Quantum and classical mechanics in the phase space representation

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The theory of Hamiltonian mechanical systems is formulated solely in terms of physical and mathematical concepts which have meaning in both classical and quantum mechanics. In particular, the observables in both mechanics are c-number functions of the coordinates and the momenta. The operations of ordinary multiplication of observables and the Poisson brackets, also treated as a form of multiplication operation, are treated as separate objects which can have structural properties, including a dependence on ħ. It is a consequence of this that the only primary difference between quantum mechanics and classical mechanics is the concrete form of one algebraic identity for the multiplication operations. All other differences are secondary. The formalism developed in the present paper is particularly convenient for quantizations and for transitions (including partial ones) to the classical limits. The transitions in both directions are perspicuous and amenable to investigation for all quantities at any stage of the calculations. A unified quantum-classical scattering theory is constructed. An integral quantum equation of Lippmann-Schwinger type is obtained, the solution of the corresponding classical problem playing the part of the free solution in this equation. Iteration of this equation gives the quantum corrections to the classical solutions.

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INTRODUCTION

The standard formulations of quantum mechanics and classical mechanics are based on systems of essentially different physical and mathematical concepts, and, as a rule, these do not "survive" transitions from the one theory to the other. In classical mechanics, there is no analog of the quantum state vector, and in quantum theory there is no analog of a classical path, etc. Each of the formulations is splendidly adapted to calculations within the framework of the corresponding mechanics. But transitions from one mechanics to the other often appear tortuous and mysterious, and seem to require not only science but also ingenuity. For example, suppose that one subsystem can be treated classically (with possible quantum corrections) but another only in quantum terms. How is one to describe the interaction between them?

Problems in which it is necessary to have a combined quantum-classical treatment occur in many and varied situations (quantization of solitons, collisions of heavy ions with transitions to excited levels, quantum corrections to classical radiation, multidimensional tunneling, etc.). Attempts to find solutions to these problems lead to the obvious idea that for the treatment of all such combined situations it would be convenient to formulate classical and quantum mechanics in terms of the same physical and mathematical concepts. Such a unified formulation exists and is presented in what follows. In Ref. 1, it is called the combined algebra for quantum and classical mechanics. In the combined algebra, it turns out that the structures of classical and quantum mechanics are not only similar but are even identical in everything except the concrete form of one identity [(12a) in classical mechanics instead of (12) in quantum mechanics].

Three groups of ideas and methods are synthesized in the construction of the combined algebra.

1. Methods employing the phase space to describe quantum states and observables derived from the pioneering investigations of Weyl,2 Wigner,3 and Moyal.4

- 2. The methods of the theory of topological vector spaces and topological algebras (see, for example, Refs. 5 and 6 for the general definitions of observables; states, pure states, and positive states).
- 3. The methods of universal algebras, which make it possible to consider algebras with several different multiplication operations (for the general theory of these methods, see, for example, Refs. 7 and 8; for their use in quantum mechanics, see Refs. 9-11).

The transition to the combined algebra gives a definite gain, at a definite price. The gain is that transitions between quantum and classical mechanics become perspicuous and amenable to direct investigation (and . completion when possible) at any stage of the calculations. The price to be paid is that both theories must be presented in terms of unfamiliar physical and mathematical concepts. Therefore, to facilitate the reading of this review and to avoid misunderstandings, we give below some notes for the reader.

- 1. Classical and quantum mechanics are regarded as special cases of Hamiltonian theories. Therefore, the epithet "Hamiltonian" is to be understood as "both classical and quantum," and statements (definitions, properties, formulas, etc.) whose region of applicability is not stated or is not clear from the context are to be assumed valid for both mechanics.
- 2. The symbols π , π_h , π_0 , Π_h , σ , σ_0 , σ_h everywhere (except cases clear from the context; for example, when π is the corresponding number) denote new objects different operations of multiplication of observables. The multiplication symbol is written to the right of the pair of multiplied objects. For example, $AB\sigma_0$ denotes multiplication of A by B by means of the operation σ_0 . In general, of course, $AB\sigma_0 \neq AB\sigma_h$, etc. In accordance with 1), π_h , σ_h , Π_h are quantum multiplications and π_0 , σ_0 are classical multiplications (in them $\hbar = 0$), and the use of the multiplications π and σ means that the corre-

sponding formula holds in both mechanics.

3. Linear operators that act on different spaces are used. The ordinary quantum-mechanical operators acting on state vectors are denoted by upper-case letters with "hats," for example, \hat{A}, \hat{B} . Aggregates of the type $B\pi$ and $B\sigma$, and also upper-case script letters [for example, $\mathcal{U}(t)$] denote operators applied to the left to observables A. As a result of such an operation, we obtain new observables $AB\pi$, $AB\sigma$, $A\mathcal{U}(t)$. By definition, $B\pi$ is the operator of multiplication to the left by B by means of the operation π , as is reflected in the notation.

Operators that act to the right on states ρ are denoted by the same symbols with arrows underneath them, for example, $B\pi$, $B\sigma$, $\mathcal{U}(t)$. By definition, for any observable A and any state ρ

$$\langle A\mathcal{H}, \rho \rangle = \langle A, \mathcal{H}\rho \rangle,$$
 (1)

where $\langle A, \rho \rangle$ is a bilinear functional whose physical meaning is that of the expectation value of the observable A in the state ρ .

4. For the understanding of the present review, no special knowledge is required of either topological or universal algebras. Mathematical results needed for understanding things such as the existence of expansions in \hbar , the mathematical correctness of various multiplication operations, and so forth, are given without proof with appropriate references.

1. OBSERVABLES, STATES, EXPECTATION VALUES

We begin the construction of the combined quantumclassical algebra for one-dimensional motion.

In any physical theory, we are interested in observables, states, and the means for calculating the expectation value of a given observable in a given state.

In the ordinary formulation of classical mechanics, every observable is a c-number function A(p,q) of the momenta and the coordinates, and each state is given by a pair of numbers p_0, q_0 . The value of the observable in such a state is simply $A(p_0,q_0)$. To get closer to the quantum treatment, we go over to a more general statistical description of the state by means of a distribution function $\rho(p,q)$ (also a c-number function) which satisfies the obvious conditions of reality, normalizability, and positivity:

$$\rho = \rho^*; \quad \int dp \, dq \rho \, (p, q) \stackrel{\text{def}}{=} \langle 1, \rho \rangle = 1; \quad \rho_{cl} \geqslant 0. \tag{2}$$

We can now introduce the expectation value $\langle A, \rho \rangle$ of the observable A in the state ρ :

$$\langle A, \rho \rangle \stackrel{\text{def}}{=} \int dp \, dq A(p, q) \, \rho(p, q).$$
 (3)

For a completely determined (determinate) state, $\rho = \delta(p - p_0)\delta(q - q_0)$, we obtain the old result $\langle A, \rho \rangle = A(p_0, q_0)$.

In the usual formulation of quantum theory, the observables are operators \hat{A} and are described by matrix elements $\langle q_1 | \hat{A} | q_2 \rangle \stackrel{\text{def}}{=} A_0(q_1, q_2)$. The states are described by state vectors $\psi(q)$. Instead of the state vec-

tor, one can introduce the more general concept of a density matrix $\langle q_2 | \hat{\rho} | q_1 \rangle \stackrel{\text{def}}{=} \rho_0(q_2, q_1)$:

$$\langle q_2 | \hat{\rho} | q_1 \rangle = \sum_n \lambda_n \psi_n (q_2) \psi_n^* (q_1), \tag{4}$$

where $\lambda_n \ge 0$ and $\sum_n \lambda_n = 1$. The expectation value of the observable \hat{A} in the state $\hat{\rho}$ is written in the form

$$\langle A, \rho \rangle = \operatorname{Sp}(\hat{A} \hat{\rho}) = \int dq_1 dq_2 A_0(q_1, q_2) \rho_0(q_2, q_1).$$
 (5)

To make the quantum description closer to the classical one, we go over from the functions A_0 and ρ_0 by a linear nondegenerate transformation

$$A_{0}(q_{1}, q_{2}) = \frac{1}{2\pi\hbar} \int dp \, dq A(p, q) \exp\left\{i\hbar^{-1}p(q_{1}-q_{2})\right\} \times \delta\left\{q - \frac{1}{2}(q_{1}+q_{2})\right\};$$

$$\rho_{0}(q_{2}, q_{1}) = \int dp \, dq \exp\left\{i\hbar^{-1}p(q_{2}-q_{1})\right\} \times \delta\left\{q - \frac{1}{2}(q_{1}+q_{2})\right\}\rho(p, q)$$
(6)

to the Weyl representation of operators² by c-number functions A(p,q) and to the Wigner³ density matrix $\rho(p,q)$. The transformations (6) have the following properties, which make the new functions A and ρ more similar to the classical quantities:

- 1) the variables p and q of the functions A(p,q) are associated with the momentum and coordinate operators \hat{p} and \hat{q} , respectively;
- 2) for any observable A(p,q), the quantum Poisson brackets $(i\hbar)^{-1}[\hat{A},\hat{p}]$ and $(i\hbar)^{-1}[\hat{A},\hat{q}]$ are associated with the functions $\partial A/\partial q$ and $-\partial A/\partial p$;
- 3) the functions A(p,q) and $\rho(p,q)$ are real if they are associated with self-adjoint operators \hat{A} and $\hat{\rho}$:
- 4) the expression (5) for the expectation value takes the same form (3) as in the classical case.

However, it is well known that the Wigner density matrix is not always positive definite. Therefore, of the three conditions (2) only the first two hold for both mechanics. Below, in Sec. 3, we shall see that the difference in the third of the conditions (2) is not a primary but only a secondary difference.

2. CLASSICAL AND QUANTUM OPERATIONS OF MULTIPLICATION OF OBSERVABLES

We now turn to the key question of the operations of multiplication of observables. We give the name multiplication operation π to any rule that uniquely and bilinearly associates with any ordered pair (A,B) of observables a third observable C, which is called their product: $(A,B) \leftarrow C^{\text{def}}AB\pi$. The bilinearity of multiplication is expressed by the equations

 $(\alpha A_1 + \beta A_2) B\pi = \alpha A_1 B\pi + \beta A_2 B\pi;$ $A (\alpha B_1 + \beta B_2) = \alpha A B_1 \pi + \beta A B_2 \pi,$ where α and β are complex numbers.

Note that the multiplication operation is written to the right of the multiplied entities, and not between them (see, for example, Refs. 7 and 8).

It is obvious that with such a definition one can introduce several multiplication operations, not necessarily commutative or associative, for one and the same set. We now list the independent operations over the observables A(p,q). Above all, observables can be multiplied by numbers and added to one another. This means that the set $\{A\}$ of all observables forms a vector space. In addition, in each of the forms of mechanics there exist for the observables two multiplication operations—ordinary multiplication π and Poisson multiplication σ .

The classical ordinary multiplication π_0 is associative and commutative, and is realized as the simple multiplication of functions. The classical Poisson multiplication σ_0 is anticommutative and is realized by the classical Poisson brackets:

$$AB\sigma_0 \stackrel{\text{def}}{=} \left[\frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} \underline{\pi}_0 \right]. \tag{7}$$

We recall that any pair of observables, for example, $(\partial A/\partial q)\partial B/\partial p$, becomes a product only once the corresponding multiplication operation has been written to the right. It follows from the arbitrariness of A and B that (7) can be rewritten in the form of an equation between operations:

$$\sigma_0 = (\partial_{1q} \partial_{2p} - \partial_{1p} \partial_{2q}) \,\pi_0. \tag{8}$$

Here, ϑ_{1q} is the operation of differentiation with respect to q applied to the left to the first factor, etc.

We now introduce for observables the operation of associative quantum multiplication Π_h , defining it by the requirement

$$AB\Pi_{\hbar} = C, \tag{9}$$

if for the corresponding operators $\hat{A}\hat{B} = \hat{C}$. It follows from (6) that Π_b has the form

$$\Pi_{\hbar} = \exp\left\{ (i\hbar)/2 \left(\partial_{1q} \partial_{2p} - \partial_{1p} \partial_{2q} \right) \right\} \pi_0. \tag{10}$$

The exponential of the differentiation operations is to be understood as calculated by means of Fourier transformations:

$$C(p, q) = AB\Pi_{h} = \frac{1}{(2\pi)^{2}} \int dx_{1} dx_{2} dp_{1} dp_{2} \exp \left\{ i p \left(x_{1} + x_{2} \right) - i p_{1} x_{1} - i p_{2} x_{2} \right\} A\left(p_{1}, q - \frac{\hbar x_{2}}{2} \right) B\left(p_{2}, q + \frac{\hbar x_{1}}{2} \right) = \frac{1}{(\pi \hbar)^{2}} \int dq_{1} dq_{2} dp_{1} dp_{2} A\left(p_{1}, q_{1} \right) B\left(p_{2}, q_{2} \right) \times \exp \left\{ \frac{2i}{\hbar} \left(pq_{2} - pq_{1} - p_{1}q_{2} + p_{2}q_{1} + qp_{1} - qp_{2} \right) \right\}.$$

$$(11)$$

Formula (11) was obtained by Moyal.⁴ In the ordinary formalism, the quantum Poisson brackets have the form $(i\hbar)^{-1}[\hat{A},\hat{B}]$. It follows from this that the operation of quantum Poisson multiplication σ_h can be related to Π_h by the equation

$$\Pi_h - \Pi_h^T = i\hbar \sigma_h, \tag{12}$$

where Π_{\hbar}^{T} is the transposed Π_{\hbar} multiplication:

$$AB\Pi_{h}^{T} \stackrel{\text{def}}{=} BA\Pi_{h}. \tag{13}$$

One can also introduce a commutative but not associative quantum multiplication π_n :

$$\pi_h = (\Pi_h + \Pi_h^T)/2, \tag{14}$$

corresponding to half of the anticommutator. The multiplication π_h is called Jordan multiplication. In accordance with (10), (12), and (14),

$$\sigma_{\hbar} = (2/\hbar) \sin(\hbar D_{12}/2) \,\pi_0;$$
 (15)

$$\pi_{\hbar} = \cos\left(\hbar D_{12}/2\right) \pi_{0},$$
(16)

where $D_{12} = \partial_{1q}\partial_{2p} - \partial_{1p}\partial_{2q}$.

It can be seen from (10), (15), and (16) that as $\hbar \to 0$ (more precisely, as $\hbar \to +0$)

$$\Pi_h \to \pi_0; \quad \pi_h \to \pi_0; \quad \sigma_h \to \sigma_0.$$
 (17)

Therefore, one should take either Π_h or π_h as the operation of ordinary quantum multiplication corresponding to π_0 . In Refs. 9 and 10, in which operations of multiplication of quantum observables were apparently introduced for the first time as independent entities, and also in Refs. 1 and 12, Jordan multiplication π_h was taken as the quantum analog of π_0 . However, in Sec. 3 we shall see that it is correct to take Π_h as the ordinary quantum multiplication, since it is precisely for this choice that we can formulate the principal assertion of the present paper: the only primary difference between quantum and classical mechanics is the difference between the pairs of multiplications π_0 , σ_0 and Π_h , σ_h reflected in the fact that the multiplication π_0 is commutative, i.e., it satisfies the identity

$$\pi_0 - \pi_0^T = 0, \tag{12a}$$

whereas Π_h satisfies the identity (12). All the remaining necessary and sufficient basic propositions can be formulated in terms of the multiplications π and σ in the same way for both forms of mechanics.

