

$$S'(y; Y) = S(x; X) + \epsilon^{\mu\nu} (x_\mu y_\nu - X_\mu Y_\nu) \tag{1.12}$$

We stress that the functions S and S' give two possible descriptions of one and the same canonical transformation and that the relation between them is a local one in phase space.

2. The quantum mechanical case

We now consider a quantum-mechanical system describable in terms of n canonically conjugate pairs of position and momentum operators q_r, p_r, $r = 1, 2, \ldots n$. (The symbols q, p, x, y, ... of the last section will be used again here, though now they denote linear operators on a Hilbert space; this makes the writing easier and causes no confusion). These operators are assumed to be hermitian and irreducible or complete and to obey the fundamental commutation relations

$$[q_r, q_s] = [p_r, p_s] = 0, \; [q_r, p_s] = i\hbar\delta_{rs} \tag{2.1}$$

(h is Planck's constant and $\hbar = h/2\pi$). For definiteness we assume that each of the operators q_r, p_r has all real numbers from $-\infty$ to $+\infty$ for eigenvalues, analogous to their being Cartesian position and momentum operators for particles. The property of irreducibility or completeness may be described in two ways: one is that, roughly speaking, all dynamical variables for the system can be constructed as functions of the q's and p's; the other is that any operator that commutes with all the q's and p's is necessarily a C-number.

Subsets of operators $x = \{x_\mu\}$, formed out of the q's and p's in the manner described in the classical case, have now a simple description in the standard terminology of quantum mechanics (Dirac 1958): they are just the complete commuting sets of operators that one can pick out of the complete set of operators q_r, p_r, and there are exactly 2^n such complete commuting sets. Further, if x is one of these sets, so is the complementary set of operators $\tilde{x}$. The simultaneous eigenvectors of the operators x_μ are non-degenerate and form a basis for the Hilbert space. We will write x', x'', ... for collections of eigenvalues of the x; x' stands for a set of numbers $\{x'_\mu\}$, with a particular entry being zero if the corresponding operator entry in x is zero. Thus the n non-vanishing real numbers in x' denote a set of eigenvalues for the corresponding n commuting operators in x. The main properties of the normalised simultaneous eigenvectors of the x are summarised by

$$x_\mu \,|\, x'\rangle = x_\mu' \,|\, x'\rangle, \;\; \langle x'' \,|\, x'\rangle = \prod_\mu \delta(x_\mu'' - x_\mu') \tag{2.2}$$

where in the second equation the product is taken over those values of μ for which x_μ is not zero. The phases of these basis vectors $|\, x'\rangle$ are not determined by these equations, but they can be adjusted so that the complementary set of operators $\tilde{x}$ has the representation

$$\tilde{x}_\mu \,|\, x'\rangle = -\,i\hbar\epsilon_{\mu\nu} \frac{\partial}{\partial x'_\nu} \,|\, x'\rangle, \;\; \langle x' \,|\, \tilde{x}_\mu = i\hbar\epsilon_{\mu\nu} \frac{\partial}{\partial x'_\nu} \langle x' \,| \tag{2.3}$$

Again, we restrict μ to values for which $\tilde{x}_\mu$ is not zero.

We can now state the quantum-mechanical analogue of Carathéodory's theorems. Let U be any fixed unitary transformation and let us write Q_r, P_r for the transforms of q_r, p_r by U:

$$Q_r = Uq_r U^{-1}, \; P_r = Up_r U^{-1}, \; r = 1, 2, \ldots, n \tag{2.4}$$

Then the Q's and P's also obey eq. 2.1, are irreducible and complete, and analogs to eqs 2.2, 2.3 for subsets X, $\tilde{X}$ of them can be written down. We assert: Given a complete commuting subset x of the operators q_r, p_r and a definite unitary operator U, one can always find a complete commuting subset X of the operators Q_r, P_r, such that the $2n$ operators contained in x and X form an irreducible and hence complete set.

