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Lie Group Dynamical Formalism and the Relation between Quantum Mechanics and Classical Mechanics

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I. INTRODUCTION

SOME general structural features of dynamical theories can be exhibited in a study of the relation between classical and quantum mechanics; the essential dynamical structure of these theories is that of a Lie algebra of functions of the basic dynamical variables which provides the infinitesimal generators of the group of dynamical transformations. While the particular representation (real variables or operators) which is chosen for this algebra may be important in the formulation of the kinematics of the theory and for a physical interpretation, it is not important for the dynamical structure analysis. We illustrate this point of view by considering the possibility of a transcription of classical and quantum mechanics each into the natural representation of the other. This point of view leads us to outline a formal theory of generalized dynamics by constructing a class of Lie algebras which includes those of classical and quantum mechanics as special cases.

It is well known that the formal relationship between quantum mechanics and classical mechanics is expressed in the analogy between commutator brackets and Poisson brackets, and between Heisenberg's equations of motion and Hamilton's equations of motion.[1] However, it has been shown by Moyal[2] that quantum mechanics can be formulated in a natural manner in terms of functions on the classical phase space such that there corresponds to the commutator of two operators, not the Poisson bracket of the functions corresponding to the operators, but a somewhat more complicated function which may also be associated with the two original functions by a bracket-type mapping. This bracket is shown to have the properties of a Lie bracket. We are thus led to consider the functions on the phase space as forming a Lie algebra with this bracket. The elements of this algebra act as generators for the dynamical transformations which are elements of the corresponding Lie group. The operator representation of this algebra and group provides, of course, the usual formulation of quantum mechanics.

With these ideas in mind we begin with a discussion in II of classical mechanics, developing the usual phase space formulation and noting that we may choose any power series in the dynamical variables as the Hamiltonian. Hence the set of such quantities are generators for the canonical dynamical transformations on the system. Since the Poisson bracket has the properties of a Lie bracket, this set is a Lie algebra and we identify the canonical transformations with elements of the corresponding Lie group. We then outline formally an operator representation for the algebra and group and thus show how classical mechanics would look in the natural representation of quantum mechanics.

In III we note that a parallel discussion is possible for quantum mechanics, and since we have a phase space formulation and an operator formulation of both classical and quantum mechanics at our disposal, comparisons are immediately evident. Both classical and quantum dynamics have the structure of a Lie group of transformations associated with a Lie algebra of functions of the dynamical variables. We regard the phase space and operator formulations as different representations of these. From this point of view the main difference between the two mechanics is in the choice of the Lie bracket. Many of the other features of the two formalisms become identical; for example, the commutator of the operators corresponding to two canonical variables q and p has the value 1 in both the classical and quantum cases.

In IV we note that the classical formalism may be considered as the limit as $\hbar\rightarrow 0$ of the quantum, but we prefer to take the limit in the equations of motion and not in commutator brackets. We consider the connection with the WKB approximation. In V we note that there is a general form of a Lie bracket which includes the brackets of classical and quantum mechanics as special cases and we are thus led to consider the possibility of more general mechanical formalisms.

Since these topics have been of long-standing interest they have been considered by various authors from many different points of view. It was shown by Koopman[3] how the dynamical transformations of classical mechanics, considered as measure preserving transformations of the phase space, induce unitary transformations on the Hilbert space of functions which are square integrable with respect to a density function over the phase space. This Hilbert space formulation

[1] P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford University Press, New York, 1958), Chaps. IV, V.

[2] J. E. Moyal, Proc. Cambridge Phil. Soc. **45**, 99 (1949).

[3] B. O. Koopman, Proc. Natl. Acad. Sci. **17**, 315 (1931).

of classical mechanics was further developed by von Neumann.[4] It is to be noted that this Hilbert space corresponds not to the space of state vectors in quantum mechanics but to the Hilbert space of operators on the state vectors (with the trace of the product of two operators being chosen as the scalar product). A comparison of classical and quantum mechanics in terms of these analogous Hilbert spaces and the unitary dynamical transformations on them has been carried out by Uhlhorn,[5] who noted that any linear correspondence between phase space functions and operators would provide an isomorphism of these Hilbert spaces and used the phase space formulation of quantum mechanics to investigate the possible isomorphism of the dynamical groups. His result, that there is no isomorphism of the full groups but that there is an isomorphism of the subgroups generated by Hamiltonians which are of at most quadratic degree in the dynamical variables, is in agreement with our conclusions (see Sec. III). The association of classical mechanical phase space functions with quantum mechanical operators and Poisson brackets with commutator brackets has also been studied by Groenwold[6] and Bopp,[7] among others. The possible isomorphism of the dynamical groups of classical and quantum mechanics was investigated by Van Hove[8] who also found that the isomorphism does exist for the subgroup generated by Hamiltonians of quadratic or lower degree in the canonical variables. In general the isomorphism of the dynamical groups will depend on the rule one uses to associate phase space functions with operators. This led Rivier[9] to propose a rule of association which is invariant under simultaneous infinitesimal transformations of the classical and quantum dynamical variables generated by Poisson brackets and commutator brackets, respectively. However we shall show in Sec. III that this rule does not in general associate Poisson brackets with commutator brackets. In this paper we have chosen to use the correspondence rule of Moyal, Wigner,[10] and Weyl,[11] according to which these dynamical groups are explicitly nonisomorphic. The various possible rules for associating function with operators have been studied by Shewell.[12]