These propositions single out classical mechanics as $\pi \to \pi_0$, $\sigma \to \sigma_0$ and quantum mechanics as $\pi \to \Pi_h$, $\sigma \to \sigma_h$. In particular, one can obtain from (8), (10), and (15) identities for all observables A, B, C:

$$AB\pi C\sigma = AC\sigma B\pi + ABC\sigma\pi; \tag{18}$$

$$AB\sigma C\sigma = AC\sigma B\sigma + ABC\sigma\sigma, \tag{19}$$

which hold (as is indicated by the notation) for both forms of mechanics. In Ref. 11, these identities were called the conditions for Hamiltonicity of the theory. Their meaning is explained in Sec. 5.

In the mathematical sense, the observables of each of the mechanics form an algebra with the two multiplications π and σ . One can go even further and define a combined quantum-classical algebra with four multiplication operations $\pi_0, \sigma_0, \Pi_h, \sigma_h$, since both algebras are realized on the same entities—the functions A(p,q). It is only necessary to remember that in the algebra each operation must exist for any pair of elements and lead to another element of the algebra. This requirement imposes fairly stringent restrictions on the set of elements $\{A\}$ of the vector space of observables. These restrictions were analyzed in Ref. 1, and it was shown that in the space $\{A\}$ one can include all infinitely differentiable functions that increase at infinity (together with all their derivatives) not faster than polynomials.

The quantum algebra of observables with Moyal multiplication (10) has been investigated on many occasions (see, for example, Refs. 13–17, in which references to earlier papers can be found), in which, however, the space $\{A\}$ was either not defined at all (for example, in Refs. 13 and 14) or was assumed to be the space of infinitely differentiable functions that decrease rapidly (faster than any polynomial in $|p|^{-1}$ and $|q|^{-1}$) at infinity (for example, in Ref. 15) or was assumed to

be isomorphic to the space of bounded operators. However, the restriction to either rapidly decreasing functions or functions corresponding to bounded operators means that one cannot consider observables such as the momentum and kinetic energy. In addition, for functions corresponding to bounded operators differentiation, and thus the multiplication σ_0 itself, is not defined almost everywhere.

3. CONDITIONS OF REALITY AND POSITIVITY OF OBSERVABLES AND STATES

Beginning with this section, we shall work toward the establishment of the main assertion of the paper. The set of observables $\{A\}$ is the same for the classical and quantum theories. Since quantum theory also uses non-self-adjoint operators, we must assume that the functions A(p,q) can be not only real but also complex. We then encounter a new operation over observables—the involution J, which in the operator formulation corresponds to Hermitian conjugation, $\hat{A} + \hat{A}^{\dagger}$, and in the phase space realization to complex conjugation, $A(p,q) + A^{*}(p,q)$. We shall assume that the involution operation acts to the left, so that

$$AJ = A^*. (20)$$

Obviously, $J^2=1$.

Real (or, which is the same thing, Hermitian) observables are now distinguished by the condition

$$AJ = A$$
, i.e., $A = A^*$. (21)

In the complete state space $\{\rho\}$ we include all real and complex functions $\rho(p,q)$ for which $\langle A,\rho\rangle$ in (3) exists for all A in $\{A\}$. In this case, $\{\rho\}$ will be a vector space containing all ordinary and generalized functions that decrease rapidly at infinity (together with all their derivatives). In particular, $\{\rho\}$ will include the determinate classical states $\delta(p-p_0)\delta(q-q_0)$.

In the space $\{\rho\}$, we also introduce the involution operation \underline{J} , which it is convenient to assume acts to the right and realizes complex conjugation:

$$J_0 = 0^*$$
. (22)

The operations J and J are connected by the further relation $\langle AJ, \rho \rangle = \langle A, J\rho \rangle^*$. In complete analogy with (21), real states are distinguished by the condition

$$J\rho = \rho$$
, i.e., $\rho = \rho^*$. (23)

The bilinear form $\langle A, \rho \rangle$ is real for real A and ρ . We emphasize that the exposition applies throughout to both forms of mechanics.

In physics, one encounters observables (for example, the kinetic energy) for which measurements of them give only non-negative results. Such observables are called positive. By definition, an observable B is positive if it can be represented in the form

$$B_{pos} = AA^*\pi, \tag{24}$$

where A is some other (not necessarily real) observable. Here one encounters in a typical form one of the secondary differences between quantum and classical mechanics. The condition (24) holds for both forms of

mechanics, but it contains the multiplication operation π , which has different properties in the different mechanics. In classical mechanics $\pi = \pi_0$, so that (24) reduces to

$$B_{\text{pos. cl}} \geqslant 0.$$
 (24a)

In quantum mechanics, the positive elements are the ones that can be represented in the form

$$B_{\text{pos. qu}} = AA^*\Pi_h. \tag{24b}$$

We have here a manifestation of the difference noted in the previous section between the definition $\pi = \Pi_h$ adopted here for the ordinary quantum multiplication and the definition $\pi = \pi_h$ adopted in Refs. 1, 9, 10, and 12. For example, the observable

$$p^2 + q^2 - \hbar = (p + iq) (p - iq) \Pi_h$$

is positive with respect to the first definition and nonpositive with respect to the second. Note that if only real observables are used, then the two definitions are identical.

The only physically admissible states are those in which the expectation values of positive observables are non-negative, i.e., for all A:

$$\langle AA^*\pi, \rho \rangle \geqslant 0.$$
 (25)

This condition is also valid for both forms of mechanics. Here too the difference between the multiplications π_0 and Π_h results in a secondary difference between the sets $[\rho]_{\rm cl}$ and $[\rho]_{\rm qu}$ of classical and quantum positive states, respectively. For classical positive states, the condition (25) is equivalent to non-negativity of ρ :

$$\rho_{\rm cl} \geqslant 0.$$
 (25a)

As one would expect, the set $[\rho]_{\mathrm{cl}}$ is composed of the classical distribution functions $\rho(p,q)$. The set of quantum states $[\rho]_{\mathrm{qu}}$ coincides with the set of admissible Wigner density matrices (6). It differs, on the one hand, from $[\rho]_{\mathrm{cl}}$ so fundamentally that there exists no linear transformation that carries the one set into the other.\(^1\) On the other hand, there are "rather many" functions that occur in both sets. For example, there are the Gaussian functions

$$(2\pi QP)^{-1} \exp\left\{-(1/2)\left[(q-q_0)^2 Q^{-2} - (p-p_0)^2 P^{-2}\right]\right\},$$
 (26)

for which the widths Q>0 and P>0 are compatible with the uncertainty relation $QP \ge \hbar/2$. Note that these Gaussian functions satisfy the inequality $|\rho(p,q)| \le (\pi\hbar)^{-1}$ obtained in Sec. 13 for ρ in $[\rho]_{qp}$.

It is well known that there exist Wigner density matrices ρ in $[\rho]_{qu}$ that are not positive definite, i.e., do not belong to $[\rho]_{cl}$. Less well known is the dual property¹: there exist classical states that do not satisfy the quantum positivity condition. In particular, the classical states $\rho_{cl} = \delta(p-p_0)\delta(q-q_0)$ corresponding to exact fixing of the momentum and coordinate are "quantum nonpositive"; indeed, for the observable $A = (p^2 + q^2)/2$ we obtain

$$\langle AA^*\Pi_\hbar, \; \rho_{\rm cl} \; \rangle = (p_{\rm o}^2 + q_{\rm o}^2)^2/4 - \hbar^2/4,$$

i.e., an expression that is negative for $p_0^2 + q_0^2 < \hbar$. Verifying that a quantum state is positive is frequently a

technically complicated problem. This difficulty can be avoided by going over from the states $\rho_{\rm qu}$ to the new quantities $\Psi_{\rm qu}(p,q)$, which can be called state amplitudes. We define the amplitude of a quantum state by the relation

$$\rho_{qu}(p, q) = \Psi_{qu}(p, q) \Psi_{qu}^*(p, q) \widetilde{\Pi}_h, \qquad (27)$$

where Π_{k} is the operation of associative multiplication

$$\widetilde{\Pi}_{h} = \exp\left(i\hbar D_{12}/2\right) \pi_{0}. \tag{28}$$

It can be seen that $\tilde{\Pi}_h$ coincides with Π_h . But this coincidence is, in a certain sense, accidental. The multiplication $\tilde{\Pi}_h$ is not defined on the same entities as Π_h and, in addition, it transforms differently under linear transformations. By direct verification one can show that states represented in the form (27) satisfy the condition of quantum positivity.

Positive states will also be called physical states, since only these states describe real physical systems.

4. PURE AND MIXED STATES

Physical states ρ are divided into pure and mixed states. A definition common to both forms of mechanics is as follows. A positive normalized state ρ is said to be mixed if it can be represented in the form

$$\rho = \lambda_1 \rho_1 + \lambda_2 \rho_2, \tag{29}$$

where $\lambda_1, \lambda_2 > 0$, $\lambda_1 + \lambda_2 = 1$, $\rho_1 \neq \rho$, $\rho_2 \neq \rho$, and ρ_1 and ρ_2 are also positive normalized states. A positive state that cannot be represented in the form (29) is said to be pure. Geometrically, the set of positive states $[\rho]$ in each of the mechanics forms a cone. In accordance with (29), mixed states are interior points of the cone. Pure states are extreme points of the cone. Because of the difference between the cones $[\rho]_{cl}$ and $[\rho]_{qu}$ (ultimately, this again derives from the difference between the multiplication operations π_0 and Π_h), classical pure states differ radically from quantum pure states. Namely, the former have the form

$$\rho_{\text{cl. pure}} = \delta (p - p_0) \delta (q - q_0), \tag{30}$$

i.e., they correspond to the complete absence of statistical spread for all observables. Quantum pure states can be represented in the form

$$\rho_{\text{qu. pure}}(p, q) = \frac{1}{2\pi\hbar} \int dq' \exp(-i\hbar^{-1}pq') \,\psi\left(q - \frac{q'}{2}\right) \psi^*\left(q + \frac{q'}{2}\right), \tag{31}$$

i.e., they admit description in terms of state vectors (not to be confused with a state amplitude $\Psi_{qu}(p,q)$!).

One can say that the ordinary formalisms in each form of mechanics are constructed to describe only pure states, and it is for this reason that they are not well suited for transitions from the one form of mechanics to the other.

5. GENERATORS

In the operator formulation of quantum mechanics, each observable \hat{A} is simultaneously the generator of some one-parameter Lie group. In particular, the Hamiltonian \hat{H} is the generator of time displacements. In classical mechanics, the observables themselves are not generators. However, with each observable there is uniquely associated a corresponding generator. In the most general form, these relations were formulated in Ref. 11. In the approach developed here, the connection is established in the same way for both forms of mechanics. The operation of Poisson multiplication σ is used to obtain the generators. We note first that the expression $AB\sigma$, by definition, admits two (of course, mutually consistent) interpretations. First, one can imagine that the brackets are placed in the manner $(AB)\sigma$ and then assume that this expression is the product of two elements in the space $\{A\}$. Second, one can equally well imagine the brackets in the form $A(B\sigma)$. In this case, the aggregate $B\sigma$ can be interpreted as a linear operator applied to the left on the vector space $\{A\}$ of the functions A(p,q) in accordance with the rule $A \rightarrow AB\sigma$. This operator is then the generator of the corresponding one-parameter Lie group. In order to be the generator of a Lie group, an operator must satisfy definite mathematical relations. One of the forms of these relations is that each generator Co must be a differentiation operator, i.e., it must satisfy the rule for the differentiation of a product for all products $AB\pi$ and $AB\sigma$. But it is precisely this rule that is expressed by the identities (18) and (19), which show that to each observable C in each of the mechanics there corresponds the generator Co.

It follows from (18) and (19) that the operator $\exp(zC\sigma)$ of a finite transformation of the Lie group (z is the group parameter) satisfies the relations

$$A(0) B(0) \pi \exp(zC\sigma) = A(z) B(z) \pi;$$
 (32)

$$A(0) B(0) \sigma \exp(zC\sigma) = A(z) B(z) \sigma,$$
 (33)

where $A(z) = A(0) \exp(zC\sigma)$ and $B(z) = B(0) \exp(zC\sigma)$. We shall not pause here to consider the purely mathematical problem that for some elements of the Lie algebra there need not exist corresponding elements of the Lie group. Using (19) (which is none other than the Jacobi identity), we can readily show that if the set of observables $L_m(m=1,2,\ldots,M)$ forms with respect to Poisson multiplication a Lie algebra with the structure constants G_{mn}^I :

$$L_m L_n \sigma = G_{mn}^l L_l, \tag{34}$$

then the operators $L_m \sigma$ form the same Lie algebra with respect to the operation of commutation of operators:

$$(L_n\sigma)(L_n\sigma) - (L_n\sigma)(L_m\sigma) = L_m(L_n\sigma)\sigma = G_{mn}^l(L_l\sigma).$$
(35)

Here too the brackets are inserted only for convenience.

Our most important achievement in this section is to have obtained three entities that are uniquely related to one another: the observable A(p,q), the classical generator

$$A\sigma_0 = \left(\partial_{\boldsymbol{q}} \frac{\partial A}{\partial p} - \partial_{p} \frac{\partial A}{\partial q}\right) \pi_0$$

¹⁾Mathematically, observables are contravariant symbols (see Ref. 17), while ρ , Ψ , Ψ^* are covariant. Therefore, the multiplication operations Π_h and $\tilde{\Pi}_h$ have different transformation properties.

and the quantum generator $A\sigma_h$. At the same time, the observable itself can be assumed to be simultaneously classical and quantum. Note that the generators $A\sigma_0$ and $A\sigma_h$ coincide only for observables A that are polynomials in p and q of degree not higher than the second. The existence of the triplet $A, A\sigma_0, A\sigma_h$ makes it possible to formulate clearly and simply the problem of transitions between classical and quantum mechanics: Under such transitions, the observables need not be changed at all, while the generators are mapped into each other; $A \leftarrow A, A\sigma_0 \leftarrow A\sigma_h$.

6. HEISENBERG EQUATIONS OF MOTION

The Heisenberg equations of motion describe an evolution of the observables in time that is completely determined by the specification of the observable H(p,q), i.e., the Hamiltonian function. To this observable there correspond two generators of time displacement—the classical $H\sigma_0$ and the quantum $H\sigma_h$. Thus, for each observable A(p,q) there are two evolutions in time. The classical evolution is described by the equation

$$\partial A_{cl}(p, q, t)/\partial t = A_{cl}(p, q, t) H(p, q) \sigma_0,$$
 (36a)

and the quantum evolution by the equation

$$\partial A_{qu}(p, q, t)/\partial t = A_{qu}(p, q, t) H(p, q) \sigma_{h}.$$
 (36b)

These are Heisenberg equations, since they describe the time evolution of observables. At the initial time, the observables can be chosen coincident:

$$A_{cl}(p, q, 0) = A_{qu}(p, q, 0) = A(p, q).$$
 (37)

However, because of the difference between σ_0 and σ_h , this correspondence between the classical and quantum observables is lost at subsequent times (except for the quadratic Hamiltonian for a free nonrelativistic particle and for a harmonic oscillator, for which the classical evolution coincides with the quantum evolution).

