

Descriptions of operators in quantum mechanics

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Abstract. The problem of expressing a general dynamical variable in quantum mechanics as a function of a primitive set of operators is studied from several points of view. In the context of the Heisenberg commutation relation, the Weyl representation for operators and a new Fourier-Mellin representation are related to the Heisenberg group and the group $SL(2, R)$ respectively. The description of unitary transformations via generating functions is analysed in detail. The relation between functions and ordered functions of noncommuting operators is discussed, and results closely paralleling classical results are obtained.

Keywords. Heisenberg group; Weyl representation; Fourier-Mellin representation for operators; functions of operators.

1. Introduction

The study of quantum mechanics brings one into contact in a natural way with several areas of mathematics. These include the theory of Hilbert space; the eigenvalue and eigenfunction analysis of hermitian and unitary operators; expansion theorems using various complete orthonormal systems of functions; elements of the theory of Lie groups and Lie algebras, and the construction of their unitary as well as non-unitary representations. There is, however, a subject of general mathematical and conceptual significance that is not dealt with in most discussions of the subject. This is an analysis of the sense or senses in which all dynamical variables of a physical system can be thought of as being functions of a primitive set of variables. The study of a specific system begins with a statement of its kinematic structure: a set of primitive dynamical variables is chosen and definite commutation relations are postulated among them. The adjective 'primitive' means that by forming all functions (suitably understood) of these variables, one obtains all the dynamical variables pertaining to the system. In practice one is usually interested in a small number of dynamical variables, each having a well-defined physical interpretation, and these are explicitly given in terms of the primitive set. With the use of the basic commutation relations, one then studies the eigenvalue and eigenfunction problems for these important physical quantities. The relations between the different descriptions of the Hilbert space corresponding to one or another physical quantity being diagonal can also be worked out; these relations connect the various possible representatives of abstract state vectors to one another.

The phase space description of a classical dynamical system uses a canonical set of variables made up of coordinates q and conjugate momenta p as a primitive set. At least in an intuitive and immediate sense one understands how every dynamical

variable is some function of the q and p : the values of the latter determine that of the former. Indeed, dynamical variables are so defined. It would be valuable to have a similar simple understanding of the way in which any operator dynamical variable for a quantum system can be understood to be some function of the primitive variables of the system. In quantum mechanics one imposes the property of irreducibility on the primitive set of operators, ensuring that all other operators are indeed functions of them. One's understanding of the situation would be enhanced if this property could be made more tangible. This would be achieved by having ways in which, at least in principle, all dynamical variables, or at any rate a large and interesting class of them, could be explicitly written as functions of the primitive set.

The problem of explicit description of operators in quantum mechanics is naturally somewhat more complicated and subtle than the corresponding problem in classical mechanics. In making this remark we do not refer to the possible need for greater mathematical rigour in dealing with unbounded operators, their domains and ranges and the like, but rather merely to the complications arising from having to deal with noncommuting quantities in quantum mechanics. The purpose of this paper, written to some extent from a pedagogical point of view, is to give a discussion of these matters at a level accessible to anyone who is familiar with quantum mechanics as presented, say, in Dirac's classic book (Dirac [8]). Two approaches to the problem of operator description will be given, one based on group representation theory and the other on the transformation theory of dynamics. The former is in essence due to Racah and Wigner and is familiar from applications to atomic and nuclear spectroscopy (see, for instance, Fano and Racah [11]). The transformation theoretical approach is an extension of ideas pioneered by Dirac (Dirac [7]).

The arrangement of the material of this paper, and a brief description of it, are as follows. § 2 recalls the theory of tensor operators and unit tensors for the three-dimensional rotation group when one is dealing with an irreducible representation of this group. The basic ideas behind the group theoretical method are exhibited most simply via this example. §§ 3 and 4 use this method to give two possible descriptions of operators when the primitive set consists of two hermitian operators obeying the canonical Heisenberg commutation relation. In § 3 the discussion is based on the Heisenberg Lie algebra and its hermitian representations. On passing from the representation acting on vectors to that acting on operators one is led immediately to the Weyl representation for operators, which has been known and used for a long time (Weyl [21] p. 274). This is the quantum analogue of the Fourier integral representation for classical dynamical variables defined on a two-dimensional phase space. § 4 uses in a similar spirit the group $SL(2, R)$; this is the group of real linear transformations that preserves the Heisenberg commutation relation. One is now led to the quantum analogue to the Fourier-Mellin representation in the classical case. The remainder of the paper is devoted to systems with a general even number, $2n$, of canonical degrees of freedom. § 5 recapitulates the generating function description of classical canonical transformations, especially the distinctions between the so-called nondegenerate and degenerate cases (Whittaker [22] § 126; Caratheodory [5] Chapter 6). With such a description of a canonical transformation, one can try to give a mixed description for general dynamical variables. This involves expressing each dynamical variable as a function of a mixed set of $2n$ variables, half of which belong to the 'old' canonical set of variables and half to the 'new' set obtained after the canonical transformation. To the best of our knowledge some of the results found

here are new and not available in the literature; they turn out most useful for an appreciation of the quantum mechanical case. § 6 describes two definitions of the concept of a function of a given set of operators. The first is the one generally to be found in discussions on operator theory and representations of algebras of operators (for a simple discussion see Jordan [15] Chapter 4). The second, due to Jordan and Dirac, is based on the idea of ordered functions of operators; it is in general somewhat more special and restrictive than the first definition (Jordan [14]; Dirac [6, 7]). Using all this, § 7 gives a discussion of the generating function description for unitary transformations in quantum mechanics, paying special attention to the distinct cases that arise and stand in direct correspondence with the classical alternatives. As a result one sees clearly the connections between irreducibility, the set of all functions, and the set of all ordered functions, of a set of operators formed in the mixed manner as in the classical case.

Astonishingly close parallels exist at all stages between classical and quantum mechanics, and an effort will be made to bring this out clearly.

2. The Racah-Wigner method

Consider the hermitian irreducible representations of the angular momentum commutation relations in quantum mechanics (Edmonds [9]):

$$[J_k, J_l] = i \epsilon_{klm} J_m, \quad klm = 1, 2, 3. \quad (1)$$

In every dimension there is, upto unitary equivalence, exactly one such representation. The dimension written as $(2j + 1)$ with $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ is related to the value of the Casimir invariant J^2 by

$$J^2 \equiv J_1^2 + J_2^2 + J_3^2 = j(j + 1). \quad (2)$$

The odd (even) dimensional representations integrate to single (double) valued representations of the three dimensional rotation group $R(3)$. Thus for each rotation R there is a unitary operator $U(R)$ fixed upto a phase such that

$$U(R') U(R) = \omega(R', R) U(R' R), \quad (3)$$

with ω also a phase. For integral j the phases of the U s can be adjusted so that $\omega = +1$ for all arguments; for half-odd-integral j one can only achieve the restriction $\omega = \pm 1$.

Fix attention now on a definite value of j . The $(2j + 1)$ eigenvectors $|j m\rangle$ of J_3 with eigenvalues $m = j, j - 1, \dots, -j$ form an ortho-normal basis for the representation space. The effect of $U(R)$ on these basis vectors is given by the well-known D -matrices of angular momentum theory. Now the set of linear operators acting on the representation space itself forms a linear space of dimension $(2j + 1)^2$. Given the action of rotations on vectors through the operators $U(R)$, there follows an action on operators by the rule

$$A \rightarrow \mathcal{U}(R) A = U(R) A U(R)^{-1}, \quad (4)$$

A being a general operator. This rule being linear in A , \mathcal{U} is a linear operator on the set of linear operators A . This is similar to the passage from the Schrödinger picture to the Heisenberg picture in quantum mechanics. One obtains the unitary property for $\mathcal{U}(R)$ by defining an inner product among operators as

$$(A, B) = \text{Tr}(A^\dagger B). \quad (5)$$

Now, whatever be the value of j , $\mathcal{U}(R)$ obeys

$$\mathcal{U}(R') \mathcal{U}(R) = \mathcal{U}(R' R), \quad (6)$$

so that we always have here a unitary, single-valued representation of $R(3)$. The angular momenta J_k act as generators for $U(R)$ in the sense that the latter are exponentials of suitable linear combinations of the former. Similarly we can find the generators \mathcal{J}_k for $\mathcal{U}(R)$ by examining the form of (4) for infinitesimal rotations. One gets

$$\mathcal{J}_k A = [J_k A]. \quad (7)$$

These generators are hermitian with respect to the inner product (5).