We shall first prove a particular case of this result, and then explain how the general case follows. Let the complete commuting set x consist of the operators q_r, $r = 1, 2, \ldots, n$. Consider now some subset of the operators Q_r, say $\{Q_\rho\}$ with ρ running over a selection of the numbers $1, 2 \ldots, n$. We shall say that the property Θ holds for $\{Q_\rho\}$ if the following is true: if we choose any one of the Q's in $\{Q_\rho\}$, it is possible to find an operator that does not commute with it but that commutes with the remaining Q's in $\{Q_\rho\}$ as well as with all the q's. In such a case, none of the operators in $\{Q_\rho\}$ can be expressed as a function of the remaining ones and the q's. If Θ fails for $\{Q_\rho\}$, it must fail with respect to at least one of these Q's. Let us now start with the full set of Q's, namely $Q_1, Q_2, \cdots, Q_n$, and enquire if Θ holds for this set. If it does, then none of the Q's can be expressed as a function of the other Q's and all the q's. In this case, our proof when completed will show that the $2n$ operators $q_1, \ldots, q_n$, $Q_1, \ldots, Q_n$ are irreducible and so complete. More generally, let us suppose Θ fails for $Q_1, Q_2, \ldots, Q_n$, and for simplicity of notation suppose it fails with respect to Q_n. That means that any operator commuting with the $(2n-1)$ operators $q_1, \ldots, q_n, Q_1, \ldots Q_{n-1}$ automatically commutes with Q_n as well; we may conclude that Q_n is some function of $q_1, \ldots, q_n, Q_1, \ldots, Q_{n-1}$. (Jordan 1969). Consider next the set $Q_1, \ldots, Q_{n-1}$ and suppose Θ fails again, and once more for notational simplicity suppose it fails with respect to Q_{n-1}. We then conclude as before that Q_{n-1} is some function of $q_1, \ldots, q_n, Q_1, \ldots, Q_{n-2}$; using this expression for Q_{n-1} in the previously established expression for Q_n, we find that the latter is also some function of $q_1 \ldots, q_n, Q_1, \ldots, Q_{n-2}$. Proceeding in this way, we may end up with all the Q's being expressed as functions of the q's, which means that Θ fails for every subset $\{Q_\rho\}$ of the Q's. In this case, we can see that the $2n$ operators $q_1, \ldots, q_n, P_1, \ldots, P_n$ form an irreducible set. For, any operator F commuting with these $2n$ operators also obviously does so with $Q_1, \ldots, Q_n, P_1, \ldots, P_n$; but the latter set is irreducible, so F must be a C-number. More generally, we will end up with a subset of Q's for which Θ holds, and each of the remaining Q's is some function of the Q's in the subset and all the q's. Again for simplicity of notation suppose Θ holds for $Q_1, \ldots, Q_A$, and that each Q_r for $r = A + 1, \ldots, n$ is some function of the n q's and the first A Q's. We shall now show that the $2n$ operators $q_1, \ldots, q_n, Q_1, \ldots, Q_A, P_{A+1}, \ldots, P_n$ form an irreducible set. Let F be an operator commuting with each of these $2n$ operators:

$$[F, q_r] = 0, \; r = 1, 2, \ldots, n \tag{2.5 a}$$

$$[F, Q_r] = 0, \; r = 1, 2, \ldots, A \tag{2.5 b}$$

$$[F, P_r] = 0, \; r = A + 1, \ldots, n \tag{2.5 c}$$

Since each Q_r for $r = A + 1, \ldots, n$ is a function of the q's and $Q_1, \ldots, Q_A$, from eqs 2.5 *a, b* we conclude that

$$[F, Q_r] = 0, \; r = A + 1, \ldots, n \tag{2.6}$$

Thus F commutes with all the q's and likewise with all the Q's. Recalling that each of these is a complete commuting set by itself, we see that F must on the one hand be a function of the q's alone, and on the other hand it must be a function of the Q's alone:

$$F = \psi(q_1, \ldots, q_n) = \phi(Q_1, \ldots, Q_n) \tag{2.7}$$

Using this expression of F in terms of the Q's and imposing eq. 2.5 *c*, we see that in fact ϕ is a function of $Q_1, \ldots, Q_A$ alone, so we henceforth write $\phi(Q_1, \ldots, Q_A)$. If both ψ and ϕ had no genuine dependences on their arguments but were merely constants, that would be proof that F is a C-number and so the irreducibility of $q_1, \ldots q_n, Q_1, \ldots, Q_A, P_{A+1}, \ldots, P_n$, would be established. But this must necessarily be the case! If ϕ has some essential dependence on its arguments, so must ψ on *its* arguments; the second equality in eq. 2.7 could be written as

$$\Phi(Q_1, Q_2, \ldots, Q_A, \psi(q)) = 0 \tag{2.8}$$

denoting some functional relation among the operators appearing inside Φ. Now in general the Q's and the q's do not mutually commute, so any relation connecting them cannot be handled as a classical equation. But in eq. 2.8, the q's appear only in the combination $\psi(q)$, and this combination *does* commute with each Q, by virtue of eq. 2.7. Thus eq. 2.8 is a connection among mutually commuting operators, so it can be handled just like a classical equation. To the extent that there is some dependence on the Q's, we can use eq. 2.8 to solve for and express one of the operators $Q_1, \ldots, Q_A$ as a function of the remaining Q's in this set, and the function $\psi(q)$. But this must be impossible since the property Θ holds for $Q_1, \ldots, Q_A$! Hence there can be no essential dependence on any Q in eq. 2.8, and none on the q's either. Thus the operator F must be a C-number, and the irreducibility of the set $q_1, \ldots, q_n$, $Q_1, \ldots, Q_A$, $P_{A+1}, \ldots, P_n$ is proved.

We thus see that for the special case when the complete commuting set x chosen from the q's and p's consists of the q's, we can find a complete commuting set X from the Q's and P's, namely $Q_1, \ldots, Q_A$, $P_{A+1}, \ldots, P_n$, such that x and X are together irreducible. It is now easy to generalise to any other choice of x. A general choice of x differs from the choice $q_1, \ldots, q_n$ by having some of these q's replaced by their canonically conjugate p's. But, the interchange

$$q_r \rightarrow p_r, \, p_r \rightarrow -q_r \tag{2.9}$$

carried out for any collection of values of r constitutes, as is well known, a unitary transformation (or more precisely, there is a unitary transformation that implements it); it is just the Fourier transformation with respect to the relevant set of q's. Given any complete commuting set x chosen from the q's and p's, and the operators Q_r, P_r resulting from q_r, p_r by a unitary transformation U, we can introduce an intermediate set of operators $\bar{q}_r$, $\bar{p}_r$ such that x consists of $\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_n$. These operators $\bar{q}, \bar{p}$ will be unitarily related both to q, p and to Q, P. The theorem in the form already proved applies to the transition $\bar{q}, \bar{p} \rightarrow Q, P$, showing that a complete commuting set X out of Q_r, P_r, can be adjoined to the complete commuting set $\bar{q}_1, \ldots, \bar{q}_n$ to yield an irreducible set. But since the set $\bar{q}_1, \ldots, \bar{q}_n$ consists of precisely the initially chosen set x picked up from the operators q_r, p_r, the quantum-mechanical version of Carathéodory's theorem, as stated following eq. 2.4, is seen to be proved.

3. Representations of a unitary transformation

We shall now show that equations similar to eq. 1.11 can be set up to characterise a unitary transformation in quantum mechanics, thereby further developing the analogies existing between classical and quantum mechanics.