We give a simple example. For the Hamiltonian function $H = p^2/2m + aq^4$, the classical and quantum Heisenberg equations of motion are

$$\begin{split} \partial A_{\mathrm{cl}} \left(p,\,q,\,t \right) / \partial t &= \left(p/m \right) \left(\partial A_{\mathrm{cl}} \left/ \partial q \right) - 4aq^3 \, \partial A_{\mathrm{cl}} \left/ \partial p \right; \\ \partial A_{\mathrm{qu}} (p,\,q,\,t) / \partial t &= \left(p/m \right) \partial A_{\mathrm{qu}} ' \partial q - 4aq^3 \left(\partial A_{\mathrm{qu}} / \partial p \right) + \hbar^2 aq \, \partial^3 A_{\mathrm{qu}} / \partial q^3. \end{split}$$

For the classical evolution in time, one can go over from (36a) to the classical Hamilton equations for the functions P(t) and Q(t):

$$\frac{dP(t)/dt = -\partial H(P, Q)/\partial Q;}{dQ(t)'dt = \partial H(P, Q)/\partial P.}$$
 (38)

The possibility of this transition is due to the fact that, in accordance with (8), Eq. (36a) is linear and is of first order in t, p, q. It is known from the theory of such equations that each of them is equivalent to the system of ordinary differential Hamilton equations (38). If P(p,q,t), Q(p,q,t) is a solution of the system (38) with the initial conditions P(p,q,0) = p and Q(p,q,0) = q, then, in complete agreement with (32), the solution of Eq. (36a) with the initial condition (37) will be

$$A_{cl}(p, q, t) = A_{cl} \{ P(p, q, t), Q(p, q, t), 0 \}$$

= $A \{ P(p, q, t), Q(p, q, t) \}.$ (39)

We emphasize that the solution of the quantum equa-

tion (36b) does not have the property (39). This means that Eq. (36a) and the system (38) are equivalent within the limits of classical mechanics but are not equivalent when one takes into account the quantum properties. To Eq. (36a), one can add the quantum corrections, but to the system (38) one cannot. This asymmetry between quantum and classical mechanics is due to the fact that our observables are realized by c-number functions, i.e., they are constructed out of the generators p and q of the algebra by means of classical multiplications π_0 . This asymmetry is eliminated by noting that the observables of not only quantum but also classical mechanics can be realized on a "quantum" set of linear operators. 13

7. SCHRÖDINGER EQUATIONS OF MOTION

In the Heisenberg picture, the states ρ do not change in time, so that the expectation values change in time because of the change of the observables:

$$\langle A_{\mathfrak{s}} \ \rho \rangle_t = \langle A(t), \ \rho \rangle.$$
 (40)

In the Schrödinger picture, in contrast, the states change in time, while the observables are constant:

$$\langle A, \rho \rangle_t = \langle A, \rho (t) \rangle.$$
 (41)

To go over to the Schrödinger picture, we use the mathematical concept of the operator dual to the original operator in the sense of the theory of topological vector spaces (this is neither the complex nor the Hermitian conjugate!).

An operator \mathcal{U} , which acts to the right on the states ρ , is said to be dual to the operator \mathcal{U} , which acts to the left on the observables, if (1) is satisfied for all A and ρ . It follows that if the operators \mathcal{U} and \mathcal{U} are represented by their kernels, these kernels coincide:

$$\langle p, q | \mathcal{U} | p', q' \rangle = \langle p, q | \mathcal{U} | p', q' \rangle. \tag{42}$$

It follows from (36a), (36b), and (40)-(42) that the required Schrödinger equation of motion has the form of the Liouville equation:

$$\partial \rho / \partial t = H \sigma \rho,$$
 (43)

which holds of course, for classical mechanics when $\sigma = \sigma_0$ and for quantum mechanics when $\sigma = \sigma_{h}$.

In particular, for the Hamiltonian introduced above

$$\begin{split} H &= p^2/2m + aq^4; \\ \partial \rho_{\text{cl}} / \partial t &= (-p/m) \, \partial \rho_{\text{cl}} / \partial q + 4aq^3 \, \partial \rho_{\text{cl}} / \partial p; \\ \partial \rho_{\text{qu}} / \partial t &= (-p/m) \, \partial \rho_{\text{qu}} / \partial q + 4aq^3 \, \partial \rho_{\text{qu}} / \partial p - \hbar^2 a q \partial^3 \rho_{\text{qu}} / \partial p^3. \end{split}$$

By analogy with (39), the solution of the classical equation (43) has the form

$$\rho_{cl}(p, q, t) = \rho_{cl}\{P(p, q, -t), Q(p, q, -t), 0\}. \tag{44}$$

Note the difference between the signs of the time in (39) and (40). From the point of view of the physical meaning, states can be assumed to be simultaneously classical and quantum only in the common domain of the set-theoretical intersection $[\rho]_{\rm cl} \cap [\rho]_{\rm qu}$. But mathematically both equations (43) have meaning in the complete space $\{\rho\}$ of not necessarily positive nor even necessarily real states.

We introduce now the concept of the amplitude $\Psi(p,q)$ of a state in Hamiltonian mechanics defined by [cf. Eq. (27)

$$\rho = \Psi \Psi \widehat{\pi}, \tag{45}$$

where $\tilde{\pi} = \tilde{\Pi}_{n}$ from (28) for quantum mechanics and $\tilde{\pi} = \pi_{0}$ for classical mechanics. It is readily verified that the amplitude satisfies the same equation as ρ :

$$\partial \Psi(p, q, t)/\partial t = H\sigma\Psi(p, q, t).$$
 (46)

The amplitudes of physical states need be neither positive nor real. This makes it possible to obtain quantum positive states approximately by solving the classical $(\sigma = \sigma_0)$ equation (46) and making the transition to $\rho(t)$ in accordance with (27).

We note finally that, representing the Hamiltonian function in the form

$$H = H_0 + H_I, \tag{47}$$

we can introduce the interaction representation, in which

$$\partial A(t)/\partial t = A(t) H_0 \sigma; \quad \partial \rho/\partial t = (H_I(t)) \rho(t).$$
 (48)

Here, the dependence of $H_I(t)$ (and the other observables) on the time is determined by the first of Eqs. (48).

8. STATIONARY STATES

We say that a state ρ_{stat} is stationary if it does not change in time:

$$\partial \rho_{\text{stat}} / \partial t = H \sigma \rho_{\text{stat}} = 0.$$
 (49)

The stationarity condition depends twice on the operations of multiplication of observables. First, Eq. (49) explicitly contains the Poisson multiplication σ. Second, the ordinary multiplication π occurs in the definition of the set $[\rho]$ of positive states. Therefore, the states $[\rho_{\rm stat}]_{\rm cl}$ and $[\rho_{\rm stat}]_{\rm qu}$ are essentially different. The classical stationary states can all be represented in the form

$$\rho_{\text{cl. stat}}(p, q) = \int dt \rho_{\text{cl}} \{ P(p, q, -t), Q(p, q, -t), 0 \}
= \int dt \rho_{\text{cl}}(p, q, t),$$
(50)

where the integral is between infinite limits for nonperiodic motion and over the period for periodic motion (this means that the limits of integration may depend on p and q). In accordance with (50), the function $\rho_{\rm cl.stat}$ is constant on each path in the phase space. A classical stationary state can be pure only in the exceptional case of a particle at rest, when the function $\rho(p,q) = \delta(p)\delta(q-q_0)$ is a solution of the equation of motion (43) for $\sigma = \sigma_0$. The classical stationary states that are most nearly pure have the form

$$\rho_{\text{cl. stat}}(p, q) = \int dt \delta\{p_0 - P(p, q, -t)\} \delta\{q_0 - Q(p, q, -t)\}, \quad (51)$$

in which the function ρ is nonzero only on one phase path.

In quantum mechanics, in contrast, there are many pure stationary states. All functions ρ in (31) for which $\psi(q)$ is an eigenfunction of the Hamiltonian \hat{H} are such

states. In our formalism, the conditions of purity of a stationary state have the form

$$\frac{H\Pi_{h}\rho_{\text{qu. pure}} = E\rho_{\text{qu. pure}}}{H\Pi_{h}^{T}\rho_{\text{qu. pure}} = E\rho_{\text{qu. pure}}}$$
(52)

We emphasize that classical and quantum stationary states have an important common property, namely, in the case of infinite motion they cannot be normalized. For example,

$$\rho\left(p,\;q\right) = \int\limits_{-\infty}^{\infty} dt \,\delta\left(p_{0}-p\right) \,\delta\left\{q_{0}-\left(q-\frac{p}{m}\;t\right)\right\} = \frac{m}{\mid p_{0}\mid} \,\delta\left(p_{0}-p\right)$$

is a classical (and quantum!) state of free motion that cannot be normalized. Here, the difference between classical and quantum mechanics is that only in quantum theory can non-normalizable states of infinite motion be pure.

9. DIFFERENT QUANTIZATIONS

In the preceding sections, we have constructed a combined algebra for classical and quantum mechanics. In this algebra, the transitions $\pi_0 \longrightarrow \Pi_h$ and $\sigma_0 \longrightarrow \sigma_h$ establish a one-to-one correspondence between the two forms of mechanics. It is, however, well known that the transition from classical to quantum mechanics (which is called quantization) is to a high degree nonunique. In our formalism, this lack of uniqueness admits a simple and complete description. Speaking figuratively, we can say that it arises because in the linear space $\{A\}$ of observables and in the linear space $\{\rho\}$ of all (not necessarily positive) states, linear transformations can be performed that "rotate" the quantum algebra with respect to the classical algebra. Namely, in the quantum algebra we perform the nondegenerate linear transformations

$$A_{\mathcal{V}^{0}} = A_{\text{qu}} \mathcal{V} (\hbar); \tag{5.3}$$

$$A_{\mathcal{P}^{0}} = A_{\mathbf{q}\mathbf{u}} \mathcal{V}(\hbar); \tag{53}$$

$$\rho_{\mathcal{W}^{0}} = \underbrace{\mathcal{V}^{-1}(\hbar)}_{h} \mathcal{W}_{h}(\hbar) \rho_{\mathbf{q}\mathbf{u}} \stackrel{\text{def}}{=} \mathcal{V}^{-1}(\hbar) \rho_{\mathcal{P}^{0}}. \tag{54}$$

It is obvious that the transformations (53) and (54) must in the first place exist in some sense for all observables A(p,q) in $\{A\}$ and for all states ρ in $\{\rho\}$; it is also necessary that these transformations have inverses. The words "in some sense" emphasize the following circumstance. An operator [to be specific, 1/(ħ)] maps the vectors A of the space $\{A\}$ into the vectors A_{γ} of some other space $\{A_{\gamma}\}$. If the space $\{A\}$ contains infinitely differentiable functions, which can have growth not stronger than polynomial at infinity, then the space $\{A_{\gamma}\}$ may contain not only ordinary functions but also generalized functions. Moreover, in practical calculations, situations arise in which generalized functions are encountered that do not fit into the schemes with which physicists are accustomed to deal (see, for example, Refs. 18 and 19). It was shown in Ref. 12 that the appearance of generalized functions of any known class does not lead to new difficulties (any more than the use of transformations $V(\hbar)$ that "improve" the properties of the functions A(p,q) leads to real simplifications). These difficulties with spaces of generalized functions will be demonstrated in Sec. 11 in the exposition of Wick and anti-Wick quantization. The transformations $V(\hbar)$ act on all entities of the quantum algebra, i.e., on Π_h , σ_h , and J_{qu} , and also on the form of the expressions for the expectation values and on the equations of motion. The corresponding transformations to $\Pi_{q'}$, $\sigma_{q'}$, $J_{q'}$ are

$$\Pi \hbar = \mathcal{V}'(1) \mathcal{V}'(2) \Pi_{\mathcal{V}} \mathcal{V}^{-1};
\sigma_{\hbar} = \mathcal{V}'(1) \mathcal{V}'(2) \sigma_{\mathcal{V}} \mathcal{V}^{-1};$$
(55)

$$J_{\text{qu}} = \mathcal{V} J_{\mathcal{V}} \mathcal{V}^{-1} = \mathcal{V} (\mathcal{V}^*)^{-1} J_{\mathcal{V}^{\circ}}. \tag{56}$$

The bilinear form for the expectation values becomes

$$\langle A_{qu}, \rho_{qu} \rangle = \langle A_{qo} \mathcal{V}^{-1}, \mathcal{V} \mathcal{W} \rho_{qoq \mathcal{W}} \rangle = \langle A_{qo} \mathcal{W}, \rho_{qoq \mathcal{W}} \rangle. \tag{57}$$

In the Heisenberg picture, the transformed equations of motion have the form

$$\partial A_{qo}(t)/\partial t = AH_{qo}\sigma_{qo}, \tag{58}$$

and in the Schrödinger picture the form

$$W \partial \rho_{\mathcal{F} \circ \mathcal{W}} / \partial t = H_{\mathcal{F} \circ \mathcal{F} \circ \mathcal{W}} \rho_{\mathcal{F} \circ \mathcal{W}}, \tag{59}$$

or

$$\partial \rho_{\gamma \rho}/\partial t = H_{\gamma \rho} \sigma_{\gamma \rho} \rho_{\gamma \rho}.$$
 (59a)

The set of admissible transformations $V(\hbar)$, $W(\hbar)$ is very large, including, in particular, the transformations (6) to operator multiplication of observables and to the von Neumann density matrix. To single out in this set a class of transformations $V(\hbar)$, $\mathcal{H}(\hbar)$ leading to different admissible quantizations, it is necessary to impose on these transformations definite conditions. 12 which have the following origin. We wish to retain in force our principal assertion that all the differences between classical and quantum mechanics are due to the difference between the operations of multiplication of observables. On this basis, we require that on the transition from classical to quantum mechanics the observables and states (perhaps not all) pass, without changing, from being classical to being quantum. This means that the transformed observables A_{γ} are no longer arbitrary, but are functions A(p,q) of the coordinates and the momenta, and the set (vector space) $\{A_{\gamma}\}$ of these functions has nonempty intersection $\{A_{\gamma}\}\cap\{A\}$ with the set of classical observables. The set $[\rho_{\gamma_{N}^{c}}]$ of physical (i.e., positive) quantum states must satisfy similar conditions. If the new quantum algebra is to be a quantization of the classical algebra, the following conditions must also be satisfied: a) the identity, and also the observables p and q, must not change under the action of the transformations y and W:

$$1\mathcal{V} = 1\mathcal{W} = 1; \ p\mathcal{V} = p\mathcal{W} = p; \ q\mathcal{V} = q\mathcal{W} = q; \tag{60}$$

b) the generators $p\sigma$ and $q\sigma$ must not change under the action of the transformations V and W; for example,

$$p\sigma_{\gamma \circ} = p\sigma_{\hbar} = \partial_{q}; \tag{61}$$

c) the transformations $V(\hbar)$ and $\mathcal{H}(\hbar)$ must depend on \hbar and must be infinitely differentiable with respect to \hbar as $\hbar \rightarrow +0$. There must also exist the limits

$$\lim_{\hbar \to 0} \mathcal{V}(\hbar) = \lim_{\hbar \to 0} \mathcal{W}(\hbar) = 1; \tag{62}$$

d) the set-theoretical intersections $\{A\}\cap\{A_{g'}\}$ and $[
ho]_{\mathtt{cl}}$ $\cap [\rho_{q,q}]$ must contain sufficiently many elements. The meaning of the expression "sufficiently many" may be

different in different problems.

Let us elucidate the meaning of the requirements a) and b). Condition a) requires that the observables p and q have the meaning of the coordinate and momentum in every combined algebra. Through condition b), the observable p is associated with the generator of a coordinate shift, and the observable -q with the generator of a momentum shift.