II. CLASSICAL MECHANICS

The classical statistical mechanical state of a physical system is represented by a probability distribution function $\rho(M)$ on the phase space $\{M\}$ of the system. (In the usual case $\{M\}$ is the $2n$-dimensional Euclidean space of n pairs of canonical coordinates and momenta q_i, p_i, $i=1, 2, \cdots, n$). It is required that $\rho(M)$ be normalized

$$\int \rho(M)\,dM=1; \tag{1}$$

and the expectation value, for this state, of a function $A(M)$ of the dynamical variables is defined by

$$\langle A\rangle=\int A(M)\rho(M)\,dM. \tag{2}$$

We call a pure state that limiting state in which the system exists with unit probability at the point M'

$$\rho_{M'}(M)=\delta(M-M'). \tag{3}$$

For such a state the time evolution of the system is given by Hamilton's equations of motion for functions $A(M)$ of the dynamical variables

$$(\partial/\partial t)A_t(M)=[A_t(M), H(M)]_{\text{PB}}, \tag{4a}$$

where the bracket is the Poisson bracket and $H(M)$ is the Hamiltonian function. For a state specified by the density function $\rho(M)$, the expectation value at time t of the physical quantity A will then be given by

$$\langle A\rangle_t=\int \rho(M)A_t(M)\,dM, \tag{5a}$$

where $\rho(M)$ is taken to be constant in time and $A_t(M)$ satisfies Eq. (4). Here we have let each individual point in the phase space move along the trajectory given by Eq. (4) and have averaged over the initial distribution, since we know by Liouville's theorem that the amount of density at an infinitesimal element of phase space remains constant as that element moves along its trajectory. But we could just as well consider the physical function A of the dynamical variables to be constant and average with respect to a distribution which has undergone the inverse time transformation

$$\langle A\rangle_t=\int \rho_t(M)A(M)\,dM \tag{5b}$$

$$(\partial/\partial t)\rho(M)=-[\rho_t(M), H(M)]_{\text{PB}}. \tag{4b}$$

Now a Hamiltonian $H(M)$ generates according to Eq. (4) an element of the group of canonical transformations on the dynamical variables. But as yet H is an arbitrary function of the dynamical variables. For definiteness we will limit ourselves to Hamiltonians which have a power series expansion and will illustrate our ideas for a system with one pair of canonical coordinate and momentum q and p. Then we may write

$$H(p,q)=\alpha_{m,n}q^m p^n,$$

and the two alternative forms of the equations of

[4] J. von Neumann, Ann. of Math. **33**, 587 (1932).
[5] U. Uhlhorn, Arkiv. Fysik. **11**, 87 (1956).
[6] H. J. Groenewold, Physica **12**, 405 (1946).
[7] F. Bopp, preprint. We are grateful to Professor Bopp for providing us with a copy of his work.
[8] L. Van Hove, Acad. roy. Belg. Bull. Classe Sci. Mém. (5) **37**, 610 (1951).
[9] D. C. Rivier, Phys. Rev. **83**, 862 (L) (1951).
[10] E. Wigner, Phys. Rev. **40**, 749 (1932).
[11] H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dover Publications, Inc., New York, 1950), p. 275.
[12] J. R. Shewell, Am. J. Phys. **27**, 16 (1959).

motion [Eq. (4)] take the form

$$(\partial/\partial t)A(q,p)=[A(q,p),\, q^m p^n]_{\mathrm{PB}}\alpha_{m,n}, \tag{6a}$$

$$(\partial/\partial t)\rho(q,p)=-[\rho(q,p),\, q^m p^n]_{\mathrm{PB}}\alpha_{m,n}. \tag{6b}$$

Or we can absorb the time dependence into the constants α_{mn} and write

$$dA(q,p)=[A(q,p),\, q^m p^n]_{\mathrm{PB}}d\alpha_{m,n} \tag{7a}$$

$$d\rho(q,p)=-[\rho(q,p),\, q^m p^n]_{\mathrm{PB}}d\alpha_{m,n}. \tag{7b}$$

Here the $d\alpha_{mn}$ appear as a countable set of parameters which characterize the infinitesimal transformation. The Poisson bracket has the properties that for any real numbers a and b and functions A, B, C

$$[A,\, aB+bC]_{\mathrm{PB}}=a[A,\, B]_{\mathrm{PB}}+b[A,\, C]_{\mathrm{PB}}, \quad \text{(linearity)} \tag{8a}$$

$$[A,\, A]_{\mathrm{PB}}=0 \qquad \text{(antisymmetry)} \tag{8b}$$

or, equivalently,

$$[A,\, B]_{\mathrm{PB}}=-[B,\, A]_{\mathrm{PB}},$$

$$[A,\,[B,\, C]_{\mathrm{PB}}]_{\mathrm{PB}}+[B,\,[C,\, A]_{\mathrm{PB}}]_{\mathrm{PB}} +[C,\,[A,\, B]_{\mathrm{PB}}]_{\mathrm{PB}}=0 \quad \text{(Jacobi identity)}. \tag{8c}$$

Hence the real linear space of power series in the dynamical variables forms an infinite dimensional Lie algebra[13] with the Poisson bracket as Lie bracket. Evidently the dynamical transformations (7) are elements of the corresponding Lie group.

This association would become clearer if we could find an operator representation for this Lie algebra and dynamical group. Hence we will outline in a purely formal way the essential properties of such a representation. To every real function $A(M)$ we would want to correspond a Hermitian operator A on a Hilbert space so that the correspondence is linear, to the Poisson bracket of two functions $A(M)$ and $B(M)$ there corresponds the commutator bracket of the operators A and B, and

$$\int A(M)B(M)dM=\mathrm{Tr}(AB). \tag{9}$$

We would be interested in the operators $\rho_{M'}$ corresponding to the pure-state distributions (3) and, since all other functions can be written as an integral superposition of these, we could accomplish our purpose by letting

$$A(M)=\mathrm{Tr}[AL(M)], \tag{10a}$$

$$A=\int A(M)L(M)dM, \tag{10b}$$

where

$$L(M)=\int \rho_{M'}\rho_{M'}(M)dM'=\int \rho_{M'}\delta(M-M')dM'. \tag{11}$$

Then, since

$$\int \rho_{M'}(M)\rho_{M''}(M)dM=\int \delta(M-M')\delta(M-M'')dM =\delta(M'-M''),$$

we will need to require that

$$\mathrm{Tr}(\rho_{M'}\rho_{M''})=\delta(M'-M'') \tag{12}$$

One can easily check that these are formally consistent, that (9) is satisfied, and that we can write

$$A=\int A(M')\rho_{M'}dM'$$

$$A(M')=\mathrm{Tr}(A\rho_{M'})$$

The operators corresponding to real functions will be Hermitian if we require $\rho_{M'}$ to be Hermitian. Also we will assume that

$$\int \rho_M{}'dM'=1, \tag{13}$$

which implies that

$$\int A(M)dM=\mathrm{Tr}(A), \tag{14}$$

and the normalization condition (1) for probability distributions becomes

$$\mathrm{Tr}(\rho)=1 \tag{15}$$

for density operators ρ. Conditions (15) and (9) allow us to let ρ represent the state of the system and to form expectation values of physical quantities according to

$$\langle A\rangle=\mathrm{Tr}(A\rho). \tag{16}$$

Since all A and ρ are Hermitian, $\langle A\rangle$ will be real.