The complete set of operators q_r, p_r, $r = 1, 2, \ldots, n$, and the unitary operator U being given, we have first the transformed operators Q_r, P_r which are also complete. Next, with any given complete commuting set x out of the q's and p's, we associate a complete commuting set X out of the Q's and P's, such that the $2n$ operators in x and X are together irreducible. Given x, there exists at least one such X, as shown in the previous section. The simultaneous eigenvectors of the x's give a basis for the Hilbert space, characterised by eqs 2.2, 2.3. Similarly the simultaneous eigenvectors of the X_μ also define a basis for the Hilbert space, and we have the properties

$$X_\mu \mid X' \rangle = X_\mu' \mid X' \rangle \, , \quad \langle X'' \mid X' \rangle = \prod_\mu \delta(X_\mu'' - X_\mu')$$

$$\tilde{X}_\mu \mid X' \rangle = - i\hbar \epsilon_{\mu\nu} \frac{\partial}{\partial X_\nu'} \mid X' \rangle \, , \quad \langle X' \mid \tilde{X}_\mu = i\hbar \epsilon_{\mu\nu} \frac{\partial}{\partial X_\nu'} \langle X' \mid \tag{3.1}$$

With the forms chosen for $\tilde{x}$ and $\tilde{X}$ in the respective bases, there are no phase ambiguities either in $\mid x' \rangle$ or in $\mid X' \rangle$ (except for overall constant phase factors). The unitary transformation U is then completely characterised by the scalar products of vectors drawn from these two bases, namely, by

$$\langle x' \mid X' \rangle \tag{3.2}$$

taken for all allowed values of the eigenvalue sets x' and X'. We know in advance that x and X together constitute a complete set, so that any other operator can be expressed as a function of these. Using a result of Dirac, we then see that the scalar product 3.2 will not vanish for any values of x' and X' in their allowed domains of variation (Dirac 1945). (Qualitatively speaking, if there had been any functional relations among the x_μ's and X_μ's, that would have led to the scalar product 3.2 being proportional to one or more delta functions with arguments depending on x' and X', but we are assured this will not happen). A general operator F is fully determined by its "mixed x-X representative" which consists of the "matrix elements":

$$F(x'; X') = \langle x' \mid F \mid X' \rangle \tag{3.3}$$

(However, these mixed representatives must not be treated the way one treats matrices, since the x-X representative of the product FG of two operators F, G is not simply the "matrix product" of the individual x-X representatives but involves an intermediate integration with a non-trivial factor). To express F explicitly as a function of x and X, we consider the function of x' and X' defined by

$$\frac{F(x'; X')}{\langle x' \mid X' \rangle} = \frac{\langle x' \mid F \mid X' \rangle}{\langle x' \mid X' \rangle} \tag{3.4}$$

which we may since by Dirac's result $\langle x' \mid X' \rangle$ never vanishes, and then expand its x' and X' dependences in the general form

$$\frac{F(x'; X')}{\langle x' \mid X' \rangle} = \sum_n u_n(x') \, v_n(X') \tag{3.5}$$

For example, one can expand the X'-dependence of the left hand side of eq. 3.5 in terms of some complete set of functions $v_n(X')$, and denote the expansion coefficients by $u_n(x')$. (The choice of the complete set $v_n(X')$ is arbitrary and does not influence what follows). Using eq. (3.5), one can express F as a "well-ordered" function of x and X, namely, the dependences on x always stand to the left of dependences on X:

$$\begin{aligned} \langle x' \mid F \mid X' \rangle &= \Sigma_n \langle x' \mid u_n(x') \, v_n(X') \mid X' \rangle \\ &= \Sigma_n \langle x' \mid u_n(x) \, v_n(X) \mid X' \rangle \\ F &= \Sigma_n u_n(x) \, v_n(X) \end{aligned} \tag{3.6}$$

We now use the above formulae to compute the mixed x-X representatives of the operators $\tilde{x}_\mu$, $\tilde{X}_\mu$, and then deduce their expressions in terms of x and X. Following Dirac (Dirac 1933), we introduce a function $S(x';\ X')$ by setting

$$\langle x' \mid X' \rangle = \exp(\mathrm{i}S(x';\ X')/\hbar) \tag{3.7}$$

and denote the corresponding well-ordered *operator* obtained via eqs 3.5, 3.6 by $S(x;\ X)$. This operator need not be hermitian. Making use of eqs 2.3, 3.7, we get:

$$\langle x' \mid \tilde{x}_\mu \mid X' \rangle = \mathrm{i}\hbar\epsilon_{\mu\nu}\frac{\partial}{\partial x_\nu'}\langle x' \mid X' \rangle = -\epsilon_{\mu\nu}\frac{\partial S(x';\ X')}{\partial x_\nu'}\langle x' \mid X' \rangle$$

$$= -\epsilon_{\mu\nu}\langle x' \mid \frac{\partial S(x_2;\ X)}{\partial x_\nu} \mid X' \rangle$$

$$\tilde{x}_\mu = -\epsilon_{\mu\nu}\frac{\partial S(x;\ X)}{\partial X_\nu} \tag{3.8}$$

Similarly combining eqs 3.1, 3.7 leads to

$$\tilde{X}_\mu = \epsilon_{\mu\nu}\frac{\partial S(x;\ X)}{\partial X_\nu} \tag{3.9}$$

In the above two equations, we restrict μ to values for which the left hand sides do not vanish. These are now operator equations, and the operations $\partial/\partial X_\nu$, $\partial/\partial x_\nu$ have a straightforward meaning since x and X are individually commuting sets and $S(x;\ X)$ is well-ordered. Comparing these operator equations with eq. 1.11 valid for a classical canonical transformation, (recall that there all the quantities x, X, S are classical real variables), we see that the equations are of the same form in the two cases; it is just that the meanings attached to the symbols are different.

Two different descriptions of a given canonical transformation in classical dynamics, both of the general form of eq. 1.11, involve two different generating functions related by eq. 1.12. We want to obtain the quantum-mechanical analogue of eq. 1.12. The unitary operator U being held fixed, let x, X be one complete set of operators of the type described above, and let y, Y be another. Then the transformation U is characterised by a function $S(x';\ X')$ or equally well by a function $S'(y';\ Y')$, and we seek the relation between them. In the general case, the complete commuting set y differs from the set x in that some of the q's in x are replaced by their corresponding p's, some of the p's in x by their q's, and the remaining operators in x reappear in y; X and Y are similarly related. To connect $S(x';X')$ and $S'(y';\ Y')$ in this most general case would require a massive automation of the notation. It suffices to examine a couple of special cases from which the general form of the transformation law to go from S to S' can be deduced. Let us suppose the unitary transformation U admits both $x = q_1, \ldots, q_n$, $X = Q_1, \ldots, Q_n$ and $y = p_1, \ldots, p_n$, $Y = P_1, \ldots, P_n$ as complete sets. We want to relate $S(q';\ Q')$ and $S'(p';\ P')$. For a single degree of freedom, (one q and one p), the eigenvectors of q and of p are related by Fourier transformation:

$$\mid p' \rangle = \int_{-\infty}^{\infty} \mathrm{d}q' h^{-\frac{1}{2}} \exp(\mathrm{i}p'q'/\hbar) \mid q' \rangle$$

$$\mid q' \rangle = \int_{-\infty}^{\infty} \mathrm{d}p' h^{-\frac{1}{2}} \exp(-\mathrm{i}q'p'/\hbar) \mid p' \rangle \tag{3.10}$$

For the relation between $S(q';\ Q')$ and $S'(p';\ P')$ we then get:

$$\langle p' \mid P' \rangle = \int_{-\infty}^{\infty} \left(\prod_{r=1}^{n} \mathrm{d}q_r'\,\mathrm{d}Q_r' \right) \langle p' \mid q' \rangle \langle q' \mid Q' \rangle \langle Q' \mid P' \rangle$$

$$= \int_{-\infty}^{\infty} \left(\prod_{r=1}^{n} \mathrm{d}q_r'\,\mathrm{d}Q_r' \right) h^{-n} \langle q' \mid Q' \rangle \exp\left(\frac{\mathrm{i}}{\hbar} \sum_{r=1}^{n} (P_r'Q_r' - p_r'\,q_r') \right)$$

$$\exp\left(\frac{\mathrm{i}}{\hbar} S'(p';\ P') \right) = \int_{-\infty}^{\infty} \left(\prod_{r=1}^{n} \mathrm{d}q_r'\mathrm{d}Q_r' \right) h^{-n} \times$$

$$\times \exp\left(\frac{\mathrm{i}}{\hbar} \left\{ S(q';\ Q') + \sum_{r=1}^{n} (P_r'Q_r' - p_r'q_r') \right\} \right) \tag{3.11}$$