The reduction of the representation $\mathcal{U}(R)$ will yield only odd-dimensional irreducible ones. From the Wigner-Eckart theorem the details of this reduction are completely known: only the representations with quantum number $K = 0, 1, 2, \dots, 2j$ occur, and each one once. That is, the space of operators considered contains spherical tensor operators of ranks $K = 0, 1, \dots, 2j$ alone; and apart from a scale factor there is just one tensor operator for each rank. Based on this, it is natural to define a set of unit tensors u_M^K through

$$\langle j m' | u_M^K | j m \rangle = \left(\frac{2K+1}{2j+1} \right)^{1/2} C(j K j | m M m'), \quad (8)$$

the C 's being Clebsch-Gordan coefficients for $R(3)$ (de Shalit and Talmi [20] p. 220). This definition is such that one has

$$(u_{M'}^{K'}, u_M^K) = \delta_{K'K} \delta_{M'M}. \quad (9)$$

The unit tensors have the following properties; under the representation $\mathcal{U}(R)$ each transforms irreducibly according to its rank; any spherical tensor operator of rank K is some multiple of the unit tensor of that rank; they form a basis for the space of operators so that a general operator A can be expressed as a sum

$$A = \sum_{K=0}^{2j} \sum_{M=-K}^K a_{KM} u_M^K, \quad (10)$$

$$a_{KM} = (u_M^K, A).$$

One obtains in this way a particular description of every operator A via the corresponding set of coefficients a_{KM} .

The unit tensors themselves are essentially polynomials in the operators J_k . Thus apart from a scale factor, u_M^1 is the spherical component J_M of angular momentum. To get u_M^2 we must form the spherical components of the symmetric traceless Cartesian second rank tensor operator

$$\frac{1}{2} (J_k J_l + J_l J_k) - \frac{1}{3} \delta_{kl} j(j+1).$$

And so on. Thus the above-mentioned description of a general operator A amounts to expressing it in a well-defined way as a polynomial in J_k .

The essential steps in the group-theoretical description of operators are then the following: one begins with a representation of a group at the level of vectors, possibly in the form (3) with nontrivial ω ; one obtains from this a true representation of the group by defining the transformation law of operators through an equation like (4); on reduction of this latter representation one obtains operators with irreducible transformation behaviours and at the same time one gets a definite description for operators in general.

3. Heisenberg group and Weyl representation

As a first application of the method outlined in the previous section, we describe what happens when the Heisenberg commutation relation of quantum mechanics is viewed as one of a set defining a Lie algebra. A Cartesian position variable q and its conjugate momentum p are hermitian operators obeying

$$[q, p] = i \hbar. \tag{11}$$

The right hand side actually stands for a numerical multiple of the unit operator. The form of (11) motivates the definition of the Heisenberg Lie algebra; this has three basis elements X, Y, Z say obeying the commutation relations

$$[X, Y] = iZ, [X, Z] = [Y, Z] = 0. \tag{12}$$

Elements g of the corresponding three-parameter Lie group can be labelled by real variables α, β, γ :

$$g(\alpha, \beta, \gamma) = \exp(i\alpha X - i\beta Y + i\gamma Z), -\infty < \alpha, \beta, \gamma < \infty. \tag{13}$$

The group multiplication law is easily obtained by using a standard formula for combining two exponentials of the above form when both X and Y commute with their commutator;

$$g(\alpha', \beta', \gamma') g(\alpha, \beta, \gamma) = g(\alpha' + \alpha, \beta' + \beta, \gamma' + \gamma + \frac{1}{2}(\alpha' \beta - \beta' \alpha)). \tag{14}$$

Let us now consider the unitary irreducible representations of this group, or equivalently the hermitian irreducible representations of the commutation relations (12).

Since Z commutes with all the generators, in any such representation it must be a real multiple of the unit operator. Now the representation will be infinite dimensional if Z does not vanish, one dimensional if it does. The former representations are essentially the familiar quantum mechanical solution to the commutation relation (11): Z may be taken as \hbar times the unit operator, $X=q$ and $Y=p$. As \hbar 'varies' without vanishing, we get a one-parameter family of inequivalent irreducible representations of the Heisenberg algebra: it consists of two continuous components for $-\infty < \hbar < 0$ and $0 < \hbar < \infty$. On the other hand if Z vanishes, the only commutation relation left to be satisfied demands that X and Y commute. There is thus a two-parameter family of such irreducible representations, each one dimensional, labelled (τ, σ) say, with $X = \tau$ and $Y = \sigma$. Here τ and σ are any two real numbers.

In a certain context, the set of one dimensional representations is assigned measure zero. Thus if one considers the Hilbert space of functions defined and square integrable over the Heisenberg group and sets up the left regular representation, say, this representation turns out to be a direct integral of the infinite dimensional unitary irreducible representations alone. However as we shall soon see in the problem of operator description only the one-dimensional representations appear.

Let \hbar now be given its 'actual' value, so that we are dealing with a specific infinite dimensional irreducible representation of the Heisenberg Lie algebra. The group element $g(\alpha, \beta, \gamma)$ is represented by the unitary operator

$$U(\alpha, \beta, \gamma) = \exp(i\alpha q - i\beta p + i\gamma \hbar), \quad (15)$$

acting on the vectors of the Hilbert space. (This space could be explicitly realised as consisting of all square integrable functions of q on which p acts as $-i\hbar$ times the derivative with respect to q). These unitary operators follow a composition rule exactly like (14). We must now define an action of the Heisenberg group on operators acting on the Hilbert space. Here we encounter a feature absent in the finite dimensional example of §2. There we were able to consider all operators acting on the space on which an irreducible representation of $R(3)$ was first given, and could define a suitable inner product for them. In the present case, the set of 'all' operators acting on the Hilbert space is a very large one, and it is quite impractical to deal with them all at once. One must restrict one self to some usefully chosen subset of them. One may choose to deal with all bounded operators; or all finite polynomials in q and p , which involves domain questions; and so on. For our present purposes we shall work with the so-called Hilbert-Schmidt ($H-S$) class of operators: an operator A is $H-S$ if and only if

$$\text{Tr}(A^\dagger A) < \infty. \quad (16)$$

Such operators form a linear set and in fact a Hilbert space of their own, provided the inner product is defined as

$$(A, B) = \text{Tr}(A^\dagger B). \quad (17)$$

The point is that in finite dimensions such an inner product makes sense for all operators, while in infinite dimensions one must restrict oneself to those operators for

which it makes sense. This is quite a restriction: for example, the unit operator, or any unitary operator, violate condition (16).