The commutator of two operators A and B will be given by

$$1/i(AB-BA)=[A,\, B]_- =\int A(M)B(M')[\rho_M,\, \rho_{M'}]_-dMdM',$$

so we see that we need to specify the commutation relations of the operators $\rho_{M'}$ in order to have the commutator bracket correspond to the Poisson bracket. For the case of one pair of canonical variables q and p we let

$$[\rho_{qp},\, \rho_{q'p'}]_-=\rho_{q'p}(\partial/\partial q)\delta(q-q')(\partial/\partial p')\delta(p-p') -\rho_{qp'}(\partial/\partial q')\delta(q-q')(\partial/\partial p)\delta(p-p'). \tag{17}$$

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[13] C. Chevalley, *Theory of Lie Groups* (Princeton University Press, Princeton, New Jersey, 1946), p. 103.

Then

$$[A, B]_- = \int A(q, p) B(q', p') \{\rho_{q'p}(\partial/\partial q)\delta(q-q') \cdot (\partial/\partial p')\delta(p-p') - \rho_{qp'}(\partial/\partial q')\delta(q-q')(\partial/\partial p)\delta(p-p')\} \cdot dqdpdq'dp',$$

which, after integrating by parts twice (and discarding the integrated terms by assuming that ρ_{qp} is such that $q^m p^n \rho_{qp} \to 0$ as q or $p \to \infty$ for any m, n), becomes

$$[A, B]_- = \int \left\{ \left(\frac{\partial}{\partial q} \frac{\partial}{\partial p'} - \frac{\partial}{\partial q'} \frac{\partial}{\partial p} \right) A(q, p) B(q', p') \right\} \cdot \rho_{qp} \delta(q-q') \delta(p-p') dqdpdq'dp', \quad (18)$$

which is clearly the operator corresponding to the Poisson bracket of $A(q, p)$ and $B(q, p)$. The operators $(q^m p^n)_{\text{op}}$ corresponding to the functions $q^m p^n$ will then satisfy the commutation relations

$$[(q_{\text{op}})^{m_1}(p_{\text{op}})^{n_1}, (q_{\text{op}})^{m_2}(p_{\text{op}})^{n_2}]_- = (m_1 n_2 - m_2 n_1) \{ (q^{m_1+m_2} p^{n_1+n_2-1})_{\text{op}} \} \quad (19)$$

We note that the correspondence (10) does not, in general, preserve multiplication. Indeed the commutation relations (19) are inconsistent with assigning the operator $(q_{\text{op}})^m$ to q^m and $(p_{\text{op}})^n$ to p^n. To show this we note that we have

$$[q_{\text{op}}, p_{\text{op}}]_- = 1, \quad (20)$$

from which it follows that

$$[(q_{\text{op}})^2, (p_{\text{op}})^n] = n\{ (q_{\text{op}})(p_{\text{op}})^{n-1} + (p_{\text{op}})^{n-1}(q_{\text{op}}) \}$$

and

$$[(q_{\text{op}})^3, (p_{\text{op}})^n]_- = n\{ (q_{\text{op}})^2(p_{\text{op}})^{n-1} + q_{\text{op}}(p_{\text{op}})^{n-1}q_{\text{op}} + (p_{\text{op}})^{n-1}(q_{\text{op}})^2 \}.$$

Hence if $(q_{\text{op}})^3 = (q^3)_{\text{op}}$, $(p_{\text{op}})^n = (p^n)_{\text{op}}$, the right-hand side of the above equations must be the operators for $2nqp^{n-1}$ and $3nq^2p^{n-1}$ according to (19). Now, multiplying the section equation, first on the left and then on the right by q_{op} and taking half the sum of the results, we get

$$[(q_{\text{op}})^3, (p_{\text{op}})^n]_- = \tfrac{3}{4} n \{ (q_{\text{op}})^3(p_{\text{op}})^{n-1} + (q_{\text{op}})^2(p_{\text{op}})^{n-1}q_{\text{op}} + q_{\text{op}}(p_{\text{op}})^{n-1}(q_{\text{op}})^2 + (p_{\text{op}})^{n-1}(q_{\text{op}})^3 \} + [n(n-1)/4i]\{ (q_{\text{op}})^2(p_{\text{op}})^{n-2} - (p_{\text{op}})^{n-2}(q_{\text{op}})^2 \}.$$

But, using (20), we get

$$[(q_{\text{op}})^4, (p_{\text{op}})^n]_- = n\{ (q_{\text{op}})^3(p_{\text{op}})^{n-1} + (q_{\text{op}})^2(p_{\text{op}})^{n-1}q_{\text{op}} + q_{\text{op}}(p_{\text{op}})^{n-1}(q_{\text{op}})^2 + (p_{\text{op}})^{n-1}(q_{\text{op}})^3 \},$$

so that by (19) we see that the right-hand side of the above equation is the operator for $4nq^3p^{n-1}$ and only the first term in parentheses in the commutator $[(q_{\text{op}})^3, (qp^n)_{\text{op}}]_-$ is the operator for $3nq^3p^{n-1}$ which according to (19) should be equal to the commutator. Therefore, we have demonstrated that the relation between functions and operators will not preserve multiplication.