It follows from (60) and (61) that the operators $V(\hbar)$ and %(ħ) must have the form

$$\mathcal{V} = \mathcal{V}(\hat{\sigma}_p, \, \hat{\sigma}_q, \, \hbar); \, \, \mathcal{W} = \mathcal{W}(\hat{\sigma}_p, \, \hat{\sigma}_q, \, \hbar). \tag{63}$$

The dependence on the differentiation operations is understood in the sense of Fourier transformations: the Fourier transforms

$$\widetilde{A}(x, k) = \frac{1}{2\pi} \int dp \, dq \exp\left(-ipx + iqk\right) A(p, q)$$
 (64)

are related by the transformation

$$\widetilde{A}_{\mathcal{F}^0}(x, k) = \widetilde{A}(x, k) \, \mathcal{V}(\mathrm{i} x, -\mathrm{i} k, \, \hbar), \tag{65}$$

where $V(-ix, ik, \hbar)$ is an ordinary function of the c-number variables ix, -ik, and \hbar . The meaning of $\mathcal{H}(\partial_{b}, \partial_{a}, \hbar)$ is similar.

We can now particularize condition c): the functions $\mathcal{V}(\mathrm{i}x,-\mathrm{i}k,\hbar)$ and $\mathcal{W}(\mathrm{i}x,-\mathrm{i}k,\hbar)$ exist and are infinitely differentiable for all real x and k and for all \hbar in the interval from zero to any finite value of the Planck constant. In addition, for the invertibility of the transformations V and M the functions V and M must vanish nowhere. The existence of the limits (62) now acquires a clear mathematical meaning:

$$\lim_{\hbar \to 0} \mathcal{V}(\mathbf{i}x, -\mathbf{i}k, \hbar) = \lim_{\hbar \to 0} \mathcal{W}(\mathbf{i}x, -\mathbf{i}k, \hbar) = 1.$$
 (62a)

The conditions (60) also take a clear form:

$$\mathcal{V}(0, 0 \, \hbar) = \mathcal{W}(0, 0, \hbar) = 1; \tag{66}$$

$$\frac{\partial \mathcal{V}(0, 0, \hbar)/\partial x = \partial \mathcal{V}(0, 0, \hbar)/\partial k}{= \partial \mathcal{W}(0, 0, \hbar)/\partial k} = \frac{\partial \mathcal{W}(0, 0, \hbar)/\partial k}{= 0.}$$
(67)

We emphasize that the properties of growth (or decrease) of the functions ${\mathscr V}$ and ${\mathscr H}$ and their derivatives with respect to the variables ix and -ik have not yet been restricted in any way except that functions of compact support are forbidden by the requirement that these functions do not vanish.

For the existence of nonempty intersections $\{A\}$ $\cap \{A_{\gamma}\}\$ and $[\rho]_{c1} \cap [\rho_{\gamma\gamma}]$ the functions $\mathcal{V}(\partial_{\rho}, \partial_{\sigma}, \hbar)$ and $\mathcal{M}(\vartheta_p,\vartheta_q,\hbar)$ must be real: $\mathcal{V}=\mathcal{V}^*,\mathcal{M}=\mathcal{M}^*$, whence in accordance with (56),

$$J_{qp} = J. \tag{68}$$

Explicit expressions for the transformed multiplication operations $\Pi_{\mathscr{C}}$ and $\sigma_{\mathscr{C}}$ can be obtained by using the rule for differentiating a product11:

$$\pi_{\hbar}\partial_{p} = (\partial_{1p} + \partial_{2p}) \pi_{\hbar}; \quad \sigma_{\hbar}\partial_{p} = (\partial_{1p} + \partial_{2p}) \sigma_{\hbar},$$

and similarly for $\Pi_h \partial_a$ and $\sigma_h \partial_a$. Using this rule, and also (15) and (16), we obtain

$$\Pi_{\varphi \circ} = U(1, 2) \exp \left[(i\hbar/2) D_{12} \right] \pi_0; \sigma_{\varphi \circ} = U(1, 2) (2/\hbar) \sin \left[(\hbar/2) D_{12} \right] \pi_0, \tag{69}$$

where

$$U(1, 2) = \mathcal{V}^{-1}(1) \mathcal{V}^{-1}(2) \mathcal{V}(1+2); \mathcal{V}(1) = \mathcal{V}(\partial_{1p}, \partial_{1q}, \hbar);$$

$$\mathcal{V}(1+2) = \mathcal{V}(\partial_{1p} + \partial_{2p}, \partial_{1q} + \partial_{2q}, \hbar).$$

$$(70)$$

The construction of the different combined algebras is now complete. Let us summarize our results.

To every pair of transformations % and % satisfying the conditions a)-d) there corresponds a combined quantum-classical algebra, which we denote by $\mathcal{B}(\mathcal{V},\mathcal{W})$. This algebra contains the two spaces of observables $\{A\}$ and $\{A_{\gamma}\}$, the operations π_0 and σ_0 of classical multiplication defined for any pair of functions A(p,q) in $\{A\}$, the quantum multiplication operations Π_{γ} and σ_{γ} defined for any pair of quantum observables in $\{A_{\mathscr{V}}\}$, and the involution operation J, which acts on all observables in both $\{A\}$ and $\{A_{\gamma}\}$. In addition, in the algebra \mathcal{B} , $(\mathcal{V}, \mathcal{W})$ there are defined the state spaces $\{\rho\}$ and $\{\rho_{\gamma \beta \gamma}\}\$ dual to $\{A\}$ and $\{A_{\gamma}\}$, respectively. By the definition of duality, these spaces are such that the classical expectation values $\langle A, \rho \rangle$ are defined for all observables in $\{A\}$ and for all states in $\{\rho\}$, and the quantum expectation values $\langle A, \mathcal{M} \rho \rangle$ are defined for all observables in $\{A_{\gamma}\}$ and for all states in $\{\rho_{\gamma\beta\gamma}\}$. The positivity conditions (24) and (25) single out in $\{\rho\}$ the set $[\rho]_{cl}$ of positive classical states, and in $\{\rho_{VV}\}$ the set $[\rho_{ggt}]$ of positive quantum states. The connection between the classical and the quantum algebra consists of the existence of the nontrivial sets $\{A\} \cap \{A_{\gamma}\}$ and $[\rho]_{cl} \cap [\rho_{q(cl)}]$, which are fairly rich in elements and within which the quantum observables and states coincide with the classical observables and states.

To every combined algebra $\mathcal{B}(\mathcal{V},\mathcal{W})$ there corresponds a quantization of the classical system. This quantization is as follows.

- 1. At the time t=0 the classical observables A(p,q) in the set $\{A\} \cap \{A_{\gamma'}\}$ become, unchanged, the quantum observables $A_{\gamma'}(p,q)$. The classical states $\rho(p,q)$ in the set $[\rho]_{\rm cl} \cap [\rho_{\gamma'\beta'}]$ become, unchanged, the quantum states $\rho_{\gamma'\beta'}$. The classical expectation values $\langle A, \rho \rangle$ are replaced by the quantum expectation values $\langle A_{\gamma'}, \underline{\psi} \rho_{\gamma'\beta'} \rangle$ for A and ρ in the same regions.
- 2. The classical Hamiltonian function H(p,q) must belong to $\{A\} \cap \{A_\gamma\}$ and therefore becomes, unchanged, the quantum Hamiltonian function $H_\gamma(p,q)$. But the classical generator $H\sigma_0$ of the time shift is changed because the classical multiplication operations are replaced by the quantum operations:

$$\pi_0 \to \Pi_{\gamma \rho}; \sigma_0 \to \sigma_{\gamma \rho}; H\sigma_0 \to H\sigma_{\gamma \rho}.$$
 (71)

The classical equation of motion (36a) in the Heisenberg picture goes over into the quantum equations (58), and the alternative classical Liouville equation (43) in the Schrödinger picture

$$\partial \rho (p, q, \hbar)/\partial t = H\sigma_0 \rho$$

goes over into the quantum equation (59). We recall that the function $A_{\rm cl}(p,q,t)$ is related by (39) to the functions P(p,q,t) and Q(p,q,t), which satisfy the classical Hamilton equations.

Because of the differences in the equations of motion, the quantum observables and states no longer coincide with the classical ones for $t \neq 0$.

The dependence of the quantization on \mathcal{V} reflects the well-known possibility of different orderings of non-commuting operators. The dependence of the quantization on \mathcal{H} was introduced in Ref. 12. This dependence reflects the fact that for a fixed method of ordering non-commuting factors one can still associate the quantum states with the classical states in different ways.

10. WICK AND ANTI-WICK QUANTIZATION

As an illustration, we consider the important special class of algebras $\mathcal{B}(\mathcal{V},\mathcal{M})$ for which

$$\mathcal{V} = \exp\{(q_0^2 \partial_q^2 + p_0^2 \partial_p^2)/2\}; \quad \mathcal{W} = 1, \tag{72}$$

where q_0 and p_0 are positive numbers. Substituting (72) in (70), we obtain

$$U(1,2) = \exp(q_0^2 \partial_{1q} \partial_{2q} + p_0^2 \partial_{1p} \partial_{2p}). \tag{73}$$

Using (69) and (73), for the operation Π_{γ} of associative multiplication of observables we obtain

$$\Pi_{q,0} = \exp\left(q_0^2 \partial_{1q} \partial_{2q} + p_0^2 \partial_{1p} \partial_{2p} + i\hbar D_{12}/2\right) \pi_0. \tag{74}$$

If the limits (62) are to exist, we must separate the factor \hbar in the constants q_0^2 and p_0^2 . We therefore set

$$q_0 p_0 = \hbar b/2; \ q_0 = a p_0,$$
 (75)

where a and b are new positive constants.

Introducing the linear combinations

$$\sqrt{\hbar} \partial = q_0 \partial_q - i p_0 \partial_p; \quad \sqrt{\hbar} \partial^+ = q_0 \partial_q + i p_0 \partial_p,$$

we obtain

$$\hbar \partial_1 \partial_2^+ = q_0^2 \partial_{1q} \partial_{2q} + p_0^2 \partial_{1p} \partial_{2p} + i \hbar b D_{12} / 2. \tag{76}$$

Comparing (74) and (76), we see that for b=1 the operation Π_{γ} acquires a particularly simple form, which we denote by Π_a :

$$\Pi_{a} = \exp\left(\hbar \partial_{1} \partial_{2}^{+}\right) \pi_{0}. \tag{77}$$

We call the corresponding combined algebra \mathcal{B}_a . The quantization generated by the algebra \mathcal{B}_a is identical to Wick quantization (see, for example, Ref. 20). The algebra itself is intimately related to coherent states. Namely, our observables A_a coincide with the diagonal elements of the operators $A_a = \langle \alpha | A | \alpha \rangle$ for coherent states; the states ρ_a coincide with the weight functions $\rho_a = \mathcal{P}(\alpha)$ (see, for example, Refs. 18 and 19); to the operation $A_a\Pi_a$ there corresponds the set of matrix elements $\langle \alpha | \hat{A} | \beta \rangle$ between the coherent states α and β . It was found long ago (see, for example, Ref. 18) that the complete set of matrix elements $\langle \alpha | \hat{A} | \beta \rangle$ is uniquely determined by the set of diagonal elements $\langle \alpha | A | \alpha \rangle$. In the formalism developed here, this property is obvious, since the operation $A_a\Pi_a$ is uniquely determined by the element A_n .

It is of interest to examine the properties of the spaces $\{A_a\}$ and $\{\rho_a\}$ and the set $[\rho_a]$ of positive states. In the algebras \mathcal{B}_a , the function $\mathcal{V}(ix,-ik,\hbar)=\exp\{-(\hbar/4)(q_0^2k^2+p_0^2x^2)\}$ at infinity with respect to |x| and |k| has Gaussian-function decrease of a definite form. Therefore, all the Fourier transforms

$$\widetilde{A}_{a}(x, k) = A(x, k) \mathcal{V}(ix, -ik, \hbar)$$
(78)

decrease faster than the same Gaussian function multiplied by any polynomial in $|x|^{-1}$ and $|k|^{-1}$, since the Fourier transform of an infinitely differentiable function is a rapidly (faster than any polynomial) decreasing function. Note that since the functions A(p,q) can increase at infinity (but not faster than polynomials), the Fourier transforms A(x, k) can be generalized functions at finite points and, in particular, can contain δ functions and their derivatives. For example, the Fourier transform of the kinetic energy will be $-(\frac{1}{2}m)\partial^2\delta(x)/\partial x^2$. We must therefore consider the justification for the relation (65), since not every function can be multiplied by a generalized function. It is here that we need the property of infinite differentiability of the function V. since an infinitely differentiable function can be multiplied by a generalized function.

In the space $\{\tilde{A}\}$ of the functions $\tilde{A}(x,k)$ functions that decrease arbitrarily rapidly are admissible. Therefore, the functions \tilde{A}_a form a subspace $\{\tilde{A}_a\} \subset \{\tilde{A}\}$. Accordingly, for the spaces of the Fourier pre-images we have

$$\{A_a\} \subset \{A\}. \tag{79}$$

The space $\{A_a\}$ contains only entire functions, and indeed, by no means all of them. This means that in Wick quantization, in contrast to Weyl quantization, not every classical observable can be quantized. For example, the function $H_I(q) = \exp(-q^2/Q_0^2)$ does not belong in $\{A_a\}$ for $Q_0^2 < q_0^2$.

On the transition to Wick quantization, the expression for the expectation value does not change, in accordance with (57):

$$\langle A, \rho \rangle = \langle A_a, \rho_a \rangle.$$

Therefore, the "improvement" of the function A is offset by the "deterioration" of the functions ρ ; for the Fourier transforms $\tilde{\rho}(x,k)$ are subjected to the transformation

$$\widetilde{\rho}_a(x, k) = \mathcal{V}^{-1}(ix, -ik, \hbar) \widetilde{\rho}(x, k)_{\bullet}$$
(80)

It can be seen from (80) that if $\{\tilde{\rho}\}$ contained only functions that increase at infinity not faster than a polynomial, then the space $\{\tilde{\rho}_a\}$ of transformed Fourier transforms would contain functions with Gaussian growth (but not every Gaussian-function growth). Thus, the spaces $\{\rho\}$, $\{\rho_a\}$ satisfy the inclusion that is the opposite of (79):

$$\{\tilde{\rho}\}\subset \{\tilde{\rho}_a\};\ \{\rho\}\subset \{\rho_a\}.$$
 (81)

Moreover, it can be shown that this inclusion is also valid for the sets of physical (i.e., positive) states:

$$[\rho]_{cl} \subset [\rho_a].$$
 (82)

This means that in Wick quantization (again, in contrast to Weyl quantization) any classical state can be quantized, including the pure classical state $\delta(p-p_0)\delta(q-q_0)$, which corresponds to motion along a definite path. This last fact has a simple physical explanation: In Wick quantization, the classical coordinate and momentum are associated in the phase space

with the center of a Gaussian packet, whose dimensions are compatible with the uncertainty relations.

For the states $\rho_a(p,q)$, not only δ functions but also infinite series in δ functions and their derivatives of increasing orders are admissible. Summation of such series may lead to nonstandard generalized functions having nonzero values in the whole of space. This property may seem unusual. It disturbed the physicists that first encountered it (see, for example, Refs. 18, 19, and 21). Indeed, for the generalized functions with which physicists are familiar (in the spaces S' or D') only polynomials in δ functions and their derivatives are admissible. In our case, however, the appearance of the series is perfectly natural, since the dual space $\{A_0\}$ contains only entire functions, each of which at any point can be expanded in a power series and is completely determined by this series. Therefore

$$\langle A_a, \, \rho_a \rangle = \sum_{m=0, \, n=0}^{\infty} \frac{1}{m! \, n!} \, A_{mn} \, \int p^m q^n \rho_a \left(p, \, q \right) \, dp \, dq.$$

The coefficients

$$\rho_{mn} = \int p^m q^n \rho(p, q) dp dq$$

determine the series

$$\rho_{a}^{r}(p, q) \sim \sum_{m,n} (-1)^{m+n} \rho_{mn} \left(\frac{\partial}{\partial p}\right)^{m} \delta(p) \left(\frac{\partial}{\partial q}\right)^{n} \delta(q).$$

Our use of the tilde (instead of the equality sign) is to emphasize that although the coefficients ρ_{mn} are defined for all $\rho_a(p,q)$ in $\{\rho_a\}$, the series does not converge for all ρ_a to the original function and need not even converge at all.