On the space of $H-S$ operators we now define a unitary representation of the Heisenberg group in the fashion of (4):

$$\mathcal{U}(\alpha, \beta, \gamma) A = U(\alpha, \beta, \gamma) A U(\alpha, \beta, \gamma)^{-1}. \quad (18)$$

It is trivial to see that $\mathcal{U}(\alpha, \beta, \gamma)$ has actually no dependence on γ at all. We have thus obtained a representation of the Heisenberg group for which the generator Z vanishes: it follows that this representation must be a direct integral (generalisation of direct sum) of the one-dimensional representations described earlier. Denoting the generators for the representation $\mathcal{U}(\alpha, \beta, \gamma)$ by the letters X, Y, Z themselves, we get from (15):

$$\begin{aligned} X &= -i \left. \frac{\partial \mathcal{U}(\alpha, 0, 0)}{\partial \alpha} \right|_{\alpha=0}, & XA &= [q, A]; \\ Y &= -i \left. \frac{\partial \mathcal{U}(0, \beta, 0)}{\partial \beta} \right|_{\beta=0}, & YA &= [p, A]; \\ Z &= -i \left. \frac{\partial \mathcal{U}(0, 0, \gamma)}{\partial \gamma} \right|_{\gamma=0} = 0. \end{aligned} \quad (19)$$

To exhibit the representation \mathcal{U} as a direct integral, one must 'simultaneously diagonalise' X and Y , remembering that they are operators acting on $H-S$ operators. It turns out that the 'simultaneous eigenfunctions' of X and Y with real eigenvalues for both are the elementary exponentials used in (15) (Weyl [21] p. 275):

$$\begin{aligned} X \exp(i\sigma q - i\tau p) &= \tau \exp(i\sigma q - i\tau p), \\ Y \exp(i\sigma q - i\tau p) &= \sigma \exp(i\sigma q - i\tau p), \quad -\infty < \tau, \sigma < \infty. \end{aligned} \quad (20)$$

These operators do not really belong to the $H-S$ class but bear the same relation to this class of operators that momentum eigenfunctions bear to the underlying Hilbert space of square-integrable functions of q . Thus one can formally show that

$$(\exp(i\sigma'q - i\tau'p), \exp(i\sigma q - i\tau p)) = 2\pi \delta(\tau' - \tau) \delta(\sigma' - \sigma). \quad (21)$$

The 'simultaneous eigenfunctions' of X and Y can therefore be used as an orthonormal basis for operators, being normalised in the delta function sense. They give us a particular description or representation in which each $H-S$ operator can be expanded as

$$\begin{aligned} A &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\sigma \alpha(\tau, \sigma) \exp(i\sigma q - i\tau p), \\ \alpha(\tau, \sigma) &= (2\pi)^{-1/2} (\exp(i\sigma q - i\tau p), A), \end{aligned} \quad (22)$$

$$\text{with} \quad (A, A) = \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\sigma |\alpha(\tau, \sigma)|^2. \quad (23)$$

We see that this explicit representation of an operator A as a function of the primitive set of operators q and p is the quantum version of the classical Fourier integral representation for functions on a two-dimensional phase plane. It is known as the Weyl representation and has been widely used in many contexts (for a rigorous discussion of this representation see Pool [18]). The interesting point is that it emerges naturally on applying the Racah-Wigner method to the Heisenberg group: in this sense this representation is intrinsically associated with the Heisenberg commutation relation itself.

4. Fourier-Mellin representation for operators

Our second application of the Racah-Wigner method in the context of the Heisenberg commutation relation is based on the invariance of that relation under a very simple set of transformations. If a, b, c, d are four real numbers with whose help we define

$$q' = aq + bp, \quad p' = cq + dp, \quad (24)$$

then q' and p' will obey (11) provided only that

$$ad - bc = 1. \quad (25)$$

It is easy to see that this set of transformations forms a group, and furthermore for any choice of a, b, c, d obeying condition (25) there will exist a unitary transformation carrying q and p into q' and p' respectively. The group structure is best displayed by defining a real two dimensional unimodular matrix

$$g = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (26)$$

Then every matrix of this type determines a transformation (24) and conversely; and the successive application of two transformations corresponds to the product of the two associated matrices, while the inverse of a transformation goes with the inverse of the matrix. The set of all these matrices forms by definition the group $SL(2, R)$; the relation between this group and the Lorentz group in three dimensions is similar in some respects to the relation between $SU(2)$ and $R(3)$. (For descriptions of $SL(2, R)$ and its true unitary representations see Bargmann [2], Gel'fand *et al* [12] Chapter 7).

If g is any element in $SL(2, R)$ let us denote by $U(g)$ the unitary operator that implements the transformation (24):

$$\begin{aligned} U(g) q U(g)^{-1} &= aq + bp, \\ U(g) p U(g)^{-1} &= cq + dp. \end{aligned} \quad (27)$$

Evidently $U(g)$ is determined only upto a g -dependent phase. Next, if g' and g are

any two elements of $SL(2, R)$, one sees that $U(g') U(g)$ and $U(g'g)$ produce the same changes in q and p . They can therefore differ at most by a phase:

$$U(g')U(g) = \omega(g', g) U(g'g). \quad (28)$$

The freedom to alter $U(g)$ by a g -dependent phase leads to a corresponding degree of freedom in the phase ω , but it can be shown that even so we cannot reduce ω identically to unity. Thus we have a 'representation upto a factor' of the group $SL(2, R)$ at the level of vectors.

One important difference between the previous section and the present one must be noticed. In the case of the Heisenberg group the unitary operators forming a representation of the group were directly defined in terms of their generators by (15); based on this, a representation acting on operators was set up in (18). In the present case, the operators $U(g)$ are themselves defined by (27) which is in the form of (4) and (18), except that at the moment only q and p have been subjected to transformation. We must therefore use (27) to determine the generators of $U(g)$, and then extend (27) to all H - S operators. For the former purpose, it is useful to define three one parameter subgroups of $SL(2, R)$ in this way:

$$\begin{aligned} g_0(\theta) &= \begin{pmatrix} \cos \theta/2 & \sin \theta/2 \\ -\sin \theta/2 & \cos \theta/2 \end{pmatrix}, & 0 \leq \theta \leq 4\pi. \\ g_1(\lambda) &= \begin{pmatrix} \cosh \lambda/2 & \sinh \lambda/2 \\ \sinh \lambda/2 & \cosh \lambda/2 \end{pmatrix}, & -\infty < \lambda < \infty. \\ g_2(\mu) &= \begin{pmatrix} \exp(\mu/2) & 0 \\ 0 & \exp(-\mu/2) \end{pmatrix}, & -\infty < \mu < \infty. \end{aligned} \quad (29)$$

A general group element can be obtained as a suitable product of these special ones. (Bargmann [2]). Let the three generators J_0, J_1, J_2 be defined thus:

$$\begin{aligned} U(g_0(\theta)) &= \exp(i\theta J_0), & U(g_1(\lambda)) &= \exp(i\lambda J_1), \\ U(g_2(\mu)) &= \exp(i\mu J_2). \end{aligned} \quad (30)$$

We get equations to determine them by specialising (27) to each one-parameter subgroup in turn and then making the parameter infinitesimally small:

$$\begin{aligned} [J_0, q] &= -ip/2, & [J_0, p] &= iq/2; \\ [J_1, q] &= -ip/2, & [J_1, p] &= -iq/2; \\ [J_2, q] &= -iq/2, & [J_2, p] &= ip/2. \end{aligned} \quad (31)$$

The J s are fixed upto additive constants; let us take them to be

$$J_0 = \frac{1}{4}(p^2 + q^2), \quad J_1 = \frac{1}{4}(p^2 - q^2), \quad J_2 = \frac{1}{4}(qp + pq). \quad (32)$$

They then obey the commutation relations (Goshen and Lipkin [13]):

$$[J_0, J_1] = iJ_2, \quad [J_0, J_2] = -iJ_1, \quad [J_1, J_2] = -iJ_0. \quad (33)$$