We have seen that the kinematics of the system will be specified by (16) in terms of a density operator ρ. Since an arbitrary distribution $\rho(M)$ is an integral with a positive weighting function of the pure state distributions $\rho_{M'}(M) = \delta(M-M')$, but the delta function cannot be a sum with positive weights of positive functions having nonvanishing values at points $M \neq M'$, we see that the densities ρ form a convex set with the pure states $\rho_{M'}$ forming the extremal elements. Hence in studying the properties of the density operators we can confine our attention to the pure states. To include the property (9) we are forced to condition (12) for these operators. From this and (15) we can conclude that $\rho_{M'}$ cannot be positive definite and have a discrete spectrum. For then we would have $\text{Tr}(\rho_{M'}^2) \leq \text{Tr}(\rho_{M'}) = 1$, which contradicts (12). But then $\rho_{M'}$ cannot be positive definite. For if it were it would have a discrete spectrum since it has all of the other properties of the quantum mechanical density operator.[14] Also it is obvious that $\rho_{M'}^2 \neq \rho_{M'}$, so that this operator will not be a projection. This means that the pure state of the system cannot be associated with a vector of the Hilbert space. Similarly, the lack of positive definiteness means that each vector cannot be associated with a physical state of the system (there is no superposition principle in classical mechanics). In particular the state in which a set of quantities have precisely determined values will not be represented by a common eigenvector of the corresponding operators. The density operator $\rho_{q'p'}$ does, however, represent a state with definite values for the quantities q and p corresponding to the noncommuting operators q_{op} and p_{op} for we have that

$$\langle q^m p^n \rangle = \langle q \rangle^m \langle p \rangle^n = q'^m p'^n$$

or

$$\text{Tr}[\delta_{q'p'}(q^m p^n)_{\text{op}}] = [\text{Tr}(\rho_{q'p'} q_{\text{op}})]^m [\text{Tr}(\rho_{q'p'} p_{\text{op}})]^n = q'^m p'^n$$

This reflects the idea that when we say a quantity has a definite value in a probabalistic scheme we mean that the expectation values of all powers of the quantity are determined to satisfy relations of the above type.

Since the commutator bracket is known to satisfy linearity, antisymmetry, and Jacobi identity relations corresponding to Eq. (8), we see that the operators corresponding to power series in the dynamical variables will form a representation of this Lie algebra.

The dynamics of the system in the operator repre-

[14] J. von Newmann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1955), p. 189.

sentation is obtained by replacing Eqs. (4) and (5) by

$$(\partial/\partial t)A_t=[A_t, H]_- \tag{21a}$$

or

$$(\partial/\partial t)\rho_t=-[\rho_t, H]_- \tag{21b}$$

and

$$\langle A\rangle_t=\mathrm{Tr}(\rho A_t) \tag{22a}$$

or

$$\langle A\rangle_t=\mathrm{Tr}(\rho_t A), \tag{22b}$$

the choice of the (a) or (b) equations again depending on whether one chooses to regard the functions of the dynamical variables or the density of the state of the system as changing in time. Similarly the Eqs. (7) become

$$dA=[A, (q^m p^n)_{\mathrm{op}}]_- d\alpha_{mn} \tag{23a}$$

$$d\rho=-[\rho, (q^m p^n)_{\mathrm{op}}]_- d\alpha_{mn} \tag{23b}$$

showing how the operators $(q^m p^n)_{\mathrm{op}}$, which form a basis of the Lie algebra, act as the generators for the transformation specified by the parameters $d\alpha_{mn}$. The infinite parameter Lie group associated with this Lie algebra will have finite elements of the form of the operator

$$U=\exp\{\alpha_{mn}(q^m p^n)_{\mathrm{op}}\},$$

where the α_{mn} are the infinite set of parameters of the group and the

$$(q^m p^n)_{\mathrm{op}}=1/i(\partial U/\partial\alpha_{mn})_{\alpha_{ij}=0}$$

are the infinitesimal generators of the group.[15] These operators will produce dynamical transformations on the system according to

$$A\rightarrow UAU^{-1} \tag{24a}$$

or

$$\rho\rightarrow U^{-1}\rho U, \tag{24b}$$

which for the special case of a Hamiltonian of the (time-independent) form

$$H=\alpha_{mn}(q^m p^n)_{\mathrm{op}},\quad U=e^{iHt}$$

become

$$A_t=e^{iHt}A_0e^{-iHt} \tag{25a}$$

$$\rho_t=e^{-iHt}\rho_0{}^{iHt}, \tag{25b}$$

which are solutions of (21).

We note that the kinematical formalism of (16) or (22) shows explicitly that we can use either the (a) or (b) equations, since for either (24a) or (24b) we get that

$$\langle A\rangle\rightarrow\mathrm{Tr}(UAU^{-1}\rho)=\mathrm{Tr}(AU^{-1}\rho U)$$

Since the operators $(q^m p^n)_{\mathrm{op}}$ are Hermitian, U is unitary, which ensures that the Hermitian nature, as well as the other required properties, of A and ρ will be preserved under the dynamical transformations, and that the expectation values will remain real.

[15] G. Racah, Nuovo cimento Suppl. **14,** 67 (1959).

III. QUANTUM MECHANICS

To each quantum-mechanical state of a physical system one can associate, as Moyal[2] has shown, a quasi-probability distribution function $\rho(M)$ on the phase space $\{M\}$ of the canonical variables of the system. Similarly, to any physical quantity represented by the operator A there corresponds the function $A(M)$ which classically represents this quantity. The distribution is normalized according to (1) and expectation values are taken according to (2). To the commutator $[A, B]_-$ there corresponds a function which we shall call the Moyal bracket of the functions $A(M)$ and $B(M)$ and shall denote by $\sin[A(M), B(M)]$. We will illustrate our arguments with one pair of variables q and p which, as in classical mechanics, is easily generalized to n pairs of variables. Then the Moyal bracket has the form

$$2\sin\tfrac{1}{2}\left[\frac{\partial}{\partial q_A}\frac{\partial}{\partial p_B}-\frac{\partial}{\partial q_B}\frac{\partial}{\partial p_A}\right]A(q,p)B(q,p)$$
$$=2\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}}{k!(2n+1-k)!}\left(\frac{1}{2}\right)^{2n+1}\frac{\partial^{2n+1}A(q,p)}{\partial q^{2n+1-k}\partial p^k}\cdot\frac{\partial^{2n+1}B(q,p)}{\partial q^k\partial p^{2n+1-k}}, \tag{26}$$