This example is an extreme case in the sense that none of the operators in the set x, X appears in y, Y. The classical relation corresponding to eq. 3.11 arises from specialising eq. 1.12 appropriately and reads:

$$S'(p;P) = S(q;\ Q) + \sum_{r=1}^{n} \ (P_r\,Q_r - p_r q_r) \tag{3.12}$$

As another example, one in which $(x,\ X)$ and $(y,\ Y)$ possess common elements, consider a unitary transformation U that admits $x = q_1, \ldots, q_n$, $y = p_1 \ldots, p_n$, $X = Y = Q_1, \ldots, Q_n$. That is, both q, Q and p, Q form irreducible sets. Then eq. 3.11 gets replaced by

$$\exp\left(\frac{\mathrm{i}}{\hbar} S'(p';\ Q') \right)$$

$$= \int_{-\infty}^{\infty} \left(\prod_{r=1}^{n} \mathrm{d}q_r' \right) h^{-n/2} \exp\left(\frac{\mathrm{i}}{\hbar} \left\{ S(q';\ Q') - \sum_{r=1}^{n} p_r'q_r' \right\} \right) \tag{3.13}$$

whereas the corresponding classical relation would have been:

$$S'(p;Q) = S(q;\ Q) - \sum_{r=1}^{n} \ p_r q_r \tag{3.14}$$

From these examples one quickly realises that the general rule for obtaining $S'(y';\ Y')$ from $S(x';\ X')$ is to "exponentiate the classical relation" eq. 1.12 and integrate with respect to the eigenvalues of those operators in $(x,\ X)$ that do not appear in $(y,\ Y)$:

$$\exp\left(\frac{\mathrm{i}}{\hbar} S'(y';\ Y') \right) = \int_{-\infty}^{\infty} \left(\prod_{\mu}^{*} h^{-\frac{1}{2}}\,\mathrm{d}x'_\mu \right) \left(\prod_{\nu}^{*} h^{-\frac{1}{2}}\,\mathrm{d}X'_\nu \right) \times$$

$$\times \exp\left(\frac{\mathrm{i}}{\hbar} \left\{ S(X';x') + \epsilon^{\mu\nu}\,(x_\mu' y_\nu' - X_\mu' Y_\nu') \right\} \right) \tag{3.15}$$

The asterisk on the product over μ means that μ runs over those values for which the operator x_μ is absent in the set y; and similarly for the product over ν. If a particular operator from $x(X)$ reappears in $y(Y)$, then the same numerical eigenvalue of it appears as one of the arguments of $S(x'; X')$ and of $S'(y'; Y')$ (and clearly this eigenvalue is *not* integrated over).

The interesting point that emerges is that while the equations that determine a canonical transformation on the one hand, and those that determine a unitary transformation on the other, have exactly similar forms, namely eq. 1.11 and eqs 3.8, 3.9, the laws relating different descriptions of a given transformation are rather different in the two cases. In the classical case, eq. 1.12 connecting two possible generating functions is a local one in phase space. The corresponding connection in the quantum case is a nonlocal one; examples are provided by eqs 3.11, 3.13.

Concluding remarks

We have formulated and proved a quantum-mechanical analogue of Carathéodory's theorem in classical mechanics, and derived quantum analogues to several classical equations. To conclude, we make several comments that help interpret our results and further illumine the relationship between classical and quantum mechanics.