At this point we briefly describe some features of the $SL(2, R)$ representation provided by the operators $U(g)$. It is, as already mentioned, a representation upto a factor. It is, moreover, reducible into a direct sum of two irreducible parts. The set of three commutation relations (33) is very similar in appearance to the $R(3)$ set, there being a difference in sign in just one of them. Correspondingly there is a quadratic Casimir invariant in the $SL(2, R)$ case given by

$$Q \equiv J_1^2 + J_2^2 - J_0^2. \quad (34)$$

But substitution of the expressions (32) reduces Q to a number, $Q=3/16$, so this does not help achieve the reduction. This can be done using the properties of J_0 . From the theory of the harmonic oscillator in quantum mechanics we see that J_0 has the eigenvalues $1/4, 3/4, 5/4, \dots$, with multiplicity one each. On the other hand, as in the $R(3)$ case, the combinations $J_1 \pm iJ_2$ raise and lower the eigenvalue of J_0 by unity. Thus the space spanned by the eigenvectors of J_0 with eigenvalues $1/4, 5/4, 9/4, \dots$ forms one irreducible subspace for the $SL(2, R)$ Lie algebra; this is the space of even parity wavefunctions. And the complementary space spanned by the eigenvectors with eigenvalues $3/4, 7/4, 11/4, \dots$ forms a second irreducible subspace; this consists of all odd parity wave functions. Another easy way to arrive at this reduction is to notice that $\exp(2\pi i J_0)$ is an invariant of the $SL(2, R)$ algebra; and this operator takes on the values $+i$ and $-i$ respectively on the even and odd parity subspaces.

Let us now generalise (27) to get an $SL(2, R)$ representation acting on $H-S$ operators:

$$A \rightarrow \mathcal{U}(g) A = U(g) A U(g)^{-1}. \quad (35)$$

(g and p do not, of course, have the $H-S$ property). This is again a unitary representation, and a true one:

$$\mathcal{U}(g') \mathcal{U}(g) = \mathcal{U}(g'g). \quad (36)$$

The generators \mathcal{J} act on an operator A thus:

$$\mathcal{J}_0 A = [J_0, A], \quad \mathcal{J}_1 A = [J_1, A], \quad \mathcal{J}_2 A = [J_2, A]. \quad (37)$$

We must now express this representation as a direct integral (and sum) of irreducible ones. Doing this amounts to constructing a certain family of 'irreducible tensor operators', each transforming under \mathcal{U} according to its own unitary irreducible $SL(2, R)$ representation; taken together they will form a basis for a new description of ($H-S$) operators.

The most efficient way to do all this is to use the Wevl representation for operators already considered in the previous section. If we combine (22) and (27), we see that

the effect of $\mathcal{U}(g)$ on A given in (35) amounts to the following change in the function $a(\tau, \sigma)$:

$$g \in SL(2, R): a(\tau, \sigma) \rightarrow a(a\tau + b\sigma, c\tau + d\sigma). \quad (38)$$

This gives us a unitary $SL(2, R)$ representation on all square integrable $a(\tau, \sigma)$ which is in essential respects 'the same' as the representation $\mathcal{U}(g)$ on $H-S$ operators; so we need to effect reduction of the former. The generators $\mathcal{J}_0, \mathcal{J}_1, \mathcal{J}_2$ of $\mathcal{U}(g)$, when their action on operators A is expressed as an action on their 'Weyl weight functions' $a(\tau, \sigma)$, appear as the following differential operators:

$$\begin{aligned} \mathcal{J}_0 &= \frac{i}{2} \left(\tau \frac{\partial}{\partial \sigma} - \sigma \frac{\partial}{\partial \tau} \right), \quad \mathcal{J}_1 = -\frac{i}{2} \left(\tau \frac{\partial}{\partial \sigma} + \sigma \frac{\partial}{\partial \tau} \right), \\ \mathcal{J}_2 &= \frac{i}{2} \left(\sigma \frac{\partial}{\partial \sigma} - \tau \frac{\partial}{\partial \tau} \right). \end{aligned} \quad (39)$$

The simultaneous eigenfunctions of \mathcal{J}_0 and Q , the Casimir invariant formed from the \mathcal{J} 's, will form a complete orthonormal set. Both operators must, of course, have real eigenvalues. If we introduce radial and angular variables ρ, ϕ , by

$$\tau = \rho \sin \phi, \quad \sigma = \rho \cos \phi, \quad 0 \leq \rho < \infty, \quad 0 \leq \phi < 2\pi, \quad (40)$$

the integration volume is $\rho d\rho d\phi$, and \mathcal{J}_0 and Q become

$$\mathcal{J}_0 = -\frac{i}{2} \frac{\partial}{\partial \phi}, \quad Q = -\frac{1}{4} \rho \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} + 2 \right). \quad (41)$$

A simple calculation gives the following eigenfunctions and eigenvalues for these operators:

$$\begin{aligned} \psi_{sm}(\rho, \phi) &= (1/\pi\sqrt{2}) \rho^{-1+2is} \exp(2im\phi), \\ &-\infty < s < \infty, \quad m = 0, \pm \frac{1}{2}, \pm 1, \pm \frac{3}{2}, \dots; \\ \mathcal{J}_0 \psi_{sm} &= m \psi_{sm}, \quad Q \psi_{sm} = \left(\frac{1}{4} + s^2 \right) \psi_{sm}; \\ \int_0^\infty \rho d\rho \int_0^{2\pi} d\phi \psi_{s'm'}(\rho, \phi)^* \psi_{sm}(\rho, \phi) &= \delta_{m'm} \delta(s' - s). \end{aligned} \quad (42)$$

For a given eigenvalue m for \mathcal{J}_0 , the eigenvalues of Q are doubly degenerate.

The use of $\psi_{sm}(\rho, \phi)$ as a basis reduces the $SL(2, R)$ representation (38) acting in the space of square integrable functions $a(\tau, \sigma)$. For a given s , the set of functions $\psi_{s,m}$ with $m = 0, \pm 1, \pm 2, \dots$ carries a unitary irreducible representation conventionally denoted as C_q^0 ($q = \frac{1}{4} + s^2$); these representations constitute the so-called continuous integral class. Again with s fixed but $m = \pm \frac{1}{2}, \pm \frac{3}{2}, \dots$ one gets a unitary irreducible representation $C_q^{\frac{1}{2}}$ belonging to the continuous half-integral class. (The terminology is due to Bargmann [2]). Since reversing the sign of s does not alter the representation, each representation present occurs twice.

Using elements of the basis $\psi_{sm}(\rho, \phi)$ in the Weyl representation (22), we get an operator basis $u_{sm}(q, p)$:

$$u_{sm}(q, p) = (1/2\pi^{3/2}) \int_0^\infty d\rho \int_0^{2\pi} d\phi \rho^{2is} \exp [2im\phi + i\rho (q \cos \phi - p \sin \phi)]. \quad (43)$$

These operators form a complete orthonormal set for the space of $H-S$ operators:

$$(u_{s'm'}, u_{sm}) \equiv \text{Tr} (u_{s'm'}^\dagger u_{sm}) = \delta (s' - s) \delta_{m'm}. \quad (44)$$

Moreover, for fixed s the set of operators u_{sm} for $m = 0, \pm 1, \pm 2, \dots, (\pm \frac{1}{2}, \pm \frac{3}{2}, \dots)$ transforms irreducibly according to the representation $C_q^0 (C_q^{\frac{1}{2}})$ under the action of the operators $\mathcal{U}(g)$. This property can be expressed using the generators thus:

$$\begin{aligned} \mathcal{J}_0 u_{sm}(q, p) &= [J_0, u_{sm}(q, p)] = m u_{sm}(q, p), \\ (\mathcal{J}_1 + i\mathcal{J}_2) u_{sm}(q, p) &= [J_1 \pm iJ_2, u_{sm}(q, p)] = (m \pm \frac{1}{2} \mp is) u_{s, m \pm 1}(q, p). \end{aligned} \quad (45)$$

The effect of finite transformations involves using the infinite dimensional unitary matrices corresponding to elements of $SL(2, R)$ in the relevant representations; if these matrices are written as $D_{m'm}^{(s, \epsilon)}(g)$ with the subscripts enumerating the infinite number of rows and columns, and the superscripts specify the representation, we have:

$$\begin{aligned} \mathcal{U}(g) u_{sm}(q, p) &\equiv u_{sm}(aq + bp, cq + dp) \\ &= \sum_{m'} D_{m'm}^{(s, \epsilon)}(g) u_{sm'}(q, p). \end{aligned} \quad (46)$$

$\epsilon=0, \frac{1}{2}$ distinguishes the integral from the half-integral cases.