where we take $\hbar=1$ ($\hbar$ actually enters the quantity $\sin[\ \ ]$ in such a way that in the limit as $\hbar\rightarrow 0$ only the first term, which is the Poisson bracket, remains nonvanishing). From this form we see that the Moyal bracket reduces to the Poisson bracket if one of the functions A or B is of quadratic or lower order in the variables q and p. These ideas have been put into a more rigorous mathematical formalism by Baker,[16] who has found an integral expression for the Moyal bracket and developed a set of postulates for quantum mechanics, in terms of the distributions $\rho(M)$, in analogy to classical mechanics. Instead of delta functions, the pure states are represented by functions $\rho(M)$ which satisfy

$$\rho(M)=\tfrac{1}{2}\cos[\rho(M),\rho(M)] \tag{27}$$

where the $\cos[\ \ ]$ is defined in complete analogy to the $\sin[\ \ ]$ and corresponds to the anticommutator of the operators corresponding to the functions. The set of all (physically allowed) densities is the convex set generated by these. The time evolution of the system is given by equations of the forms (4) and (5) with the Poisson bracket replaced by the Moyal bracket. We can also write Eqs. (7) with this replacement of brackets and we can show (see Appendix) that the Moyal bracket satisfies linearity, antisymmetry, and

[16] G. A. Baker, Jr., Phys. Rev. **109,** 2198 (1958). This problem was also considered by T. Takabayasi, Progr. Theoret. Phys. (Kyoto) **11,** 341 (1954), and the phase-space formulation was reviewed by H. Rubin, Proc. International Symposium on Axiomatic Method at Berkeley (North-Holland Publishing Company, Inc., Amsterdam, 1959).

Jacobi identity relations corresponding to (8). Hence the linear space of power series in the dynamical variables forms a Lie Algebra with the Moyal bracket as the Lie bracket. Evidently the dynamical transformations are again elements of the corresponding Lie group.

The operator representation is of course the usual formalism of quantum theory in terms of Hermitian density operators and operators representing physical quantities. Stratonovich[17] has explicitly shown that the linear correspondence between the phase space and operator representations which satisfies (9) and associates commutators with Moyal brackets is given by Eqs. (10), now with

$$L(M)=\sum_i A_i{}^+A_i(M),$$

where the operators A_i form a basis in the linear space of operators corresponding to functions of the dynamical variables, the inner product being $(A,B)=\mathrm{Tr}(AB^+)$; that is,

$$\mathrm{Tr}(A_iA_j{}^+)=\delta_{ij} \tag{28}$$

and the corresponding functions $A_i(M)$ satisfy

$$\int A_i(M)A_j{}^*(M)dM=\delta_{ij}.$$

[Actually, if we want to maintain the condition (15) we need to replace (1) by $\int\rho(M)\lambda(M)dM=1$, where $\lambda(M)=\mathrm{Tr}L(M)$.] Condition (28) does not lead to any of the restrictions that resulted from (12) in the case of classical mechanics. In fact we can have that for pure state density operators

$$\rho^2=\rho,$$

which is the operator equivalent of (27) and the condition that the Hermitian normalized ρ be a projection. Hence we can identify the pure states with vectors of the Hilbert space. The superposition principle requirement that every normalized vector be associated with a physical state means that ρ must be positive definite and thus have a discrete spectrum, which Baker has shown is indeed the case. The operators then have all the properties of the quantum mechanical density operators and (16) gives the usual quantum kinematics.

While we have a positive definite density operator and a one-to-one correspondence between physical states and vectors which was not possible in classical mechanics, the functions $\rho(M)$, in general, take negative values (hence the term quasi-probability distribution function). This means that not all distributions represent physical states of the system; e.g., the distribution concentrating all the probability at a point M' at which some $\rho(M')<0$ (i.e., we do not have positive definite distribution functions or a one-to-one correspondence between distribution functions and physical states). This is clearly related to the uncertainty principle.

In the operator representation the dynamics of the system is given by equations which are identical in form to Eqs. (21)–(25); this is, of course, the usual form of quantum dynamics. The quantum formalism differs from the classical only in the properties of the operators. The density operators belong to the convex set generated by projections, and the operators corresponding to functions of the dynamical variables have commutators corresponding to Moyal brackets. It is interesting to note that for the case of one pair of variables, having specified the operators q_{op} and p_{op} to satisfy (20) which, while sometimes called the "quantum condition," is characteristic of both classical and quantum mechanics, we can complete the dynamical formulation with one simple postulate: the operators $(q^mp^n)_{\mathrm{op}}$ are taken to be the symmetrized products of the operators $(q_{\mathrm{op}})^m$ and $(p_{\mathrm{op}})^n$. That is these operators will satisfy

$$[(q^{m_1}p^{n_1})_{\mathrm{op}},(q^{m_2}p^{n_2})_{\mathrm{op}}]_-=C_{m_1n_1m_2n_2}{}^{mn}(q^mp^n)_{\mathrm{op}}, \tag{29}$$

where the $C_{m_1n_1m_2n_2}{}^{mn}$ are determined from the Moyal bracket by

$$\sin[q^{m_1}p^{n_1},q^{m_2}p^{n_2}]=C_{m_1n_1m_2n_2}{}^{mn}q^mp^n.$$

Equation (29) is the quantum analog of (19). Since this determines the structure of the Lie algebra corresponding to power series in the dynamical variables, it determines the dynamics of the system within the formalism which we have seen to be descriptive of both quantum mechanics and classical mechanics.

We also note that with this quantum mechanical choice of operators the correspondence between functions and operators preserves multiplication except for a symmetrization of noncommuting factors, e.g., we have $(q^m)_{\mathrm{op}}=(q_{\mathrm{op}})^m$, $(p^n)_{\mathrm{op}}=(p_{\mathrm{op}})^n$. However the association does not preserve multiplication in general, as has been pointed out by Shewell.[12] For example if H_{op} is the operator corresponding to the function $H=p^2+q^2$ one can easily check that $(H^2)_{\mathrm{op}}\neq(H_{\mathrm{op}})^2$. This forces us to conclude that while these studies facilitate a comparison of quantum to classical mechanics the phase-space formulation is not completely suitable for a physical interpretation of quantum mechanics, for a function of a physically measurable quantity must correspond to the same function of the operator representing that quantity.