We see that a change of the quantization significantly changes the sets of observables and states for which the quantization is possible. These changes are different for different combined algebras $\mathcal{B}(\mathcal{V},\mathcal{H})$. For example, for anti-Wick quantization, for which

$$\mathcal{V}(ix, -ik, \hbar) = \exp\{(\hbar/4)(q_0^2k^2 + p_0^2x^2)\}$$

with the same restriction $q_0 p_0 = \hbar/2$, the inclusions (79), (81), and (82) are replaced by the opposite ones:

$$\{A\} \subset \{A_{\overline{a}}\}; \{\rho_{\overline{a}}\} \subset \{\rho\}; [\rho_{\overline{a}}] \subset [\rho].$$

Here, the subscript \overline{a} refers to anti-Wick quantization. In this quantization, ¹⁹ the physical quantum density matrices are positive definite entire functions, and the observables can even be series in δ functions.

11. DIFFERENT CLASSICAL LIMITS

It is not infrequently asserted or assumed that the transition from quantum to classical mechanics is uniquely determined by the limit $\hbar - 0$. In reality, the particularization of such a transition is to a high degree nonunique, as has been noted, in particular, in Refs. 22 and 23. This lack of uniqueness generates discussions. For example, Kobe²⁴ stated that the passage to the limit made by Cohn^{25} is incorrect because in it some expression $\hbar/\Delta p$ is made to tend to zero, and this expression can be replaced by the width Δx of the coordinate packet and does not tend to zero. Arguments of this kind can be neither proved nor disproved. An ex-

perimental verification is impossible because there is no instrument that "switches on or off" the quantum effects. And in any theoretical expression \hbar can be introduced and removed by different definitions of the quantities occurring in a formula. There then follows directly the apparently paradoxical conclusion that for the transition to the classical theory it is by no means necessary to make ħ tend to zero wherever it is encountered. This circumstance was noted by Faddeev.23 who divided the Planck constant into an "internal" and an "external" part and made the quasiclassical expansion only with respect to the external ħ. This conclusion also follows from physical considerations. It is known, for example, that in many situations the atoms of noble gases can be treated as classical particles. But in this classical approximation a nonzero constant \hbar is needed for the stability of the atoms themselves. Therefore, ħ occurs in the expression for the classical potential of the interaction between the atoms.

It frequently happens that the straightforward limit $n \to 0$ is quite meaningless. The simplest example is the Schrödinger equation in the coordinate representation.

The aim of the present section is to find consistent and, in a certain sense, complete answers to the questions of precisely where one must go to the limit $\hbar \to 0$ on the transition to the classical theory and where not, in what cases the transition is possible, and what is the degree of nonuniqueness of the transition.

Since the straightforward prescription of the transition $\hbar - 0$ turns out not to have a clear meaning, we begin with a definition: The transition to the classical theory means that the quantitative result calculated in the quantum theory is replaced by the result calculated in the classical theory. Here, it is possible that some classical quantities (for example, the Hamiltonian function) will depend on \hbar . In other words, on the transition the quantum theory must go over into the classical theory. Therefore, the limiting process must be considered for the theory as a whole, and not for individual quantities, as is usually done.

Now the combined algebra is maximally suited for such "global" limiting processes, since in it all entities "survive" the transition from the one theory to the other. In other formulations, the question of the entity involved in the transition is nontrivial (as was emphasized in Ref. 26). In the combined algebra, the answer to the question is obvious: On the transition from the quantum to the classical theory, the quantum algebra must become the classical algebra. Therefore, the quantum multiplication operations Π_h and σ_h must necessarily go over into the classical ones:

$$\Pi_h \to \pi_0, \ \sigma_h \to \sigma_0. \tag{83}$$

A nonuniqueness arises because the quantum observables and states can also be specified as certain functions of \hbar :

$$A_{qu} = A(p, q, \hbar); \ \rho_{qu} = \rho(p, q, \hbar), \tag{84}$$

and these have definite limits as $\hbar \rightarrow 0$. The problem of finding of all possible transitions to the classical theory

can now be formulated as equivalent to that of establishing the restrictions on all possible dependences on π in (84) and in a constructive description of the remaining arbitrariness.

To preserve the linear properties of the vector spaces spaces $\{A\}$ and $\{\rho\}$, the limiting processes in (83) must be linear. Then the dependence of A and ρ on \hbar can be represented in the forms (53) and (54), respectively. And this, in its turn, means that one can always get rid of the (admissible) dependence of A and ρ on \hbar by the transition to a certain quantum algebra $\mathcal{B}(\mathcal{V},\mathcal{M})$. In this algebra, the transition to the classical theory then reduces to the transformations

$$\Pi_{\gamma \rho} \to \pi_0, \ \sigma_{\gamma \rho} \to \sigma_0.$$
 (85)

We have obtained what at first sight appears to be an unexpected result, though it becomes obvious on reflection, namely, every admissible method of quantization is in a one-to-one correspondence with an admissible method of transition to the classical theory.

The rules for the transition to the classical theory can now be formulated as follows. First, one fixes the algebra $\mathcal{B}(\mathcal{V},\mathcal{W})$, so that all the observables (including the Hamiltonian!) are realized by functions $A_{\gamma}(p,q)$, which are different for different algebras and which in general depend on \hbar . Further:

a) at time t=0 the quantum observables and the states in the regions $A_{\gamma'} \in \{A_{\gamma'}\} \cap \{A\}$ and $\rho_{\gamma' \gamma'} \in [\rho_{\gamma' \gamma'}] \cap [\rho]_{c1}$, respectively, that are common to the classical spaces become, unchanged (even if they depend on $\hbar!$), classical observables and states:

$$A_{\mathcal{I}^{\circ}}(p, q) \rightarrow A(p, q) = A_{\mathcal{I}^{\circ}}; \rho_{\mathcal{I}^{\circ}}(p, q) \rightarrow \rho(p, q) = \rho_{\mathcal{I}^{\circ}}(p, q)$$
 (86)

b) the quantities $\Pi_{\gamma'}, \sigma_{\gamma'}, \mathscr{W}(\hbar)$ are replaced by the classical limits

$$\Pi_{\mathcal{V}^{\circ}} \to \pi_0, \, \sigma_{\mathcal{V}^{\circ}} \to \sigma_0, \, \mathcal{W}^{\circ}(\hbar) \to \mathcal{W}^{\circ}(0) = 1; \tag{87}$$

c) the quantum Hamiltonian function $H_{\gamma}(p,q)$ must belong to $\{A_{\gamma}\} \cap \{A\}$; therefore, unchanged, it becomes the classical Hamiltonian function:

$$H_{\mathcal{V}^0} = H. \tag{88}$$

But in accordance with (87) the quantum generator of time displacement is changed:

$$H_{\gamma \circ \sigma_{\gamma \circ}} \to H_{\gamma \circ \sigma_0}.$$
 (89)

Therefore, the quantum equation of motion [Heisenberg (58) or Schrödinger (59)] goes over into the corresponding classical equation. To the classical equations of motion, one can add quantum corrections, which are obtained by expanding σ_{γ} in powers of \hbar . The equations with corrections will no longer reduce to the classical Hamilton equations. This last circumstance is not always noted. For example, in Ref. 14 equations of the type (58) were written down with total (not partial) time derivatives.

Admissible transitions from quantum to classical mechanics corresponding to different algebras $\mathscr{B}(\mathcal{V},\mathcal{W})$ will give similar results in the essentially classical regions. However, the results may differ strongly in the essentially quantum regions. This can be used to

achieve practically convenient classical and semiclassical approximations to quantum problems.

To conclude this section, we emphasize two principal features of the developed approach.

First, it is neither the states nor the observables that change on the transition from quantum to classical mechanics (and vice versa) but rather the operations of multiplication of the observables.

Second, the treatment goes through for not only pure but also mixed states. This circumstance is important because for the most natural Weyl quantization all the classical states and many of the quantum states are outside the common domain $[\rho]_{\rm cl} \cap [\rho]_{\rm qu}$, whereas the mixed states include "many" that are in this domain. It is for this reason that the transition to classical mechanics is particularly clear for coherent states (see, for example, Refs. 18 and 19) corresponding to Wick quantization (see Sec. 10), for which the inclusion (82) holds.

As an example, we find approximately, by a suitable transition to classical mechanics, the energy of the lowest state for the Hamiltonian

$$\hat{H} = \hat{\mathbf{p}}^2 / 2m + H_I(\mathbf{q}) \tag{90}$$

of a quantum particle in a central attractive field $(\partial H_I/\partial |\mathbf{q}| \ge 0)$. The three-dimensional generalization of the technique developed here is obvious $(D_{12} = \partial_{1q}\partial_{2p} - \partial_{1p}\partial_{2q}$, etc.). The lowest state in the classical theory is trivial, the particle lying on the bottom of the potential well, so that

$$\rho = \delta^3(\mathbf{p}) \, \delta^3(\mathbf{q}); \, E_0 = H_I(0).$$
 (91)

To use this classical property to solve the quantum problem, we must choose the algebra $\mathcal{B}(\mathcal{V},\mathcal{W})$ in such a way that this solution belongs to $[\rho_{\gamma'}]$. In accordance with (81), this condition is satisfied for Wick quantization, i.e., for the algebras \mathcal{B}_a defined by (77). In the algebra \mathcal{B}_a , the Hamiltonian (90) takes in accordance with (78) the form

$$H_{a} = \frac{\mathbf{p}_{2}}{2m} + \frac{3\hbar}{4am} + \frac{1}{(\pi a \hbar)^{3/2}} \int d^{3}\mathbf{q'} H_{I}(|\mathbf{q} - \mathbf{q'}|) \exp\left(-\frac{\mathbf{q'}^{2}}{a\hbar}\right). \tag{92}$$

This Hamiltonian has two corrections of quantum scale, namely, a constant correction to the kinetic energy and a spreading of the potential. With the Hamiltonian (92), the classical solution (91) in fact already takes into account the uncertainty relation, i.e., it has a quantum meaning. It gives the ground-state level

$$E_0 = -H_a(0,0). (93)$$

Even for the Coulomb potential $H_I = -e^2/|\mathbf{q}|$, for which classical solutions are not present in the Weyl algebra $\mathcal{B}(1)$, (93) gives (after minimization with respect to a) the ground-state level of the hydrogen atom

$$E_0 = (-4/3\pi) e^4 m/\hbar^2, \tag{94}$$

which coincides with the exact value to within 15%. Note that the constant \hbar occurs nontrivially in the solution (94), which was obtained by a passage to the limit of classical mechanics.

12. GENERALIZATION TO MANY DEGREES OF FREEDOM

Our treatment can be naturally generalized to the case of any finite number of canonical degrees of freedom. The generalization reduces to the replacement of (69) by

$$\Pi_{\mathcal{V}} = U(1, 2) \exp \{ (i\hbar/2) (D_{12}^{(1)} + \ldots + D_{12}^{(n)}) \}.$$
 (95)

The multiplicative structure of $\Pi_{\gamma'}$ provides the possibility for a systematic treatment of semiquantum approximations in which some degrees of freedom are treated in a quantum manner, while others are treated classically with quantum corrections. For this, it is necessary to expand the corresponding operations $\Pi_{\gamma'}$ and $\sigma_{\gamma'}$ only with respect to some of the terms $D_{12}^{(i)}$. The variables with respect to which the problem remains a quantum one can also be noncanonical variables, for example, spin variables.

If the theory contains a continuous symmetry group, the choice of the quantization (i.e., the choice of the operator V) is subject to an additional restriction, ^{27,12} which takes the form that the generators of this group must correspond to the same observables L_i in the classical and quantum theories, i.e., for all i, j = 1, 2, ..., N:

$$L_i L_j \sigma_{\gamma \circ} = L_i L_j \sigma_0. \tag{96}$$

Note that, from the point of view of preserving the symmetry on quantization, Weyl quantization is advantageous, because in it the set of observables L_i satisfying (96) is the largest possible.

As an example of the semiquantum treatment of several degrees of freedom, let us consider the motion of a nonrelativistic electron in an arbitrary external electromagnetic field. The Pauli equation in the gauge $\varphi = 0$,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} \left\{ \hat{\mathbf{p}} - \frac{e}{c} \mathbf{A} \left(\hat{\mathbf{q}}, t \right) \right\}^2 \psi + \frac{\hbar g}{2} \hat{\mathbf{\sigma}} \mathbf{H} \left(\hat{\mathbf{q}}, t \right) \psi, \tag{97}$$

goes over in Weyl quantization into a system of equations for the four components $\{\rho_0, \rho\}$ of the density matrix $\hat{\rho} = \hat{\rho}_0 + \hat{\sigma}\hat{\rho}$:

$$\frac{\partial \rho_0 \left(\mathbf{p}, \mathbf{q}, t \right) / \partial t = H_1 \rho_0 \sigma_h + \left(g \hbar / 2 \right) \mathbf{H} \rho \sigma_h;}{\partial \rho \left(p, q, t \right) / \partial t = H_1 \rho \sigma_h + g \left[\mathbf{H} \rho \right] \pi_h + \left(g \hbar / 2 \right) \mathbf{H} \rho_0 \sigma_h.}$$
 (98)

Here, A(q, t) is the vector potential, H is the magnetic field, and H_1 is the spinless part of the Hamiltonian function:

$$H_1(\mathbf{p}, \mathbf{q}) = (1/2m) \{\mathbf{p} - \mathbf{A}(\mathbf{q}, t)\}^2.$$

We have used the fact that in Weyl quantization $\underline{H}\sigma_h\rho$ = $H\rho\sigma_h$, as can be shown. The component ρ_0 plays the part of the density of particles, and the components ρ describe the polarization, namely, the expectation value of spin $\hat{s}=\hbar\hat{\sigma}/2$

$$\overline{\mathbf{s}} = \frac{\hbar}{2} \langle 1, \, \boldsymbol{\rho} \rangle = \frac{\hbar}{2} \int d^3\mathbf{p} d^3\mathbf{q} \boldsymbol{\rho}.$$

We now go over to a semiclassical equation by expanding σ_h and π_h on the right-hand sides of the system (98) in \hbar . To terms of order \hbar^2 , we obtain

$$\frac{\partial \rho_{0}/\partial t = H_{1}\rho_{0}\sigma_{0} + (g\hbar/2) \operatorname{H}\rho\sigma_{0} + (\hbar^{2}/2) H_{1}\rho_{0}\sigma_{0}^{"};}{\partial \rho/\partial t = H_{1}\rho\sigma_{0} + g \left[\operatorname{H}\rho\right] \pi_{0} + (g\hbar/2) \operatorname{H}\rho_{0}\sigma_{0}} + (\hbar^{2}/2) H_{1}\rho\sigma_{0}^{"} + (g\hbar^{2}/2) \left[\operatorname{H}\rho\right] \pi_{0}^{"},}$$
(99)

where $\sigma_0'' = \frac{\partial^2 \sigma_h}{\partial \hbar^2}$ for $\hbar = 0$ and $\pi_0'' = \frac{\partial^2 \pi_h}{\partial \hbar^2}$ for $\hbar = 0$. Without wasting space on the simple but length form of the system (99) when written out in full, let us discuss the meaning of the various approximations. In the zeroth order in ħ, the spin interactions do not affect the translational motion (g does not occur in the equation for ρ_0), but they give rise to Larmor precession. This is what they do in the ordinary classical calculation. In the first order in \hbar , an effect of the translational motion of the magnetic moment under the influence of the gradient of the magnetic field is manifested. The motion is non-Hamiltonian, so that such quantum corrections cannot be taken into account by the usual methods. Finally, in the second order we encounter quantum corrections to the interaction of the external field with the charge.