The new operator description arises by representing a general $H-S$ operator A in the form

$$\begin{aligned} A &= \sum_{m=0, \pm \frac{1}{2}, \pm 1, \dots} \int_{-\infty}^{\infty} ds a(s, m) u_{sm}(q, p), \\ (A, A) &= \sum_m \int ds |a(s, m)|^2. \end{aligned} \quad (47)$$

This is the quantum analogue of the classical Fourier-Mellin representation. We can see that this is so as follows. If in the above analysis we allow q and p to become classical commuting variables, then the action of $SL(2, R)$ on these variables given in (27) is identical in form with its action via (38) on the Fourier transformed variables τ, σ . We therefore expect that in the classical limit if we set $q=r \sin \theta, p=r \cos \theta$,

$u_{sm}(q, p)$ must reduce to either $r^{-1+2is} \exp(2im\theta)$ or $r^{-1-2is} \exp(2im\theta)$. This is indeed true: on carrying out the integrations the right hand side of (43) becomes

$$\frac{(-1)^{m-|m|}}{\sqrt{\pi}} 2^{2is} \left[\frac{\Gamma(\frac{1}{2} + |m| + is)}{\Gamma(\frac{1}{2} + |m| - is)} \right] r^{-1-2is} \exp(2im\theta) \tag{48}$$

So the classical limit of the operator description (47) is the expression of a classical dynamical variable $f(q, p)$ defined over a two-dimensional phase plane in the form

$$f(q, p) = \sum_m \int ds h(s, m) r^{-1-2is} \exp(2im\theta). \tag{49}$$

In concluding this section we mention briefly a different way of using the operators \mathcal{G} , due to Biedenharn and Louck (Biedenharn and Louck [3]). The triplet of operators $\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_0$ obeys the $SL(2, R)$ commutation relations whose form is given in eq. (33). Therefore the triplet $i\mathcal{G}_1, i\mathcal{G}_2, \mathcal{G}_0$ formally obeys the angular momentum commutation relations (1). However this is not a hermitian triplet (in the sense of the inner product (17)), so it does not give rise to a unitary $R(3)$ representation on $H-S$ operators. On the other hand we can consider, in place of $H-S$ operators, the set of all finite degree polynomials in q and p . In acting on them, the operators $i\mathcal{G}_1, i\mathcal{G}_2, \mathcal{G}_0$ do not increase the order of a polynomial, so we obtain finite dimensional representations of the Lie algebra of $R(3)$ which can be used to build up representations of the group itself. This way of constructing $R(3)$ (more precisely $SU(2)$) representations in the space of polynomials in q and p is known as the symplecton calculus. From the point of view of this paper, we must note that this method is not related in any way to a natural group of invariance of the Heisenberg commutation relation, at least not to a group that preserves hermiticity properties.

5. Canonical transformations and generating functions

We turn next to a class of operator descriptions based on the transformation theory of dynamics. The discussion will refer to systems with a general finite number of degrees of freedom. In comparison with the approach of the two preceding sections, the descriptions to follow will admittedly be heuristic. As preparation for the quantum mechanical discussion, we recall in this section some important results from the classical theory of canonical transformations (Some of the results of this section are well known and can be found, for example, in Caratheodory [5] Chapter 6).

Let $q_r, p_r, r = 1, 2, \dots, n$ be canonical co-ordinates for the phase space of a classical dynamical system with $2n$ degrees of freedom. A canonical transformation is the replacement of q_r, p_r by $2n$ independent functions $Q_r(q, p), P_r(q, p)$ obeying the condition

$$P_r dQ_r - p_r dq_r = \text{perfect differential.} \tag{50}$$

[Summation over repeated indices is understood]. This definition is equivalent to one stated in terms of invariance of Poisson brackets (PB) or Lagrange brackets (LB). A

canonical transformation being given, the function whose differential appears on the right in (50) can certainly be regarded as expressed explicitly in terms of q and p . However, if the transformation is such that throughout phase space the $2n$ variables q_r and Q_r are independent, these can be taken to form a non-canonical co-ordinate system. A necessary and sufficient condition for this is that the matrix

$$\| \partial Q_r (q, p) / \partial p_s \|, \quad (51)$$

have rank n . The right hand side in (50) can then be expressed as the differential of a 'generating function' $S(Q; q)$, determined by the transformation upto an additive constant, and this gives

$$p_r = - \partial S / \partial q_r, \quad (52a)$$

$$P_r = \partial S / \partial Q_r. \quad (52b)$$

Canonical transformations of this type are said to be non-degenerate, from the point of view of using q_r and Q_r as a (non-canonical) phase space co-ordinate system. In such a case, not only P_r and p_r but in fact every dynamical variable is expressible as a function of Q and q . Another important property of such transformations is that only constants can be in involution with, i.e., have vanishing PB with, all Q s and q s

$$\{Q_r, f\} = \{q_r, f\} = 0 \implies f = \text{constant}. \quad (53)$$

[Curly brackets denote PBs]. This is a direct consequence of the matrix (51) being nonsingular.

Canonical transformations of the above kind will be said to belong to the classical case I. As is well known, such transformations can be constructed by taking any function $S(Q; q)$ of $2n$ arguments obeying the hessian condition

$$\det \| \partial^2 S / \partial Q_r \partial q_s \| \neq 0, \quad (54)$$

and using (52) to define both Q and P as functions of q and p .

Transformations belonging to the degenerate case arise when the rank of the matrix (51) is m with $0 \leq m < n$. When this happens, the Q s and q s must obey $(n - m)$ independent conditions characteristic of the transformation:

$$F_\alpha(Q; q) = 0, \quad \alpha = 1, 2, \dots, n - m. \quad (55)$$

There is considerable freedom in the way these conditions are expressed but they will surely be such that no conditions can be derived on the q s alone by eliminating the Q s and conversely. These conditions imply that exactly $n - m$ out of the $2n$ variables q_r, Q_r are mutually independent. A simplifying assumption will now be made: throughout phase space there is a fixed subset of m Q s, taken without loss of generality to be Q_1, Q_2, \dots, Q_m , which can be adjoined to q_1, q_2, \dots, q_n to give $n - m$ independent variables. It follows that (55) can be solved for $Q_{m+1}, Q_{m+2}, \dots, Q_n$:

$$Q_A = f_A(Q_1, Q_2, \dots, Q_m; q_1, q_2, \dots, q_n).$$

$$A = m + 1, m + 2, \dots, n. \quad (56)$$

[We introduce the convention that indices a, b, c, \dots , run over $1, 2, \dots, m$ and indices A, B, C, \dots over $m+1, m+2, \dots, n$]. Now it turns out that even though it is not possible to express every dynamical variable as a function of Q s and q s, the function whose differential appears on the right in (50) can be expressed as a function of Q_a and q_r ; indeed when it is so expressed it is unique upto an additive constant. This happens because only the differentials of Q_a and q_r enter the left hand side of (50). Writing $S(Q_1, Q_2, \dots, Q_m; q_1, q_2, \dots, q_n)$ for this function and using (56), (50) gives;

$$p_r = -\frac{\partial S}{\partial q_r} + P_A \frac{\partial f_A}{\partial q_r}, \quad (57a)$$

$$P_a = \frac{\partial S}{\partial Q_a} - P_A \frac{\partial f_A}{\partial Q_a}. \quad (57b)$$