As an example of quantities having a Moyal bracket different from the Poisson bracket one can easily compute that

$$[q^3,p^3]_{\mathrm{PB}}=9q^2p^2,$$

while

$$\sin[q^3,p^3]=9q^2p^2-\tfrac{3}{2}.$$

[17] R. L. Stratonovich, Soviet Phys.—JETP **4**, 891 (1957); we wish to thank Dr. I. Bialynicki-Birula for bringing this work to our attention.

For the corresponding operators one obtains

$$[(q_{op})^3, (p_{op})^3]_- = 3(q_{op})^2(p_{op})^2 + 3q_{op}(p_{op})^2 q_{op} + 3(p_{op})^2(q_{op})^2$$
$$= 9(q_{op})^2(p_{op})^2\}_{\text{sym.}} - \tfrac{3}{2}$$
$$= 9/2\{(q_{op})^2(p_{op})^2 + (p_{op})^2(q_{op})^2\} + 3$$

with

$$\{(q_{op})^2(p_{op})^2\}_{\text{sym.}} = \tfrac{1}{16}\{(q_{op})^2(p_{op})^2 + q_{op}p_{op}q_{op}p_{op} + q_{op}(p_{op})^2 p_{op} + p_{op}(q_{op})^2 p_{op} + p_{op}q_{op}p_{op}q_{op} + (p_{op})^2(q_{op})^2\}$$
$$= \tfrac{1}{2}\{(q_{op})^2(p_{op})^2 + (p_{op})^2(q_{op})^2\} + \tfrac{1}{2}.$$

According to the Moyal rule of correspondence we associate the operator $\{(q_{op})^2(p_{op})^2\}_{\text{sym.}}$ with the function q^2p^2 and we see that in our example the commutator bracket corresponds to the Moyal bracket. According to Shewell,[12] River's rule of correspondence associates the function q^2p^2 with the operator

$$\tfrac{1}{2}\{(p_{op})^2(q_{op})^2 + (p_{op})^2(q_{op})^2\}$$

and our example shows that it does not make commutator brackets correspond toPoisson brackets.

We can now also see that Heisenberg's equations of motion (21a) will reduce to the form of Hamilton's equations of motion if A corresponds to a function of quadratic or lower order in the variables, for then the Moyal bracket is identical with the Poisson bracket.

The reduction of the Moyal bracket to the Poisson bracket in the quantum mechanical equation analogous to (4a) for the case that $A(q, p)$ is equal to q or p means that the points of phase space will traverse the same orbits quantum mechanically as classically. But in the quantum mechanical case the amount of probability density at an infinitesimal element of phase space will not remain constant as the element moves along its trajectory. Hence we were not really justified in assuming that we could choose either the (a)- or (b)-type equations to describe the dynamics of the system in phase space. However in the operator formulation it is clear that we do have this freedom of choice [see remarks following (25)], which means that we have the same freedom in the phase space formulation as long as we are dealing with functions which are quantum mechanically "physically meaningful," i.e., functions which have corresponding operators. We see then that the duality between the Schrödinger and Heisenberg pictures is a kind of quantum analog of Liouville's Theorem. In a similar way the fact that the operator formalism always leads to positive definite probabilities ensures that from the phase space calculations we cannot get negative probabilities for physically meaningful quantities.

Stratonovich has shown that equations of the type (1) can be used to find functions corresponding to operators which do not represent canonical coordinates and momenta, e.g., spin operators. However we can see that it is meaningless to ask for the classical analog of quantities which have no Poisson bracket relationships. For operators will be called classical if their commutators correspond to Poisson brackets and quantum if they correspond to Moyal brackets. If the properties of the quantities are known only through operator equations, this information is unavailable.

IV. THE CLASSICAL APPROXIMATION TO QUANTUM MECHANICS

Since the equations of quantum mechanics should reduce to those of classical mechanics in the limit as $\hbar \to 0$, it is of some interest to consider the explicit dependence of our quantum mechanical equations on $\hbar$. The form of the commutator bracket is then

$$[A, B]_- = 1/i\hbar(AB - BA)$$

If we were to consider the limit as $\hbar \to 0$ of Eq. (20) as the starting point for comparing the quantum and classical formalisms, we would have to conclude that the classical variables q and p commute. However we have chosen to regard the difference between the real variable and operator schemes as a choice of representation for the dynamical group. Hence we prefer to use the equations of motion as the starting point for our comparison of the two mechanics. With the above form of the commutator the Schrödinger equation (21b) is

$$i\hbar(\partial/\partial t)\rho = H\rho - \rho H$$

For the case that ρ represents a pure state which corresponds to the eigenvector ψ of the energy operator H with eigenvalue E this equation is equivalent to

$$i\hbar(\partial\psi/\partial t) = H\psi = E\psi$$

Now the right-hand sides of these equations are of the same order in $\hbar$ as commutator brackets multiplied by $\hbar$. As we have seen, taking the limit as $\hbar \to 0$ of such a quantity will not retain the operator representation features. Instead we have chosen to consider the commutator bracket which corresponds to the Moyal bracket which in turn reduces to the Poisson bracket as $\hbar \to 0$. Hence in obtaining a classical approximation to the eigenequation $H\psi = E\psi$ we should expect to retain terms of order $\hbar$ as well as of zero order in $\hbar$. The well-known WKB approximation does just this, and it turns out that the zero-order terms give the equation for Hamilton's principal function, while inclusion of the terms of order $\hbar$ leads (with some added conditions) to the Bohr quantization rules.

V. GENERALIZED MECHANICAL FORMALISMS

We have seen that both classical and quantum mechanics fit into a formal scheme which may be simply summarized. Suitable dynamical variables are chosen to describe the system and a quantity is chosen to describe the probability distribution state of the system. A bracket relation is assumed between functions of the dynamical variables by which the quantities corresponding to power series form a Lie algebra. A representation is chosen for these quantities which allows the formulation of a physically meaningful kinematical scheme. The elements of the corresponding Lie group then provide the dynamical transformations of the system.