13. PARITY OF STATES IN THE PHASE SPACE REPRESENTATION

As was noted in Sec. 3, the Wigner density matrix $\rho_{av}(p,q)$ is not a positive definite function. It therefore cannot be interpreted as a probability density, and it is usually concluded that ρ_{qu} is not a distribution function (see any discussion of this question, for example, Refs. 18 and 19). This conclusion, however, contains a non sequitur of the following kind. The real (i.e., experimentally verified) meaning of a distribution function is that, using it, one can calculate the expectation values of observables. And in this sense the positivity properties of ρ_{au} are as irreproachable as those of ρ_{c1} , but with respect to a different operation of multiplication of the observables. Giving $\rho(p,q)$ the meaning of a probability density is a further assertion that has nothing to do with the explanation and prediction of observable facts. From this point of view, $\rho(\mathbf{p}_0, \mathbf{q}_0)$ can be given meaning as the expectation value of the observable $\delta^3(\mathbf{p} - \mathbf{p}_0)\delta^3(\mathbf{q} - \mathbf{q}_0)$. We then arrive at the conclusion that this observable is positive in classical theory and nonpositive in quantum theory. The physical meaning of this nonpositivity is elucidated in Ref. 28, in which a simple and interesting fact was noted, namely, that the quantum observable

$$\mathcal{F} = \hbar^3 \pi^3 \delta^3 (\mathbf{p}) \, \delta^3 (\mathbf{q}) \tag{100}$$

is carried by the transformation (6) into a matrix element of the parity operator $\hat{\mathcal{P}}$. Therefore, in particular.

$$\mathcal{F}\mathcal{F}\Pi_h=1. \tag{101}$$

The observable $\hbar^3\pi^3\delta^3(\mathbf{p}-\mathbf{p}_0)\delta^3(\mathbf{q}-\mathbf{q}_0)$ is obtained from $\mathscr P$ by shifts. Therefore, the square of this observable is also equal to 1. From this we obtain the simple and useful estimate

$$\pi^3 \hbar^3 \left| \rho_{\mathbf{q}\mathbf{u}}(\mathbf{p}, \mathbf{q}) \right| \leqslant 1,$$
 (102)

and the function $\rho_{qu}(p,q)$ can attain the extremal values ± 1 at not more than one point. We note also that the operator $\mathcal{P}\Pi_h$ realizes a Fourier transformation with the substitution $p \leftrightarrow q$:

$$A(\mathbf{p}, \mathbf{q}) \mathcal{P}\Pi_{h} = \frac{1}{(\pi h)^{3}} \int d^{3}\mathbf{p}' d^{3}\mathbf{q}'$$

$$\times \exp\left\{\frac{2i}{h} (\mathbf{q}\mathbf{p}' - \mathbf{p}\mathbf{q}')\right\} A(\mathbf{p}', \mathbf{q}') \stackrel{\text{def}}{=} \widetilde{A}(\mathbf{p}, \mathbf{q}). \tag{103}$$

This means that the space $\{A\}$ of observables for the quantum algebra can be extended by adding to it all Fourier transforms, i.e., functions $A(\mathbf{p},\mathbf{q})$ that are generalized functions with respect to both variables at finite points but decrease rapidly at infinity.

14. PERTURBATION THEORY FOR OBTAINING THE QUANTUM CORRECTIONS

For the construction and analysis of any perturbation theory, it is always convenient to go over from the differential equation to the corresponding integral equation with explicit allowance for the initial conditions, the perturbation series then being obtained by simple iteration. A typical example is the Lippmann-Schwinger equation for the scattering of two particles. We show that in the representation of the combined algebra (and only in it!) one can construct an analog of the Lippmann-Schwinger equation, in which the classical solution plays the part of the free solution and the quantum solution the part of the complete solution.²⁹

We restrict ourselves to the motion of one particle in an external field. In the Heisenberg picture, the observables $A_{\rm cl}({\bf p},{\bf q},t)$ satisfy the three-dimensional analog of Eq. (36a):

$$\partial A_{cl} (\mathbf{p}, \mathbf{q}, t)/\partial t = A_{cl} H \sigma_0,$$
 (104)

where $\sigma_0 = D_{1,2}\pi_0$; at the same time,

$$D_{12} = (\partial_{1q}\partial_{2p} - \partial_{1p}\partial_{2q}). \tag{105}$$

The quantum observables $A_{qu}(\mathbf{p},\mathbf{q},t)$ in the algebra $\mathcal{B}(V,\mathcal{M})$ satisfy the three-dimensional analog of Eq. (58):

$$\partial A_{\mathbf{q}\mathbf{u}}(\mathbf{p}, \mathbf{q}, t)/\partial t = A_{\mathbf{q}\mathbf{u}}H\sigma_{q/o},$$
 (106)

where σ_{γ} is determined, as before, by Eqs. (55), but with D_{12} from (105) and with the function $U = U(\partial_{\mathbf{q}}, \partial_{\mathbf{p}})$. In accordance with (86), in the initial state for t = 0,

$$A_{qu}(\mathbf{p}, \mathbf{q}, 0) = A_{cl}(\mathbf{p}, \mathbf{q}, 0) \equiv A_{0}(\mathbf{p}, \mathbf{q}).$$
 (107)

In accordance with (39),

$$A_{cl}(\mathbf{p}, \mathbf{q}, t) = A_0 \{ P(\mathbf{p}, \mathbf{q}, t), Q(\mathbf{p}, \mathbf{q}, t) \},$$
 (108)

where P(...), Q(...) is the solution of the classical Hamilton equations with initial conditions P(p,q,0) = p, Q(p,q,0) = q. Our problem can now be formulated as follows: to obtain for $A_{qu}(p,q,t)$ an inhomogeneous integral equation whose first iteration is the function $A_{cl}(p,q,t)$.

We first find the retarded Green's function $G(\mathbf{p},\mathbf{q},t,\mathbf{p}',\mathbf{q}',t')$ of the classical equation (104). This function satisfies the equation

$$\partial G/\partial t - GH\sigma_0 = \delta^3(\mathbf{p} - \mathbf{p}') \,\delta^3(\mathbf{q} - \mathbf{q}') \,\delta(t - t'). \tag{109}$$

It follows from the property (108) that the retarded solution of Eq. (109) has the form

$$G = \delta^{3} \{ \mathbf{p}' - \mathbf{P} (\mathbf{p}, \mathbf{q}, t - t') \} \delta^{3} \{ \mathbf{q}' - \mathbf{Q} (\mathbf{p}, \mathbf{q}, t - t') \} \Theta (t - t').$$
 (110)

This solution has a clear physical meaning, namely, at the point p', q' of the phase space at the time t' the classical phase path is generated. Denoting now $A_1 = A_{qu} - A_{cl}$, we obtain from (104) and (106)

$$\partial A_1(\mathbf{p}, \mathbf{q}, t) \partial t - A_1 H \sigma_0 = A_{00} H(\sigma_{V} - \sigma_0).$$
 (111)

Remembering that $A_1(\mathbf{p}, \mathbf{q}, 0) = 0$ in accordance with (107), we can rewrite Eq. (111) in the integral form

$$A_{1}\left(\mathbf{p},\,\mathbf{q},\,t\right)=\int\limits_{0}^{\infty}dt'd^{3}\mathbf{p}'d^{3}\mathbf{q}'G\left(\mathbf{p},\,\mathbf{q},\,t;\,\mathbf{p}',\,\mathbf{q}',\,t'\right)\{A_{\mathbf{q}\mathbf{u}}H\left(\mathbf{\sigma}_{\mathcal{V}^{\infty}}--\sigma_{\mathbf{0}}\right)\}_{\mathbf{p}',\,\mathbf{q}',\,t'}.$$

Hence, integrating with respect to the δ functions in G, we obtain the required integral equation for $A_{qq}(\mathbf{p},\mathbf{q},t)$:

$$A_{qu}(\mathbf{p}, \mathbf{q}, t) = A_{cl}(\mathbf{p}, \mathbf{q}, t) + \int_{0}^{t} dt' A_{qu}(\mathbf{p}', \mathbf{q}', t') H(\mathbf{p}', \mathbf{q}') (\sigma_{\gamma \rho} - \sigma_{0}),$$
(112)

where $\mathbf{p}' = \mathbf{P}(\mathbf{p}, \mathbf{q}, t - t')$ and $\mathbf{q}' = \mathbf{Q}(\mathbf{p}, \mathbf{q}, t - t')$. This equation can be iterated with the classical solution $A_{cl}(\mathbf{p}, \mathbf{q}, t)$ taken as the zeroth approximation. To establish whether the iterations exist, we can use the theorems proved in Refs. 1 and 12 which state that if the functions A and H belong to the set of classical (respectively, quantum) observables, the product $AH\sigma_0$ (respectively, $AH\sigma_{x'}$) also belongs to the same set.

Here too Weyl quantization is distinguished. In it, in accordance with Sec. 2, the spaces $\{A\}_{\rm cl}$ and $\{A\}_{\rm qu}$ coincide, so that all iterations exist if in the considered interval (0,t) the corresponding classical solutions exist. For other quantizations, the spaces $\{A\}_{\rm cl}$ and $\{A_{\gamma}\}$ no longer coincide. Therefore, even for the first iteration, it may happen that the product $A_{\rm cl}H\sigma_{\gamma}$, and thus the iteration itself, does not exist.

Of course, the existence of all iterations does not ensure convergence of the series to a solution. In fact, the series are as a rule asymptotic.

In the Schrödinger picture, an equation analogous to (112) can be obtained for the state $\rho_{\gamma}(\mathbf{p},\mathbf{q},t)$:

$$\rho_{\mathcal{F}^{\circ}}(\mathbf{p}, \mathbf{q}, t) = \rho_{cl}(\mathbf{p}, \mathbf{q}, t)$$

$$+ \int_{0}^{t} dt' \left\{ \underbrace{H(\mathbf{p}'', \mathbf{q}'') \sigma_{\mathcal{F}^{\circ}} - H(\mathbf{p}'', \mathbf{q}'') \sigma_{0}}_{\rightarrow} \right\} \rho_{\mathcal{F}^{\circ}}(\mathbf{p}'', \mathbf{q}'', t'). \qquad (113)$$

Here, p'' = P(p, q, t' - t) and q'' = Q(p, q, t' - t). Note that the time has the opposite sign to p' and q' in (112).

Iterations of Eq. (113) exist under the same conditions as iterations of Eq. (112). But if the iterated solution leaves the common domain $[\rho]_{c1} \cap [\rho_{\gamma\gamma}]$ of the physical states, positivity of the state may be lost.

The difficulty associated with positivity can be completely avoided by going over from the quantum states ρ_{γ} to the state amplitudes Ψ_{γ} introduced in Sec. 3 for Weyl quantization. The transition to other quantizations for Ψ is the same as for the states

$$\Psi_{\mathfrak{P}^{\circ}} = \mathfrak{P}^{\circ_{-1}}(\hbar) \, \Psi_{\mathsf{qu}}.$$

Here, we have adopted the usual condition $\mathcal{H}=1$ for the choice of the quantization. It is readily seen that the state amplitude $\Psi_{\gamma'}$ is related to the state $\rho_{\gamma'}$ by

$$\rho_{\mathcal{T}^0} = \Psi_{\mathcal{T}^0} \Psi_{\mathcal{T}^0}^* \widetilde{\Pi}_{\mathcal{T}^0},$$

where $\tilde{\Pi}_{\mathbf{1}^{\prime}}$ is the operation of associative multiplication

$$\begin{split} &\tilde{\Pi}_{7^{\circ}} = U\,(\,-\,1,\,\,-\,2) \exp\,\left[(\mathrm{i}\hbar/2)\,D_{12} \right] \pi_{0}; \\ &U\,(\,-\,1,\,\,-\,2) = U\,(\,-\,\partial_{\,1\mathrm{p}},\,\,-\,\partial_{\,1\mathrm{q}},\,\,-\,\partial_{\,2\mathrm{p}},\,\,-\,\partial_{\,2\mathrm{q}}). \end{split}$$

The multiplication $\tilde{\Pi}_{\gamma}$ corresponds to Berezin's multi-

plication of covariant symbols.17

The multiplication $\tilde{\Pi}_{\psi}$ satisfies the Hamiltonicity property (18). Therefore, the equation for ψ_{ψ} has exactly the same form as for ρ_{ψ} :

$$\Psi_{\mathcal{F}^{\circ}}(\mathbf{p}, \mathbf{q}, t) = \Psi_{cl}(\mathbf{p}, \mathbf{q}, t)$$

$$+ \int_{0}^{t} dt' \left\{ H(\mathbf{p}'', \mathbf{q}'') \sigma_{\mathcal{F}^{\circ}} - H(\mathbf{p}'', \mathbf{q}'') \sigma_{0} \right\} \Psi_{\mathcal{F}^{\circ}}(\mathbf{p}'', \mathbf{q}'', t'). \tag{114}$$

Here, $\Psi_{\text{e}1}$ is the classical state amplitude, which satisfies the relations

$$\partial \Psi_{cl} / \partial t = H \sigma_0 \Psi_{cl} \; , \; \; \rho_{cl} = \Psi_{cl} \; \Psi_{cl}^* \; \pi_0. \label{eq:psi_cl}$$

With each iteration of Eq. (114) we can now associate the state ρ_{N} , which is definitely positive.

As an example, we write out explicitly the integral equation for the Weyl $\rho_{qu}(\mathbf{p},\mathbf{q},t)$ with the single-particle Hamiltonian (90). In accordance with (113), we obtain

$$\rho_{cl}(\mathbf{p}, \mathbf{q}, t) = \rho_{cl}(\mathbf{p}, \mathbf{q}, t)
+ \int_{0}^{t} dt' \left\{ \frac{1}{i\hbar (2\pi)^{3}} \int d^{3}\mathbf{p}_{1}d^{3}\mathbf{x} \exp \left\{ i\mathbf{x} (\mathbf{p} - \mathbf{p}_{1}) \right\} \left\{ H_{I}(\mathbf{q}' - \hbar\mathbf{x}/2) - H_{I}(\mathbf{q}' + \hbar\mathbf{x}/2) \right\} \rho_{\mathbf{q}\mathbf{u}}(\mathbf{p}_{1}, \mathbf{q}', t')
- (\partial H_{I}(\mathbf{q}')/\partial \mathbf{q}') \partial \rho_{\mathbf{q}\mathbf{u}}(\mathbf{p}', \mathbf{q}', t')/\partial \mathbf{p}' \right\},$$
(115)

where $\mathbf{p'} = \mathbf{P}(\mathbf{p}, \mathbf{q}, t' - t)$ and $\mathbf{q'} = \mathbf{Q}(\mathbf{p}, \mathbf{q}, t' - t)$. Expanding $H_I(\mathbf{q'} \mp \hbar \mathbf{x}/2)$ in a series in \hbar , we can calculate the quantum corrections as series in powers of \hbar . The series will exist everywhere where the corresponding classical solutions exist.