Now the first set of equations here state that the p_r can be expressed as functions of Q_a, q_r, P_A . These $2n$ variables must then form an independent set. We can in fact use (56) and (57) to express P_a, p_r, Q_A as the various partial derivatives of a single generating function $S'(Q_a, P_A; q_r)$:

$$S'(Q_a, P_A; q_r) = S(Q_a; q_r) - P_A f_A(Q_a; q_r), \quad (58a)$$

$$p_r = -\frac{\partial S'}{\partial q_r}, \quad (58b)$$

$$P_a = \frac{\partial S'}{\partial Q_a}, \quad (58c)$$

$$Q_A = -\frac{\partial S'}{\partial P_A}. \quad (58d)$$

We can take these equations as the replacements, in the degenerate case, for (52) of the non-degenerate case. The possibility of using Q_a, q_r, P_A as independent variables is an explicit verification of a general theorem due to Caratheodory. (Caratheodory [5], § 96; Saletan and Cromer [19] p. 213). The linearity of the dependence of the generating function S' on P_A reflects the degeneracy of the transformation from the $Q - q$ point of view (see Caratheodory [5] § 107).

As in the non-degenerate case, a degenerate canonical transformation can be constructed by taking any $(n - m + 1)$ functions S, f_A of the $(n + m)$ variables Q_a, q_r and then imposing (58). The only condition on S, f_A is that from (58b) it must be possible to get Q_a, P_A as functions of q and p : this replaces the previous condition (54).

Now the degenerate case splits further into two subcases based on the answer to the following question: are there nontrivial dynamical variables, i.e., not just

constants, that are in involution with all the Q 's and q 's? The answer depends on the nature of the set of conditions (55). It may be that from these conditions no nontrivial equation of the form

$$F(q_1, q_2, \dots, q_n) = G(Q_1, Q_2, \dots, Q_n), \quad (59)$$

is obtainable. In that case we shall say the given degenerate canonical transformation is of nonseparable kind and (as will soon be evident) we will have:

$$\{Q_r, f\} = \{q_r, f\} = 0 \implies f = \text{constant}. \quad (60)$$

This will be called the classical case IIa. To understand this case better, we remark that in view of (56), the independent conditions initially imposed on f are $(n + m)$ in number:

$$\{Q_a, f\} = 0, \quad \{q_r, f\} = 0. \quad (61)$$

However, this system of linear homogeneous first order partial differential equations on f leads in a well-known way to additional equations on f (see, for instance, Eisenhart [10] p. 6). In the present case, on using the Jacobi identity for PB 's, we see that f must obey

$$\{\{Q_a, q_r\}, f\} = 0 \quad (62)$$

and more equations of this general pattern formed from higher order PB s among the Q s and q s. It is the complete set of such conditions on f that, in the nonseparable case, leads to f being just a constant.

On the other hand, suppose there is a nontrivial f in involution with the Q s as well as with the q s. When expressed in terms of q and p it must appear as a function of q alone, $F(q)$ say; and in terms of Q and P it must appear as some $G(Q)$. Thus a nontrivial relation of the form (59) must exist. But every condition obeyed by the Q s and q s *must* be derivable from the independent set of conditions (55); hence this set permits the derivation of one or more relations in which the Q and q dependences are separated. We shall then say the degenerate canonical transformation is of separable kind and belongs to the classical case IIb.

To summarise, we see that in the nondegenerate situation or classical case I, every dynamical variable is expressible as a function of, and only constants are in involution with, the Q s and q s. If a degenerate canonical transformation belongs to the classical case IIa, certainly all dynamical variables cannot be expressed as functions of Q s and q s alone; but the fact that only constants are in involution with Q s and q s means that every dynamical variable *is* expressible as some function of Q s, q s, their first order PB s $\{Q, q\}$, their second order PB s $\{q, \{Q, q\}\}$, $\{Q, \{Q, q\}\}$ and so on upto some finite order. If the transformation belongs to the classical case IIb, then even the chain of quantities $Q, q, \{Q, q\}, \{q, \{Q, q\}\}, \dots$ fails to generate a set of $2n$ independent variables.

In concluding this section we must note that this classification is exhaustive and exclusive: every canonical transformation must belong to class I or to class IIa or to

class IIb, subject only to the one simplifying assumption made just prior to (56). However this division of the group of all canonical transformations into classes does not amount to a division into significant subgroups.

Purely for illustrative purposes, the appendix presents a degenerate case IIa canonical transformation for a system with four degrees of freedom.

6. Functions of non-commuting operators

In the present section and the following one, the symbols q_r, p_r denote hermitian operators furnishing an irreducible solution of the Heisenberg commutation relations for a quantum system with $2n$ degrees of freedom:

$$[q_r, q_s] = [p_r, p_s] = 0, \quad [q_r, p_s] = i \hbar \delta_{rs}. \quad (63)$$

Similarly, Q_r and P_r will stand for a transformed irreducible solution related to q and p by a unitary transformation U :

$$Q_r = U q_r U^{-1}, \quad P_r = U p_r U^{-1}. \quad (64)$$

To consider the question of defining functions of non-commuting operators in quantum mechanics, we begin with two noncommuting hermitian operators A and B . The conventional definition regards any formal polynomial expression written in A and B , with no attention paid to the order of factors, as a function of A and B . Thus for example, each of the expressions $AB, BA, A^2, A^2B, AB^2A^2$, etc. is viewed as a function of A and B . Moreover, since operator functions $f(A)$ of a single hermitian operator are as easy to define as numerical functions of a single classical real variable, one accepts more general expressions of the form $f(A), g(B), f(A)g(B), f(A)g(B)h(A)$, etc. as defining operator functions of A and B . More generally, all those operators that can be obtained as so-called 'weak-limits' of polynomial expressions in A and B are regarded as being functions of A and B . With this definition it is clear that numerical linear combinations and products of functions of A and B yield new functions of A and B . It is also clear that if F is a function of A and B in this sense, it will commute with every operator that commutes with A and B . It turns out that this property can be made the basis for this notion of a function of noncommuting operators. In general, given a collection \mathcal{A} of hermitian operators $\{A, B, \dots\}$, an operator F is a function of members of \mathcal{A} if it commutes with every operator that commutes with every member of \mathcal{A} :

$$[A, \Omega] = 0, \quad \text{all } A \in \mathcal{A} \implies [F, \Omega] = 0. \quad (65)$$

It is then true that such an F is the weak limit of suitable polynomial expressions in the elements of \mathcal{A} . (For a lucid discussion see Jordan [15] Chapter 4).

The notion of irreducibility of a hermitian set of operators is important in this context. \mathcal{A} is said to be irreducible if the only operators that commute with every member of \mathcal{A} are scalar multiples of the unit operator. If this is the case, then in the condition (65) the only available choices for Ω are multiples of unity and it follows that any operator F obeys this condition. Thus any F is in principle a function of

the members of an irreducible set \mathcal{A} . As examples, in § 3 and 4 we dealt with an irreducible pair q, p obeying the Heisenberg commutation relation and developed ways of expressing any ($H - S$) operator explicitly in terms of q and p .