We are thus led to ask if there are mechanical formalisms other than the classical or the quantum which can be found in this way. It is easy to see (see Appendix) that for the case of one pair of canonical variables the Poisson and Moyal brackets are special cases of a general bracket which satisfies the Lie algebra conditions and can be written as

$$[A, B]=2\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}C(n)}{D(k)D(2n+1-k)}\left(\frac{1}{2}\right)^{2n+1}\cdot\frac{\partial^{2n+1}A(q,p)}{\partial q^{2n+1-k}\partial p^{k}}\frac{\partial^{2n+1}B(q,p)}{\partial q^{k}\partial p^{2n+1-k}},$$

where $C(n)$ and $D(n)$ are functions of the index n which are restricted only by the convergence requirements of the series. Taking $C(n)=1$, $D(k)=k!$ leads to the Moyal bracket, while $C(n)=\delta_{n0}$, $D(k)=k!$ gives the Poisson bracket. However, we would not expect it to be so easy to find representations of the resulting Lie algebras which provide simple kinematical schemes. The function representation which has the most intuitive physical meaning is natural for classical mechanics while the operator representation which provides mathematical insight is natural for quantum mechanics. We have seen that each is very awkward in the natural representation of the other.

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APPENDIX

The real linear space of functions $f(q,p)$ with the composition rule $[f,g]=\sin[f,g]$ forms an infinite-dimensional Lie algebra.

Proof: We write

$$\sin[u,v]=\sum_{n=0}^{\infty}\frac{(-1)^{n}}{(2n+1)!}\left(\frac{\partial}{\partial q_u}\frac{\partial}{\partial p_v}-\frac{\partial}{\partial q_v}\frac{\partial}{\partial p_u}\right)^{2n+1}u(q,p)v(q,p)$$

$$=\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}}{k!(2n+1-k)!}\frac{\partial^{2n+1}u(q,p)}{\partial q^{2n+1-k}\partial p^{k}}\frac{\partial^{2n+1}v(q,p)}{\partial q^{k}\partial p^{2n+1-k}}\frac{\partial^{2n+1}v(q,p)}{\partial q^{k}\partial p^{2n+1-k}}.$$

(1) Then it is obvious that

$$[u, a_1v_1+a_2b_2]=a_1[u,v_1]+a_2[u,v_2]$$

$$[a_1u_1+a_2u_2, v]=a_1[u_1,v]+a_2[u_2,v],$$

where a_1, a_2 are real numbers.

(2) $[u,u]=0\Rightarrow[u+v,u+v]=0=[u,u]+[u,v]+[v,u]+[v,v]\Rightarrow[u,v]+[v,u]=0$ or $[u,v]=-[v,u]$.

(3) We need then only to prove that

$$[u,[v,w]]+[v,[w,u]]+[w,[u,v]]=0.$$

To do this we write

$$[u,[v,w]]=\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}}{k!(2n+1-k)!}\frac{\partial^{2n+1}u}{\partial q^{2n+1-k}\partial p^{k}}\frac{\partial^{2n+1}}{\partial q^{k}\partial p^{2n+1-k}}\left(\sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\frac{(-1)^{m+l}}{l!(2m+1-l)!}\frac{\partial^{2m+1}v}{\partial q^{2m+1-l}\partial p^{l}}\frac{\partial^{2m+1}w}{\partial q^{l}\partial p^{2m+1-l}}\right)$$

$$=\sum_{\substack{mn\\kl}}\frac{(-1)^{n+m+k+l}}{k!l!(2n+1-k)!(2m+1-l)!}\cdot\left(\frac{\partial^{2m+1}u}{\partial q^{2m+1-k}\partial p^{k}}\frac{\partial^{2(m+n)+2}v}{\partial q^{2m+1-l+k}\partial p^{2n+1-k+l}}\frac{\partial^{2m+1}w}{\partial q^{l}\partial p^{2m+1-l}}+\frac{\partial^{2n+1}u}{\partial q^{2n+1-k}\partial p^{k}}\frac{\partial^{2m+1}v}{\partial q^{2m+1-l}\partial p^{l}}\frac{\partial^{2(m+n)+2}w}{\partial q^{k+l}\partial p^{2(m+n)+2-k-l}}\right),$$

which we write as

$$[u,[v,w]]=\sum_{\substack{mn\\kl}}\frac{(-1)^{m+n+k+l}}{k!\,l!\,(2n+1-k)!\,(2m+1-l)!}$$

$$\left\{\begin{matrix} 2n+1 & 2(m+n)+2 & 2m+1 \\ u & v & w \\ 2n+1-k & 2m+1+k-l & l \\ k & 2n+1-k+l & 2m+1-l \end{matrix} \;+\; \begin{matrix} 2n+1 & 2m+1 & 2(m+n)+2 \\ u & v & w \\ 2n+1-k & 2m+1-l & k+l \\ k & l & 2(m+n)+2-k-l \end{matrix}\right\}$$

Hence $[u,[v,w]]+[v,[w,u]]+[w,[u,v]]=$

$$\sum_{\substack{nm\\kl}}\frac{(-1)^{m+n+k+l}}{k!\,l!\,(2n+1-k)!\,(2m+1-l)!}$$

$$\cdot\left\{\begin{matrix} 2n+1 & 2(m+n)+2 & 2m+1 \\ u & v & w \\ 2n+1-k & 2m+1+k-l & l \\ k & 2n+1-k+l & 2m+1-l \end{matrix} \;+\; \begin{matrix} 2n+1 & 2m+1 & 2(m+n)+2 \\ u & v & w \\ 2n+1-k & 2m+1-l & k+l \\ k & l & 2(m+n)+2-k-l \end{matrix}\right.$$

$$+\begin{matrix} 2n+1 & 2(m+n)+2 & 2m+1 \\ v & w & u \\ 2n+1-k & 2m+1+k-l & l \\ k & 2n+1-k+l & 2m+1-l \end{matrix} \;+\; \begin{matrix} 2n+1 & 2m+1 & 2(m+n)+2 \\ v & w & u \\ 2n+1-k & 2m+1-l & k+l \\ k & l & 2(m+n)+2-k-l \end{matrix}$$

$$\left.+\begin{matrix} 2n+1 & 2(m+n)+2 & 2m+1 \\ w & u & v \\ 2n+1-k & 2m+1+k-l & l \\ k & 2n+1-k+l & 2m+1-l \end{matrix} \;+\; \begin{matrix} 2n+1 & 2m+1 & 2(m+n)+2 \\ w & u & v \\ 2n+1-k & 2m+1-l & k+l \\ k & l & 2(m+n)+2-k-l \end{matrix}\right\}.$$