It is interesting to note that direct iteration of Eq. (115) without expansion of H_{r} in \hbar will give quantum corrections that are not analytic in ħ. In particular, beginning with the second approximation we encounter nonanalytic effects such as tunneling and above-barrier reflection. Let us establish why the tunneling effect appears only with the second order. The physical picture of barrier tunneling in the language of iterations of Eq. (115) is as follows. In the absence of perturbations, the particle moves classically. Each quantum perturbation makes possible a "jump" of the momentum, since the momentum p in $\rho_{qq}(\mathbf{p},\mathbf{q},t)$ is in no way related to the momentum p_1 in $\rho_{qq}(p_1, q', t')$. By means of these jumps, the particle can "climb over" the barrier. It is obvious that the minimal number of jumps is two (one upward and one downward).

15. COMBINED SCATTERING THEORY

In the standard formulations of classical and quantum scattering theories, completely different concepts are used, and these do not "survive" the transition from the one theory to the other. In the classical theory there is no analog of the \hat{S} matrix or the scattering amplitude, while in the quantum theory there is no impact parameter. This hinders the development of systematic semiclassical methods. In this section, we construct a unified Hamiltonian scattering theory suitable for both classical and quantum mechanics.

For simplicity, we restrict ourselves to elastic potential scattering of nonrelativistic spinless particles and Weyl quantization. The basic entity in the theory is the operator of Hamiltonian evolution:

which acts (to the left) on observables or (to the right) on states:

$$A(0) \mathcal{U}(t) = A(t); \quad \mathcal{U}(t) \rho(0) = \rho(t). \tag{117}$$

The kernel $\langle \mathbf{p}, \mathbf{q} | \mathcal{U}(t) | \mathbf{p'}, \mathbf{q'} \rangle = \langle \mathbf{p}, \mathbf{q} | \mathcal{U}(t) | \mathbf{p'}, \mathbf{q'} \rangle$ of this operator can be represented in classical theory in accordance with (39) in the form

$$\langle \mathbf{p}, \mathbf{q} | \mathcal{U}_{cl}(t) | \mathbf{p}', \mathbf{q}' \rangle = \delta^3 \{ \mathbf{p} - \mathbf{P}(\mathbf{p}', \mathbf{q}', t) \} \delta^3 \{ \mathbf{q} - \mathbf{Q}(\mathbf{p}', \mathbf{q}', t) \},$$
 (118)

and in the quantum theory it can be expressed, in accordance with (6), in terms of the matrix elements of the standard evolution operator $\hat{U}(t)$, which acts on the state vectors:

$$\langle \mathbf{p}, \mathbf{q} \mid \mathcal{U}_{\mathbf{q}\mathbf{u}}(t) \mid \mathbf{p}', \mathbf{q}' \rangle = \frac{1}{(2\pi\hbar)^3} \int d^3\mathbf{k} d^3\mathbf{k}' \exp\left(\frac{\mathbf{i}}{\hbar} \mathbf{q}' \mathbf{k}' - \frac{\mathbf{i}}{\hbar} \mathbf{q} \mathbf{k}\right)$$

$$\times \left\langle \mathbf{p} + \frac{1}{2} \mathbf{k} \mid \hat{U}(t) \mid \mathbf{p}' + \frac{1}{2} \mathbf{k}' \right\rangle \left\langle \mathbf{p}' - \frac{1}{2} \mathbf{k}' \mid \hat{U}^+(t) \mid \mathbf{p} - \frac{1}{2} \mathbf{k} \right\rangle. \tag{119}$$

It can be seen from (118) and (119) that the kernel $\langle \mathbf{p}, \mathbf{q} | \mathcal{U}(t) | \mathbf{p'}, \mathbf{q'} \rangle$ is real and that

$$\mathcal{U}^{-1}(t) = \mathcal{U}(-t) = \mathcal{U}^{T}, \tag{120}$$

where the superscript T denotes the transpose. The Hamiltonicity of the evolution is manifested in the fact that, in accordance with (32) and (33), for any pair of observables A and B

$$AB\pi\mathcal{U}(t) = A\mathcal{U}(t) B\mathcal{U}(t) \pi; AB\sigma\mathcal{U}(t) = A\mathcal{U}(t) B\mathcal{U}(t) \sigma.$$
 (121)

We recall that in nonrelativistic theory the operator $\mathcal{U}_0(t)$ of free evolution is the same in the classical and the quantum theory:

$$\langle \mathbf{p}, \mathbf{q} | \mathcal{U}_0(t) | \mathbf{p}', \mathbf{q}' \rangle = \delta^3(\mathbf{p} - \mathbf{p}') \delta^3(\mathbf{q} - \frac{\mathbf{p}'}{m}t - \mathbf{q}').$$
 (122)

We now introduce asymptotic states ρ_{in} and ρ_{out} , which are defined in the Schrödinger picture by the equations

$$\rho_{\rm in} = \lim \, \mathcal{U}_0^{-1}(t) \, \mathcal{U}(t) \, \rho(0); \tag{123}$$

$$\rho_{\text{in}} = \lim_{t \to -\infty} \underbrace{\mathcal{U}_0^{-1}(t)}_{t \to -\infty} \underbrace{\mathcal{U}(t)}_{t} \rho(0); \tag{123}$$

$$\rho_{\text{out}} = \lim_{t \to -\infty} \underbrace{\mathcal{U}_0^{-1}(t)}_{t} \underbrace{\mathcal{U}(t)}_{t} \rho(0). \tag{124}$$

The limits are understood in the topology defined in Refs. 1 and 12. In both the classical and the quantum case, the limit gives zero if finite motion is described. Therefore, in the presence of bound states, the sets $[\rho_{in}]$ and $[\rho_{out}]$ are not isomorphic to the set $[\rho]$:

$$[\rho_{\rm in}] \subset [\rho]; \ [\rho_{\rm out}] \subset [\rho]; \ [\rho_{\rm in}] \neq [\rho]; \ [\rho_{\rm out}] \neq [\rho].$$
 (125)

The next step is to introduce the generalized Møller operator $\Omega_{\bullet}(t) = \Omega(t)$ (we do not require the operator Ω_{\bullet}):

$$\Omega(t) = \lim_{\substack{t' \to -\infty \\ t' \to -\infty}} \mathcal{U}_0^{-1}(t) \,\mathcal{U}(t) \,\mathcal{U}^{-1}(t') \,\mathcal{U}_0(t'), \tag{126}$$

where the limit is taken in one of the topologies consistent with the topologies in the spaces $\{A\}$ and $\{\rho\}$. The operator $\Omega(t)$ maps from $\{\rho_{in}\}$ into $\{\rho\}$. In the presence of bound states, it therefore does not have an inverse. However, there exists the transposed operator $\Omega^{T}(t)$ from $\{\rho\}$ into $\{\rho_{in}\}$ such that

$$\Omega^{T}(t)\Omega(t)=I. \tag{127}$$

The basic entity of Hamiltonian scattering theory is the scattering operator \mathscr{G} , which relates the spaces $\{\rho_{\text{out}}\}$ and $\{\rho_{in}\}$. By definition,

$$\rho_{\text{out}} = \mathcal{F}\rho_{\text{in}}.\tag{128}$$

The spaces $\{\rho_{out}\}$ and $\{\rho_{in}\}$ are isomorphic. Therefore, the operator \mathcal{Y} is not only real but also orthogonal:

$$\mathscr{F}^T = \mathscr{F}^{-1}. \tag{129}$$

The part played by the generalized Møller operator is determined by limiting relations that follow from (123), (124), (126), and (128):

$$\lim_{t\to\infty} \Omega(t) = I; \lim_{t\to\infty} \Omega(t) = \mathcal{S}.$$
 (130)

It is therefore natural to derive and solve the integral equations describing the scattering process for $\Omega(t)$. The corresponding differential (with respect to t) equation is obtained from (116) and (126), and has the form

$$\partial \Omega(t)/\partial t = H_I \{ \mathbf{p}_{fr}(t), \mathbf{q}_{fr}(t) \}, \tag{131}$$

where $p_{fr} = p$ and $q_{fr} = q + pt/m$ (fr stands for free). The operator $\Omega(t)$ is the operator of Hamiltonian evolution in the interaction picture (48). The scattering operator satisfies the Hamiltonicity properties (32) and (33),

$$AB\sigma\mathcal{F} = A\mathcal{F}B\mathcal{F}\sigma; \ AB\pi\mathcal{F} = A\mathcal{F}B\mathcal{F}\pi, \tag{132}$$

and conserves the energy, which for the scattering states reduces to the kinetic energy:

$$H_0 \mathcal{G} = H_0. \tag{133}$$

From these properties there follow two general restrictions on the form of the matrix element $\langle \mathbf{p}, \mathbf{q} | \mathcal{P} | \mathbf{p}', \mathbf{q}' \rangle$ of \mathcal{G} .

First, taking $B = H_0$ in the first of Eqs. (132) and using (133) and the arbitrariness of A, we obtain

$$(H_0\sigma) \mathcal{F} - \mathcal{F}(H_0\sigma) = 0. \tag{134}$$

In accordance with (8) and (15), the operator $H_0\sigma$ for $H_0 = p^2/2m$ has in both the classical and the quantum theory the form

$$H_0\sigma = (\mathbf{p}/m)\,\partial_{\mathbf{q}}\pi_0,\tag{135}$$

so that the condition (134) can be represented as

$$(\mathbf{p}\partial/\partial\mathbf{q} + \mathbf{p}'\partial/\partial\mathbf{q}')\langle\mathbf{p}, \mathbf{q}|\mathcal{F}|\mathbf{p}', \mathbf{q}'\rangle = 0.$$
 (134a)

The second condition is obtained similarly by replacing the first of Eqs. (132) by the second:

$$(H_0\pi) \mathcal{S} - \mathcal{S} (H_0\pi) = 0. \tag{136}$$

Here, however, the quantum and classical analogs of (135) are different:

$$H_0 \pi_0 = (\mathbf{p}^2/2m) \,\pi_0; \ H_0 \pi_h = (1/2m) \left(\mathbf{p}^2 - \frac{\hbar^2}{4} \,\partial_{\mathbf{q}}^2\right) \pi_0.$$
 (137)

Therefore, the condition (136) for \mathscr{G}_{c1} takes the form

$$(\mathbf{p}^{2}/2m - \mathbf{p}^{\prime 2}/2m) \langle \mathbf{p}, \mathbf{q} | \mathcal{F}_{cl} | \mathbf{p}^{\prime}, \mathbf{q}^{\prime} \rangle = 0,$$
 (138a)

and for gan

$$\begin{cases}
\frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}'^2}{2m} - \frac{\hbar^2}{8m} \left(\frac{\partial}{\partial \mathbf{q}}\right)^2 + \frac{\hbar^2}{8m} \left(\frac{\partial}{\partial \mathbf{q}'}\right)^2 \\
\times \langle \mathbf{p}, \mathbf{q} \mid \mathcal{S}_{\mathbf{q}\mathbf{u}} \mid \mathbf{p}', \mathbf{q}' \rangle = 0.
\end{cases} \tag{138b}$$

We now have everything that we need to go over to the scattering cross section. This transition is made as follows. In accordance with the standard experimental situation, we choose $\rho_{in}(p',q')$ in the form

$$\rho_{\rm in}(\mathbf{p}', \mathbf{q}') = \delta^3(\mathbf{p}' - \mathbf{p}_0).$$

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This is an unnormalized stationary state, and is admissible in both the quantum and the classical theory. In this state, the momentum is fixed, the spatial density of the particles is equal to unity, and the flux is

$$\int d^3\mathbf{p} \, \frac{\mathbf{p}}{m} \, \rho_{\rm in} = \frac{\mathbf{p}_0}{m} = \mathbf{v}_{\rm in}.$$

After scattering, we obtain the state ρ_{out} :

$$\rho_{\text{out}}\left(p,\,q\right) = \int d^{3}\mathbf{q}'\,\langle\mathbf{p},\,\mathbf{q}\,|\,\mathcal{S}\,|\,\mathbf{p}_{0},\,\mathbf{q}'\rangle. \tag{139}$$

The scattering cross section is a well-defined quantity only for nonzero momentum and nonzero scattering angle. We shall therefore assume that

$$\mathbf{p} \neq \mathbf{p}_0 \neq 0$$
.

For fixed p and p', this gives the possibility of decomposing q and q' into longitudinal and transverse components:

$$\mathbf{q} = q_{||}\mathbf{p}/|\mathbf{p}| + \mathbf{q}_{\perp}; \quad \mathbf{q}' = q_{||}\mathbf{p}'/|\mathbf{p}'| + \mathbf{q}'_{\perp},$$

where

$$\mathbf{q}_{\perp}\mathbf{p}=\mathbf{q}_{\perp}^{\prime}\mathbf{p}^{\prime}=0.$$

The effect of the condition (134a) is then that $\langle \mathbf{p}, \mathbf{q} | \mathcal{S} | \mathbf{p'}, \mathbf{q'} \rangle$ depends on the difference $q_{\parallel} - q'_{\parallel}$ but not on the sum $q_{\parallel} + q'_{\parallel}$. Therefore, $\rho_{\text{out}}(\mathbf{p}, \mathbf{q})$ in (139) does not depend on q_{\parallel} :

$$\rho_{\text{out}} = \rho_{\text{out}} (\mathbf{p}, \mathbf{q}_{\perp}).$$

By the definition of the cross section.

$$\frac{d\sigma}{d^{3}p}\Big|_{p_{0}\rightarrow p}=\int d^{2}q_{\perp}\rho_{out}\left(p,\,q,\,t\right)=\int d^{3}q'd^{2}q_{\perp}\left\langle p,\,q\,\right|\mathcal{S}\left|\,p_{0},\,q'\right\rangle. \tag{140}$$

It follows from (138a) and (138b) that the classical cross sections and the quantum cross sections are proportional to an energy δ function multiplied by the cross section for scattering into the solid angle dO:

$$d\sigma/d^{3}\mathbf{p} = (1/|\mathbf{p}|m) \delta(\mathbf{p}^{2}/2m - \mathbf{p}_{0}^{2}/2m) d\sigma/dO.$$
 (141)

Note that the derivation given for Eq. (140) also holds for the inelastic scattering channel $\mathcal{G}_{\text{inel}}$ with the only difference that on the right-hand side the ratio of the velocities appears:

$$\left(\frac{d\sigma}{d^3\mathbf{p}}\right)_{\mathrm{inel}} = \frac{v_{\mathrm{out}}}{v_{\mathrm{in}}} \int \, d^3\mathbf{q}' d^2\mathbf{q}_{\perp} \, \langle \mathbf{p}, \, \mathbf{q} \, | \, \mathcal{F}_{\mathrm{inel}} \, | \, \mathbf{p_0}, \, \mathbf{q'} \rangle,$$

where $v_{\rm in} = |\mathbf{p}_{\rm o}|/m$ and $v_{\rm out} = |\mathbf{p}|/m$. We show that the general expressions (140) and (141) give the correct expressions for the cross section in the classical and quantum cases.