If a hermitian set \mathcal{A} is not irreducible, three interesting sets of operators emerge. The first is the set of all those operators that commute with every member of \mathcal{A} (the Ω s to be used in (65)): this is the commutant of \mathcal{A} . The second is the set of operators qualifying as functions of \mathcal{A} (the F s obeying (65)): this is the commutant of the commutant of \mathcal{A} . The third is the set of those F that do not obey (65) and so are not functions of \mathcal{A} . Only the first two sets possess the algebraic properties of being closed under formation of linear combinations and products of their elements.

Contrasted with the above concept of a function of non-commuting operators is the Jordan-Dirac definition of ordered functions of operators. (Jordan [14], Dirac [6, 7]). We begin again with two non-commuting hermitian operators A and B . Denote general eigenvalues of A and B by a and b respectively, and let $f(a, b)$ be any numerical (possibly complex) function of the indicated variables. With a definite order of factors chosen— A to the left, B to the right, say—each $f(a, b)$ determines uniquely an operator F by the prescription (Dirac [7]).

$$F = \sum_{a, b} f(a, b) P(A; a) P(B; b) \quad (66)$$

Here $P(A; a)$ is the projection operator onto the eigenspace of A with eigenvalue a , and is therefore a function of A ; similarly for $P(B; b)$. Thus by construction F is a sum of terms in each of which a function of A stands to the left and a function of B to the right. A direct way to construct such ordered functions of A and B is to take expressions of the general form

$$F = \sum u(A) v(B) \quad (67)$$

with u s and v s being functions of one operator each; but it is easily seen that the two alternative forms (66) and (67) lead to the same set of operators F .

A change in the ordering prescription results generally in a change in the set of operators that one obtains. Thus the set of F s obtained with the rule “ A to the right, B to the left” may not be the same as the set given by the rules (66), (67). In particular, with the latter rule AB is an ordered function of A and B , but BA may not be so.

The Jordan-Dirac definition generalises easily to the case of three or more operators, A_1, A_2, A_3, \dots , say, provided a definite sequence is prescribed for the positions of functions of A_1, A_2, \dots , in a product. We shall be interested in the next section in the case where the set A_1, A_2, \dots , consists of the $2n$ hermitian operators $q_1, q_2, \dots, q_n, Q_1, Q_2, \dots, Q_n$. Here since the q s commute among themselves and the Q s among themselves, an adequate ordering prescription is to demand that all Q s stand to the left of all q s. This then leads to a definite set of operators appearing as ordered functions of Q s and q s, characteristic of the unitary operator U present in (64).

Comparing the two definitions, we see that the concept of ordered functions of operators is more restrictive than the concept of functions of operators. For a given basic set \mathcal{A} and a chosen order, the former generally leads to fewer operators

than the latter: an ordered operator function of \mathcal{A} is also a function of \mathcal{A} but the converse may fail. For example, the commutator $[A, B]$ is a function of A and B but is not an ordered function unless one succeeds in expressing BA as a sum of terms in each of which A stands to the left of B . Further, the set of ordered functions of a basic set \mathcal{A} determined by a specific ordering rule generally does not have the property of being closed under multiplication of its members.

7. Unitary transformations and generating functions

We can now discuss the connections between the generating function description of unitary transformations in quantum mechanics and the concepts of functions and ordered functions of a mixed set of operators Q_r, q_r (cf. (63) and (64)). Denote a simultaneous eigenvector of the complete commuting set q_r by $|q'\rangle$: q' stands for n real numbers q'_1, q'_2, \dots, q'_n with q'_r being the eigenvalue of q_r . These vectors are assumed to obey

$$\langle q'' | q' \rangle = \prod_r \delta(q_r'' - q_r'), \quad (68a)$$

$$p_r |q'\rangle = (i\hbar \partial / \partial q'_r) |q'\rangle. \quad (68b)$$

Eigenvectors $|Q'\rangle$ of Q are set up in similar fashion.

Dirac's treatment rests on an analysis of the transformation function $\langle Q' | q' \rangle$ which depends on $2n$ independent variables. The original result of Jordan and Dirac is the following (Jordan [14], Dirac [6]): Assume that $\langle Q' | q' \rangle$ does not vanish for any values of Q' and q' and define a function $S(Q'; q')$ by

$$\langle Q' | q' \rangle = \exp [i S(Q'; q')/\hbar]. \quad (69)$$

Using this function in the spirit of the definition (66), we get an ordered operator function $S(Q; q)$: throughout this section the ordering rule is to place Q on the left and q on the right. By combining (69) with (68b) and a similar equation for P_r , we get operator equations having the same form as the classical relations (52):

$$p_r = - \frac{\partial S(Q; q)}{\partial q_r}, \quad P_r = \frac{\partial S(Q; q)}{\partial Q_r}. \quad (70)$$

The differentiations are to be done preserving the ordering rule.

This situation, with $\langle Q' | q' \rangle$ never vanishing, will be called the quantum mechanical case I and corresponds to the classical case I of § 5. Its further properties are as follows. Clearly an operator F is fully specified by its mixed matrix elements $\langle Q' | F | q' \rangle$ and conversely 'any' choice for the latter determines an F uniquely. Given an F , one can define a function $f(Q'; q')$ by

$$\langle Q' | F | q' \rangle = f(Q'; q') \langle Q' | q' \rangle. \quad (71)$$

One then sees that if this function is used in (66) to define an ordered operator func-

tion $f(Q; q)$, this operator must be F itself since their mixed matrix elements are, by definition, the same:

$$F = f(Q; q). \quad (72)$$

Thus in this case, as Dirac has shown, 'every' operator F is expressible as an ordered function of Q and q . We infer that the set of ordered functions of Q and q must coincide with the set of functions of Q and q , and that these $2n$ operators must be irreducible:

$$[Q_r, A] = [q_r, A] = 0 \implies A = a \cdot 1. \quad (73)$$

Suppose next that $\langle Q' | q' \rangle$ is not everywhere non-zero in the $2n$ dimensional space of the variables Q'_r, q'_r but that it vanishes everywhere except on some $(n+m)$ —dimensional hypersurface Σ defined by $(n-m)$ independent algebraic equations:

$$\Sigma : F_\alpha(Q'; q') = 0, \quad \alpha = 1, 2, \dots, n-m, \quad 0 \leq m < n. \quad (74)$$

It follows that we can no longer express 'all' operators as ordered functions of Q and q . This case has been treated by Dirac: he has shown how to develop operator equations having the same appearance as with a degenerate classical canonical transformation using the Lagrange multiplier method (Dirac [7]). We give a more detailed description of such transformations following the analysis of § 5. The transformation function must have the form

$$\langle Q' | q' \rangle = \prod_\alpha \delta(F_\alpha(Q'; q')) X(Q'; q'), \quad (75)$$

with $X(Q'; q')$ nonvanishing on Σ . The equations defining Σ must be such that it must be impossible to get a condition on $q'(Q')$ alone by eliminating $Q'(q')$. Otherwise, if a condition

$$h(q') = 0,$$

were satisfied identically on Σ , i.e. by virtue of (74), we would have

$$h(q') \langle Q' | q' \rangle = \langle Q' | h(q) | q' \rangle = 0 \implies h(q) = 0,$$

implying an operator condition on the qs alone. We now make a regularity assumption as in the classical case: we suppose that a fixed subset of m Q' variables (chosen without loss of generality to be Q'_1, Q'_2, \dots, Q'_m) along with q'_1, \dots, q'_n are independent over Σ . Equations (74) can then be solved for $Q'_A, A = m+1, \dots, n$ and Σ defined in the form

$$\Sigma : Q'_A = f_A(Q'_1, Q'_2, \dots, Q'_m; q'_1, q'_2, \dots, q'_n). \quad (76)$$

[The conventions of § 5 will be used for ranges of indices a, b, \dots, A, B, \dots]. We can replace (75) by

$$\begin{aligned} \langle Q' | q' \rangle = \prod_A \delta(Q'_A - f_A(Q'_a; q'_r)) \times \\ \exp [i S(Q'_1, \dots, Q'_m; q'_1, \dots, q'_n)/\hbar], \end{aligned} \quad (77)$$

therewith introducing a function $S(Q'_a; q'_r)$ of $(n+m)$ variables.