We now note that with the change of summation variables

$$n'=m,\quad k'=2m+1-l,\quad m'=n,\quad l'=k$$

the quantity in $\{\ \ \}$ remains unchanged, the 2nd and 3rd, 4th and 5th, and last and first terms interchanging. This is very easily seen by denoting the sets of indices by numbers

$$\left\{\begin{matrix} 2n+1 \\ 2n+1-k \\ k \end{matrix}\right\}=(1),\qquad \left\{\begin{matrix} 2m+1 \\ 2m+1-l \\ l \end{matrix}\right\}=(2),\qquad \left\{\begin{matrix} 2(m+n)+2 \\ 2m+1+k-l \\ 2n+1-k+l \end{matrix}\right\}=(3).$$

The quantity in $\{\ \ \}$ can then be written in a simple form by writing the sets of indices that occur with the u, v, w after each term has been arranged so that these appear in the order $u\ v\ w$. Thus the quantity becomes

$$(1)(3)(2)+(1)(2)(3)+(2)(1)(3)+(3)(1)(2)+(3)(2)(1)+(2)(3)(1)$$

and the change of summation variables changes the sets of indices by $(2)'=(1)$, $(1)'=(2)$, $(3)'=(3)$. Since the above quantity is just the sum of all permutations of (1)(2)(3), it is obviously unchanged under this change of indices. Now

$$k!l!(2n+1-k)!(2m+1-l)!=k'!l'!(2n'+1-k')!(2m'+1-l')!$$

but

$$n+m+k+l=m'+n'+l'+2n'+1-k'$$
$$=(n'+m'+k'+l')+2(n'-k')+1.$$

Hence

$$(-1)^{n+m+k+l}=-(-1)^{n'+m'+l'}.$$

Thus we can write

$$[u,[v,w]]+[v,[w,u]]+[w,[u,v]]=\sum_{\substack{nm\\kl}}\frac{(-1)^{n+m+k+l}}{k!l!(2n+1-k)!(2m+1-l)!}\{m,n,k,l\}$$
$$=-\sum_{\substack{n'm'\\k'l'}}\frac{(-1)^{n'+m'+l'+k'}}{k'!l'!(2n'+1-k')!(2m'+1-l')!}\{m',n',k',l'\}=-[u,[v,u]]-[v,[w,u]]-[w,[u,v]]=0,$$

which completes the proof of the Jacobi identity.

That the resulting Lie algebra is infinite dimensional can be seen by taking q^mp^n as a basis and expanding any function in the algebra in a power series

$$f=\sum_{mn}f_{mn}q^mp^n.$$

It is clear that $[u,v]=\sin[u,v]$ is not the only possible definition which gives a Lie algebra. For example, consider the same bracket changed by inserting an arbitrary function $C(n)$ as a factor:

$$[u,v]=\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}C(n)\left(\frac{\partial}{\partial q_u}\frac{\partial}{\partial p_v}-\frac{\partial}{\partial p_u}\frac{\partial}{\partial q_v}\right)^{2n+1}u(q,p)v(q,p)=\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}C(n)}{k!(2n+1-k)!}\frac{\partial^{2n+1}u}{\partial q^{2n+1-k}\partial p^k}\frac{\partial^{2n+1}v}{\partial q^k\partial p^{2n+1-k}}.$$

From the second form it is obvious that condition (1) is satisfied and from the first form (2) is also. In the proof of the Jacobi identity (3) a factor $C(n)C(m)=C(m')C(n')=C(n')C(m')$ is the only change and clearly does not alter the proof.

Of course $C(n)$ should be chosen to allow convergence of the series. If we attempt to generalize this further by an expression of the form

$$\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}C(n)}{D(k)E(2n+1-k)}\frac{\partial^{2n+1}u}{\partial q^{2n+1-k}\partial p^k}\frac{\partial^{2n+1}v}{\partial q^k\partial p^{2n+1-k}},$$

conditions (2) or (3) force us to assume that $D(n)=E(n)$.

Hence we prove that we still get a Lie algebra with

$$[u,v]=\sum_{n=0}^{\infty}\sum_{k=0}^{2n+1}\frac{(-1)^{n+k}C(n)}{D(k)D(2n+1-k)}\frac{\partial^{2n+1}u}{\partial q^{2n+1-k}\partial p^k}\frac{\partial^{2n+1}v}{\partial q^k\partial p^{2n+1-k}},$$

where C and D are restricted only by convergence requirements.

Condition (1) is still obvious and (2) is proved by writing the above expression for $[u,u]$ and introducing the new summation indices $k'=2n+1-k$, $k=2n+1-k'$.

Then, since $n+k=n+2n+1-k'=n+k'+2(n-k')+1$, we get $(-1)^{n+k}=-(-1)^{n'+k'}$, so that

$$[u,u]=\sum_{m=0}^{\infty}\sum_{k'=0}^{2n+1}\frac{-(-1)^{n+k'}C(n)}{D(k')D(2n+1-k')}\frac{\partial^{2n+1}u}{\partial q^{2n+1-k'}\partial p^{k'}}\frac{\partial^{2n+1}v}{\partial q^{k'}\partial p^{2n+1-k'}}$$
$$=-[u,u]=0$$

(3) is proved in the same manner as for $\sin[u,v]$ except the factor $1/k!l!(2n+1-k)!(2m+1-l)!$ is replaced by $C(n)C(m)/D(k)D(l)D(2n+1-k)D(2m+1-l)$ which under the change of indices

$$n'=m,\quad m'=n,\quad k'=2m+1-l,\quad l'=\mathrm{k}$$

becomes $C(m')C(n')/D(l')D(2n'+1-k')D(2m'+1-l)D(k')$, so the proof remains valid.