In accordance with the classical Hamiltonicity property (118), the classical expression $\langle \mathbf{p}, \mathbf{q} \, | \, \mathcal{G}_{\mathrm{cl}} \, | \, \mathbf{p'}, \mathbf{q'} \rangle$ can be represented in the form

$$\langle \mathbf{p}, \mathbf{q} | \mathcal{F}_{cl} | \mathbf{p}', \mathbf{q}' \rangle = \delta^{3} \{ \mathbf{p} - \mathbf{P} (\mathbf{p}', \mathbf{q}') \} \delta^{3} \{ \mathbf{q} - \mathbf{Q} (\mathbf{p}', \mathbf{q}') \},$$
 (142)

where the transformation from the pair \mathbf{p} , \mathbf{q} to the pair $\mathbf{p'}$, $\mathbf{q'}$ is canonical. At the same time, in accordance with (136) and (138a) the function $\mathbf{P}(\mathbf{p'},\mathbf{q'})$ does not depend on $\mathbf{q'}_{\parallel}$, while $\delta^3\{\mathbf{p}-\mathbf{P}(\mathbf{p'},\mathbf{q'})\}$ can be represented in the form

$$\delta^{3}\{\mathbf{p} - \mathbf{P}(\mathbf{p}', \mathbf{q}'_{-})\} = \frac{1}{m |\mathbf{p}|} \delta\left(\frac{\mathbf{p}^{2}}{2m} - \frac{\mathbf{p}'^{2}}{2m}\right) \delta^{2}\{\mathbf{n} - \mathbf{n}(E, \mathbf{n}')\}, \tag{143}$$

where, by definition, $p=n|p|, p'=n'|p'|, E=p^2/2m$,

$$\int f(\mathbf{n}, \mathbf{n}', E) \, \delta^2 \{\mathbf{n} - \mathbf{n} (E, \mathbf{n}')\} \, dO$$
= $f(\mathbf{n}, \mathbf{n}', E)$ for $\mathbf{n} = \mathbf{n} (\mathbf{n}', E)$; (144)

and dO is the element of solid angle of the vector p.

Substituting now (142) and (143) in (140) and (141), we obtain

$$\delta\left(\frac{\mathbf{p}^{2}}{2m} - \frac{\mathbf{p}_{0}^{2}}{2m}\right) \frac{d\sigma_{\mathbf{c}!}}{dO} = m \mid \mathbf{p} \mid \frac{d\sigma_{\mathbf{c}!}}{d^{3}\mathbf{p}}$$

$$= \delta\left(\frac{\mathbf{p}^{2}}{2m} - \frac{\mathbf{p}_{0}^{2}}{2m}\right) \int d^{2}\mathbf{q}_{\perp} \delta^{2}\left\{\mathbf{n} - \mathbf{n}\left(E, \mathbf{n}_{0}, \mathbf{q}_{\perp}'\right)\right\}. \tag{145}$$

In the case of elastic, azimuthally symmetric scattering, the magnitude of the vector \mathbf{q}'_{L} is equal to the impact parameter b:

$$|\mathbf{q}'_{\perp}| = b$$
,

and the standard classical expression

$$d\sigma_{\rm cl}/dO = b/\sin\vartheta \mid d\vartheta/db \mid, \tag{146}$$

where $\cos \theta = (\mathbf{n} \cdot \mathbf{n}_0)$, is obtained for the cross section (145).

In complete analogy with (119), the quantum expression $\langle \mathbf{p}, \mathbf{q} | \mathcal{G}_{\mathbf{q}\mathbf{u}} | \mathbf{p'}, \mathbf{q'} \rangle$ can be expressed in terms of the elements $\langle \mathbf{p}_1 | \hat{\mathbf{S}} | \mathbf{p}_2 \rangle$ of the S matrix:

$$\langle \mathbf{p}, \mathbf{q} \mid \mathscr{S}_{\mathbf{q}\mathbf{u}} \mid \mathbf{p'}, \mathbf{q'} \rangle = \frac{1}{(2\pi\hbar)^3} \int d^3\mathbf{k} d^3\mathbf{k'} \exp\left(\frac{\mathbf{i}}{\hbar} \mathbf{q'} \mathbf{k'} - \frac{\mathbf{i}}{\hbar} \mathbf{q} \mathbf{k}\right)$$

$$\times \left\langle \mathbf{p} + \frac{1}{2} \mathbf{k} \mid \hat{S} \mid \mathbf{p'} + \frac{1}{2} \mathbf{k'} \right\rangle \left\langle \mathbf{p'} - \frac{1}{2} \mathbf{k'} \mid \hat{S}^+ \mid \mathbf{p} - \frac{1}{2} \mathbf{k} \right\rangle; \qquad (147)$$

the \hat{S} matrix is related to the scattering amplitude $f(\mathbf{p_1},\mathbf{p_2})$ by

$$\langle \mathbf{p}_{1} | \hat{S} | \mathbf{p}_{2} \rangle = \delta^{3} (\mathbf{p}_{1} - \mathbf{p}_{2}) + \frac{i}{2\pi} \langle \mathbf{p}_{1} | \hat{R} | \mathbf{p}_{2} \rangle, \tag{148}$$

where

$$\langle \mathbf{p}_1 | \hat{R} | \mathbf{p}_2 \rangle = \delta (E_1 - E_2) f(\mathbf{p}_1, \mathbf{p}_2); E_1 = \mathbf{p}_1^2 / 2m; E_2 = \mathbf{p}_2^2 / 2m.$$

Substituting now (147) in (140) and using (141) and (148), we obtain for scattering through nonzero angle the standard quantum expression

$$d\sigma_{\mathbf{q}\mathbf{u}}/dO = m^2\hbar^2 |f(\mathbf{p}, \mathbf{p}_0)|^2$$
. (149)

Remark 1. We leave out of consideration complicating circumstances such as fall toward the center, twisting, halo, and glory scattering, since they do not have a direct bearing on our problem.

Remark 2. To the integration with respect to q and ${\bf q'}$ in the standard form of quantum theory there corresponds equating of the momenta ${\bf p}={\bf p'_1}$ and ${\bf p_2}={\bf p'_2}$ in the matrix elements $\langle {\bf p_1} | \hat{S} | {\bf p_2} \rangle$ and $\langle {\bf p'_2} | \hat{S}^* | {\bf p'_1} \rangle$. We can perform the integration with respect to q_{\parallel} by using (138b) and (134a), which corresponds to removing the standard nonrigorous operation of "squaring of the energy δ function."

16. QUANTUM-CLASSICAL INTEGRAL EQUATION FOR SCATTERING

From Eq. (131) and the initial condition (130) there follows the integral Lippmann-Schwinger equation

$$\Omega(t) = 1 + \int_{-\infty}^{t} dt' \Omega(t') H_I(t') \sigma, \qquad (150)$$

which holds for the appropriate choice of $\sigma(\sigma_0 \text{ or } \sigma_n)$ in

each of the mechanics. Of greater interest, however, is an integral equation of the type (112), (113) relating $\Omega_{\rm qu}(t)$ and $\Omega_{\rm cl}(t)$. This equation is derived similarly. Equation (131) for the quantum case can be represented in the form

$$\partial \Omega_{\mathbf{q}\mathbf{u}}(t)/\partial t - H_I \{ \mathbf{p}_{fr}(t), \mathbf{q}_{fr}(t) \} \sigma_0 \Omega_{\mathbf{q}\mathbf{u}} = H_I (\sigma_h - \sigma_0) \Omega_{\mathbf{q}\mathbf{u}}.$$
 (151)

The corresponding retarded Green's function $G_{\text{scat}}(\mathbf{p}, \mathbf{q}, t; \mathbf{p}', \mathbf{q}', t')$, which satisfies the equation

$$\frac{\partial G_{\text{stat}}}{\partial t} - H_I \sigma_0 G_{\text{stat}} = \delta^3 (\mathbf{p} - \mathbf{p}') \, \delta^3 (\mathbf{q} - \mathbf{q}') \, \delta (t - t'), \tag{152}$$

has the form

$$G_{\text{stat}} = \mathcal{U}_{0}^{-1}(t) \, \mathcal{U}_{\text{cl}}(t) \, \mathcal{U}_{\text{cl}}(t') \, \mathcal{U}_{0}(t') \, \Theta(t-t'), \tag{153}$$

whose validity can be readily established using (116). We emphasize that only in the absence of bound states can the factor in front of the θ function be replaced by $\Omega_{\rm cl}(t)\Omega_{\rm cl}^T(t)$. The required integral equation satisfying the conditions (130) can be obtained from (151) in the form

$$\Omega_{\mathbf{q}\mathbf{u}}(t) = \Omega_{\mathbf{c}\mathbf{l}}(t) + \mathcal{U}_{\mathbf{0}}^{-1}(t) \,\mathcal{U}_{\mathbf{c}\mathbf{l}}(t)
\times \int_{0}^{t} dt' \,\mathcal{U}_{\mathbf{c}\mathbf{l}}^{-1}(t') \,\mathcal{U}_{\mathbf{0}}(t') \,H_{I}\{\mathbf{p}_{\mathbf{f}\mathbf{r}}(t'), \,\mathbf{q}_{\mathbf{f}\mathbf{r}}(t')\} (\sigma_{h} - \sigma_{\mathbf{0}}) \,\Omega_{\mathbf{q}\mathbf{u}}(t').$$
(154)

In accordance with (118), the classical evolution operator is known if all the trajectories (including the finite ones!) are known. At the same time, multiplication by the operators $\mathscr U$ and $\mathscr U_0$ reduces to integration of the δ function. It follows that Eq. (154) gives a general effective method for calculating the quantum corrections to classical scattering.

We emphasize that Eq. (154) is also valid when there are additional discrete quantum degrees of freedom (particles with spin, presence of excited levels, etc.).

For relativistic scattering, it must be borne in mind that the relativistic classical evolution differs from quantum evolution even for free motion:

$$c \sqrt{\mathbf{p}^2 + m^2 c^2} \sigma_0 \neq c \sqrt{\mathbf{p}^2 + m^2 c^2} \sigma_h$$

17. AXIOMS OF HAMILTONIAN THEORY

The present paper has been based on two independent ideas: 1) presenting quantum and classical mechanics using only concepts that have meaning in both mechanics; 2) realizing observables and states by c-number functions A(p,q) and $\rho(p,q)$ in the phase space. In this section, we present the first idea independently of the second, making no use of any realization. As a result, we obtain an abstract and, at the same time, complete system of axioms for both Hamiltonian mechanics. This axiomatics is close to the axiomatics presented in Ref. 11. The small difference relates to the remark made in Sec. 3 after Eq. (24b).

Axiom 1. A Hamiltonian theory consists of a set of observables $\{A\}$ and a set of states $\{\rho\}$. The observables and states are abstract elements whose realization (by functions, operators, and so forth) is not fixed.

Axiom~2. For the observables A there are defined the operations of addition, multiplication by complex numbers, and passage to the limit. In other words, $\{A\}$

is a topological vector space.

Axiom 3. For the observables A, two bilinear multiplication operations, the ordinary π and the Poisson σ , are defined. The Poisson multiplication is anticommutative:

$$AB\sigma^{T} \stackrel{\text{def}}{=} BA\sigma = -AB\sigma$$
.

The remaining associative and commutative properties of the multiplications π and σ are as yet not determined. The set of observables contains an identity (I) with respect to the multiplication π :

$$AI\pi = IA\pi = A$$
; $IA\sigma = AI\sigma = 0$.

Axiom 4. The multiplications π and σ satisfy the Hamiltonicity properties (18) and (19)

COROLLARY. Aggregates of the type $C\sigma$ are linear operators applied to the left on observables in $\{A\}$ and they satisfy the rule for differentiating a product with respect to the multiplications π and σ . Thus, to every observable A there corresponds the element $A\sigma$ of a Lie algebra.

Axiom 5. On the set $\{A\}$ there is defined an antilinear operator J that is applied to the left and has the property

$$JJ = I$$

and also the property that for any A and any number λ

$$(\lambda A) J = (AJ) \lambda^*.$$

DEFINITIONS. The element AJ is denoted by A^+ and is called the Hermitian conjugate of A. An element A is said to be Hermitian if $A = A^+$. The element A is said to be positive if there exists an observable B such that

$$A = BB^{\dagger}\pi$$

Axiom 6. The states ρ are linear functionals on the algebra of observables. Functionals corresponding to physical states are Hermitian, multiplicatively positive, and are usually normalized. The value $\langle A, \rho \rangle$ of the functional ρ on the observable A is the expectation value of the observable A in the state ρ .

The normalization condition and the Hermiticity and positive-definiteness properties have the following forms, respectively: $\langle I,\rho\rangle=1$; for $A=A^*$, the quantity $\langle A,\rho\rangle$ is real; for all A, the relation $\langle AA^*\pi,\rho\rangle\geqslant 0$ holds. The topology in the space $\{\rho\}$ of functionals over A is consistent with the topology in $\{A\}$.

Axiom 7. In the algebra $\{A\}$ there is defined an observable H for which the corresponding generator $H\sigma$ describes the evolution in time, i.e., determines the Heisenberg equations of motion for the observables:

$$\partial A/\partial t = AH\sigma$$

Axiom 8. The multiplication π is associative, i.e., for all observables A, B, C

$$AB\pi C\pi = ABC\pi\pi$$
.

Axions 1-8 hold for both mechanics, the only difference being in Axiom 9.

Axiom 9:

a) in the classical theory, the multiplication π , denoted by π_0 , is commutative;

$$\pi_{cl} = \pi_0; (AB - BA) \pi_0 = 0;$$
 (155a)

b) in the quantum theory, the multiplication π , denoted by Π_b , satisfies the commutator relation

$$(AB - BA) \Pi_h = i\hbar AB\sigma_h, \tag{155b}$$

where σ_h is the quantum Poisson multiplication.

Using only this system of axioms, one can introduce the following.

- 1. The definitions of pure and mixed states from Sec. 4. These definitions are given in Sec. 4 in a form that does not depend on the concrete realization.
- 2. The definition of stationary states in Sec. 8. It is also independent of the realization.
- 3. The definition of canonical mechanics as an algebra with an even number of generators $p_i, q_i (i=1, 2, ..., n)$ satisfying the relations

$$p_i p_j \sigma = q_i q_j \sigma = 0; \ q_i p_j \sigma = \delta_{ij}. \tag{156}$$

4. The definitions of the Schrödinger, Heisenberg, and interaction pictures.

As is shown in Ref. 30 (for one degree of freedom) and in Ref. 31 (for many degrees of freedom) the axioms 2-8 lead for the canonical mechanics (156) to either the classical theory or the quantum theory, with, it is true, the appearance of an additional (apparently pathological) possibility, namely, quantum theory with imaginary Planck constant.

Axioms 9a and 9b, which distinguish the classical and quantum theory, are independent of the remainder. If we do not adopt Axiom 9, then we obtain a free associative Hamiltonian algebra. Classical and quantum mechanics are factor algebras of the free algebra with respect to the ideals induced by the identities of the Axioms 9a and 9b, respectively. These ideals do not have nontrivial common elements. Therefore, there do not exist homomorphisms between the classical and the quantum algebra. From this point of view, we see that one can achieve a good quantum-classical correspondence for a particular group of problems by a felicitous choice of the quantization, but this is not possible for the theory as a whole.

All known boson quantum theories are encompassed by the given system of axioms. In particular, to gauge theories and theories with constraints there correspond realizations of the observables by equivalence classes of functions or operators. The transition to fermion theories reduces to changes in the signs in some identities.

CONCLUSIONS

A direct and natural field of applicability of the method presented here is to the solution of various quantum-classical problems, especially those in which some degrees of freedom are treated quantum-mechanically and others classically.

It would be very interesting to construct a quantumclassical algebra for quantum field theory. At the formal level, such a generalization is in fact contained in Ref. 14. However, there are here various very interesting and very difficult mathematical questions associated with the choice of the realization, the spaces of observables and states, the renormalization of the operation of multiplication of observables, the choice of the vacuum (for example, can one quantize over the classical vacuum), etc.

The investigation of all these questions is currently very relevant, since both gauge and soliton theories are developed on the basis of quantum-classical methods.

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