Two interesting conclusions follow from (77). First we see that

$$\begin{aligned} (Q'_A - f_A(Q'_a; q'_r)) \langle Q' | q' \rangle = 0 \implies \\ Q_A = f_A(Q_a; q_r). \end{aligned} \quad (78)$$

This is like the classical (56) but is an operator statement; each operator Q_A is expressible as an ordered function of the $(n+m)$ operators Q_a, q_r . (Incidentally by taking the hermitian conjugates of these equations we see that each Q_A is also an ordered function with q_r to the left and Q_a to the right). Second, we know that Fourier transformation takes one from the eigenvectors of a Q to those of its conjugate P . If P'_A denote a set of eigenvalues for the $(n-m)$ operators P_A , we get from (77)

$$\begin{aligned} \langle Q'_1, \dots, Q'_m; P'_{m+1}, \dots, P'_n | q'_1, \dots, q'_n \rangle = \\ (2\pi\hbar)^{(m-n)/2} \exp [i \{S(Q'_a; q'_r) - P'_A f_A(Q'_a; q'_r)\} / \hbar]. \end{aligned} \quad (79)$$

This transformation function never vanishes (of course, in the $2n$ dimensional space of the variables Q'_a, P'_A, q'_r). So, repeating the arguments of case I, we see that 'every' operator F is expressible as an ordered function of Q_a, P_A, q_r with the (mutually commuting) Q_a and P_A always to the left and the q_r to the right. Thus this set of $2n$ operators is irreducible. This is an instance of Caratheodory's theorem in quantum mechanics (Mukunda [17]; the results of this paper have here been corrected, clarified and carried forward). In particular, we can get ordered expressions for P_a, Q_A and p_r as follows. Using the function occurring in the exponent in (79) we define the ordered operator

$$S'(Q_a, P_A; q_r) = S(Q_a; q_r) - P_A f_A(Q_a; q_r). \quad (80)$$

Then with the help of (68b) and other similar equations we get the operator equalities

$$p_r = -\frac{\partial S'}{\partial q_r}, \quad P_a = \frac{\partial S'}{\partial Q_a}, \quad Q_A = -\frac{\partial S'}{\partial P_A}, \quad (81)$$

the differentiations always respecting the ordering rule. Equations (80) and (81) are operator counterparts to the classical (58). It is interesting to note that while the linear dependence of S' on P_A classically reflects the degeneracy of the canonical transformation, in quantum mechanics it reflects the presence of the delta functions in the transformation function $\langle Q' | q' \rangle$.

Further analysis depends on whether (74) defining Σ are non-separable or separable in Q' and q' . In the former case no relation of the form

$$F(q') = G(Q'), \quad (82)$$

holds on Σ ; we call this the quantum mechanical case IIa and conclude that Q_r and q_r must together be irreducible: (73) must hold. This leads to the very interesting result that while we are not able to express every operator as an ordered function of Q and q , we *can* express it as a function of Q and q .

Finally, at least one relation of the form (82) may be valid on Σ , with non-trivial F and G . This leads to the quantum mechanical case IIb, in which there exists at least one operator A which commutes with all the Q s and q s and is not a multiple of the identity, to wit, $F(q)$ or $G(Q)$. The set Q_r, q_r is no longer irreducible, and we are unable to express every operator as a function of this set. A simple example is to take an operator B not commuting with the A above; such B must exist, and it obviously cannot be a function of Q and q .

8. Concluding remarks

We mention here some interesting features and fruitful points of view emerging from this work. The classical concept of a function of a set of variables is based on the intuitive notion of values assumed: f is a function of x, y, \dots if given values of the latter determine a definite value for the former. (We assume that all these are number-valued quantities). We are led to suggest that this stands in correspondence with the concept of ordered functions of operators in quantum mechanics. This may appear deficient in some respects. For example for a given set of classical independent real variables there is just one concept of function of them; while for a set of noncommuting hermitian operators each ordering rule leads to a corresponding set of ordered functions of them, and these sets may overlap but may not coincide. Moreover, while the product of two functions is also a function in the classical case, the product of operators ordered according to a given rule may not be similarly expressible. In spite of these drawbacks, the close similarity between the three kinds of classical canonical transformations and the three kinds of unitary transformations support our suggestion. As for the classical counterpart to the function concept among quantum mechanical operators, the situation is more satisfactory: we have the notion of a *function group* (Eisenhart [10] p. 281). A family of functions on a classical phase space is a function group if functions of its members belong to it and moreover if the *PBs* of its members with one another also belong to the family. Starting with a set of dynamical variables we can form the collection of all functions of them. If this is not a function group we may adjoin the *PBs* of the functions with one another, then their *PBs* with these *PBs*, functions of the *PBs*, and so on until we have generated the smallest function group containing the originally given set. In the classical case I the function group generated by Q and q coincides with the set of functions of these variables; similarly in the quantum case I both functions and ordered functions of Q and q yield all operators. In the classical cases IIa and IIb the function group generated by Q and q respectively does and does not yield all

dynamical variables; while in the quantum cases IIa and IIb functions of Q and q respectively do and do not yield all operators.

In most conventional treatments of quantum mechanics a general operator is regarded as completely specified or known if all its matrix elements in a chosen orthonormal basis are given. However, this is far from trying to express the operator as a function of primitive operators which may include the complete commuting set associated with the chosen basis. We have focussed attention on the latter kind of description, in contrast to the 'matrix element description'. In spite of the heuristic nature of the discussion in §§ 6 and 7, our analysis leads to a useful picture of the relations existing between the totality of dynamical variables of a quantum system and its primitive variables.

The Weyl representation for operators has been used in the literature, especially of quantum optics, as a convenient starting point for expressing operators in various ordered forms (see, for instance, Cahill and Glauber [4], Agarwal and Wolf [1], Klauder and Sudarshan [16]). The relative simplicity of the Heisenberg commutation relation makes manipulations based on Weyl's representation quite easy. Our analysis helps us to view these matters in a wider perspective and in a more general context. It would be interesting to extend the present methods to the case of Lie groups, for example, in finding ways of expressing general group elements as ordered products of specially chosen elements. It would also be worthwhile to find more compact ways of expressing and using the Fourier-Mellin description of operators discussed in § 4.

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Appendix

A classical canonical transformation belonging to case I is easily constructed by choosing a generating function $S(Q; q)$ fulfilling (54). A transformation under case IIb is also easily constructed: for example one may take the identity transformation, or a transformation in which some degrees of freedom are left unaffected. As an elementary example belonging to case IIa, we take a system with $n = 2$ and consider

$$Q_1 = p_1/p_2, \quad Q_2 = q_2 + q_1 p_1/p_2, \quad P_1 = -q_1 p_2, \quad P_2 = p_2. \quad (\text{A.1})$$

This is checked to be canonical. It is degenerate because one relation holds among Q s and q s:

$$Q_2 = Q_1 q_1 + q_2. \quad (\text{A.2})$$

But this relation is non-separable. If a function A is in involution with Q_r and q_r , it must be of the form $A(q)$ obeying

$$\{Q_1, A(q)\} = \frac{1}{p_2} \frac{\partial A}{\partial q_1} - \frac{p_1}{p_2^2} \frac{\partial A}{\partial q_2} = 0$$

identically in q_r and p_r , and this forces A to be a constant.

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