Dirac showed that the condition that must be satisfied by the operators $q_1, \ldots, q_n, Q_1, \ldots, Q_n$ in order that any other operator be expressible as a function of them is that the scalar product $\langle q' \mid Q' \rangle$ never vanish. Clearly this criterion must be the same as the condition of irreducibility of the q's and Q's taken together, for that too would permit every operator to be expressed as some function of the q's and Q's. Exactly similar results hold for the pairs of complete commuting sets (x, X) we have been considering. If (x, X) is irreducible, Dirac's work allows us to assert that $\langle x' \mid X' \rangle$ never vanishes; only then does it make sense to define a function $S(x'; X')$ as in eq. 3.7, and only then do we have a basis for deriving the quantum operator equations like eqs 3.8, 3.9. If the set (x, X) were not irreducible, there would be some relations among these operators; assuming these relations could be written in well-ordered form, they would result in $\langle x' \mid X' \rangle$ being proportional to a product of delta functions that constrain x' and X', and we would be unable to express a delta function as an exponential in the form of eq. 3.7. One could then follow Dirac's method and introduce further operators analogous to Lagrangian multipliers, but the theorem in section 2 assures us that we can avoid this by switching to some irreducible set (y, Y) which is bound to exist.

Concerning the transformation law given in eq. 3.15 in the quantum-mechanical case, the following explanatory remarks may be made. We have seen that if (x, X) is an irreducible set, then on the basis of eqs 3.3–3.6, to each function $F(x'; X')$ corresponds one well-ordered operator and conversely; quite generally, any operator can be expressed in well-ordered form. One might then be tempted to rewrite eq. 3.15 as an equation relating the operators defined by the functions $S(x'; X')$ and $S'(y'; Y')$ in their respective mixed bases, *i.e.*, convert the C-number eq. 3.15 into an operator statement hopefully similar in structure to eq. 1.12. But the problem is that there is no *simple* connection between the well-ordered form of an operator F and the well-ordered form of its exponential $\exp(F)$. All the same, there is a simple operator interpretation of eq. 3.15 which is the following. From its definition in eq. 3.7, we see that the function $\exp(iS(x'; X')/\hbar)$ is just the mixed x-X representative of the unit operator! Thus while $S(x'; X')$ corresponds to a possibly complicated operator (and it is this operator that appears in eqs 3.8, 3.9), the function $\exp(iS(x'; X')/\hbar)$ corresponds to a very simple operator. It is because we are using mixed representatives for operators that a trivial operator, namely, the unit operator, possesses a non-trivial function of the state lables x', X' as its representative. With this understanding one can claim: the quantum-mechanical analogue to the classical law eq. 1.12 relating two different generating functions for a given canonical transformation is the law that relates one mixed representative of the unit operator to another, the given unitary transformation determining which mixed representatives are allowed.

It is interesting to explore further the structure of eq. 3.15 with a view to exposing the significance of the exponentials occurring there. It is well known that a unitary transformation in quantum mechanics, which, for example, belongs to a one-parameter group of such transformations, can be written as the exponential of an antihermitian operator. Similarly, the elements of a one-parameter group of canonical transformations in classical mechanics can be written as the exponentials of a first order partial differential operator in phase space, with a structure determined by the classical PB. These two facts are really analogues of one another denoting similarity of structure, and the exponential functions appearing in the two cases are also truly analogous. However, the exponential functions $\exp(iS/\hbar)$, $\exp(iS'/\hbar)$ appearing in eq. 3.15 are of a quite different nature, and are symbolic of the relationship *between* classical mechanics and quantum mechanics. This is because there is no motivation that can be given purely within quantum mechanics for expressing the scalar product $\langle x' \mid X' \rangle$ as the exponential of some function of x' and X', and then examining the properties of this function. It is the desire to have the equations characterising a unitary transformation in quantum mechanics take up forms exactly like those characterising a canonical transformation in classical mechanics that prompts the definition of the function $S(x'; X')$ as in eq. 3.7, and this structure for $\langle x' \mid X' \rangle$ is automatically reflected in the transformation law eq. 3.15. One sees the truth of this statement also when one examines the way in which the Schrödinger equation in non-relativistic quantum mechanics, treated in the W.K.B. approximatior, yields in leading order the Hamilton-Jacobi equation of classical dynamics (Messiah 1970).

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