Towards an Autonomous Formalism for Quantum Mechanics

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A formalism is presented in which quantum particle dynamics can be developed on its own rather than ‘quantization’ of an underlying classical theory. It is proposed that the unification of probability and dynamics should be considered as the basic feature of quantum theory. Arguments are given to show that when such a unification is attempted at the configuration space level, the wave functions of Schrödinger theory appear as the natural candidates for the desired unification. A *-algebra $\mathcal{A}_Q$ of (not necessarily bounded) linear operators acting on an appropriate dense set of these wave functions appears as the arena for quantum kinematics. A simple generalization of an existing formalism in noncommutative geometry is employed to develop the notion of generalized algebraic symplectic structure (GASS) which can accommodate classical and quantum symplectic structures as special cases. Quantum kinematics and dynamics is developed in the framework of a noncommutative Hamiltonian system employing an appropriate GASS based in $\mathcal{A}_Q$. The Planck constant is introduced at only one place – in the quantum symplectic form; its appearance at conventional places is then automatic. Unitary Wigner symmetries appear as canonical transformations in the noncommutative Hamiltonian system. A straightforward treatment of quantum-classical correspondence is given in terms of appropriate GASSes.
The traditional formalism of quantum mechanics (QM) has two unsatisfactory features: (i) One all the time ‘quantizes’ classical systems. (ii) The languages employed in the traditional treatments of QM and CM (classical mechanics) are very different; this obscures the parent - daughter relationship between the two theories.

This is in marked contrast with the situation with some other pairs of parent - daughter theories in physics – for example, the pair [ special relativistic mechanics (SRM), Newtonian mechanics (NM) ] and the pair (general relativity, Newtonian theory of gravitation ). In these cases (i) the concepts and equations of the parent theory can be developed on their own; (ii) there exists a general formalism such that
(a) both the theories can be described in it;
(b) basic concepts and equations of the daughter theory can be obtained from those of the parent theory in a suitable limit, and
(c) a suitable subclass of quantities in the parent theory go over to well-defined quantities in the daughter theory (with a corresponding interpretation in the limit mentioned in (b)).

In the pair SRM - NM, for example, the concepts and equations of SRM can be developed quite independently of NM to which SRM reduces in the $c \to \infty$ limit. In this limit the relativity of simultaneity reduces to absolute simultaneity, the proper time differential $d\tau$ goes over to the Newtonian time differential $dt$, the spatial components of the equation $dp^\mu/d\tau = K^\mu$ goes over to Newton's second law, the particle energy $E = m_0c^2/\sqrt{1 - v^2/c^2}$ goes to infinity whereas the kinetic energy $K = E - m_0c^2$ goes over to the nonrelativistic kinetic energy $\frac{1}{2}m_0v^2$ etc.

The main objective of this paper is to remove the above-mentioned deficiencies in the treatment of QM and present a formalism in which one has an autonomous development of QM which permits a transparent treatment of quantum-classical correspondence. In this work we shall mainly consider particle QM. A similar autonomous treatment of quantum field dynamics is being postponed to a future publication.

To see the quantum to classical transition in a transparent form, one must translate the operator-theoretical formalism into an ‘equivalent’ one involving phase space functions (replacing commutators by the so-called Moyal brackets). One of the main concerns of the present work will be to ensure that the formalism evolved permits the description of the ‘equivalence’ referred to above as an isomorphism between appropriate mathematical structures.

What is required is a mathematical formalism employing objects of a sufficiently general type so as to include, as special cases, the algebra of phase space functions with the Poisson bracket structure defined on it and an algebra of operators in the quantum mechanical Hilbert space with the Heisenberg commutators as analogues of Poisson brackets. Noncommutative geometry (NCG) [1–4] (in which all geometry is developed in the framework of algebras) holds the key to the evolution of such a formalism. Indeed, noncommutativity is the hallmark of QM. In the paper that marked the birth of QM [5], Heisenberg’s main conclusion, based on correspondence arguments, was that the kinematics underlying QM must be based on a noncommutative algebra of observables. An intuitive formulation of noncommutative Hamilto-
nian mechanics ( matrix mechanics ) was given in ref [6-8]. Noncommutative symplectic structures yielding quantum mechanical commutators as Poisson brackets have appeared in literature[2–4,9]; however, a mathematically satisfactory treatment of quantum symplectics meeting the above mentioned needs is yet to be given. Pursuit of this objective led the present author to a generalization [10] of the NCG scheme of ref [2,3] which holds promise for interesting applications. Here we shall present this generalized formalism for NCG, use it to evolve a general framework for mechanics ( which covers CM and QM as special cases ) and give a straightforward treatment of quantum - classical correspondence in this framework.

The conceptual development of a fundamentally new theory often takes place around a unifying principle. For example, Maxwell-Lorentz electrodynamics unifies electricity and magnetism, special relativity unifies the concepts of space and time and general relativity unifies space-time geometry and gravitation. Is there a unifying principle underlying quantum mechanics? One might suggest unification of wave and particle properties of matter. ( Indeed, this was the theme underlying the work of de Broglie [11] and Schrödinger [12]. ) There is, however, in the author’s opinion, a deeper unification – that of dynamics and probability – which, when incorporated in an appropriate framework, entails the unification of wave and particle properties of matter. One possible way to understand it is this: There is a background noise field pervading all universe whose dynamics is inexorably tied up with that of matter such that the effect of of this noise field on matter cannot be adequately treated as a perturbation. This effect is presumably best treated by employing, in the description of dynamics of matter, mathematical entities that give a unified description of dynamics and probability. The resulting description of material objects is expted to involve a blend of particle - like motion with wave-like fluctuations.

In everyday use of QM, such a unification of probability and dynamics is taken for granted; indeed, we all the time employ the Schrödinger wave functions for statistical averaging as well as for describing the dynamics of atomic systems. A point brought out in the present work (section III) is that, when such a unification is attempted at the configuration space level in an appropriate setting, Schrödinger type wave functions appear as the natural candidates for such a unification, thus providing a rationale for the use of complex Hilbert spaces in QM.

Earlier works relating to the foundations of QM have been generally concerned with quantum logic [13–15], C*-algebras [16–21] or stochastic mechan-
ics [22–25]. These works have provided valuable insights into various aspects of QM; however, as far as the question of providing the initial motivation for the Schrödinger wave function is concerned, as we shall see in section III, the approach adopted here is much more direct and intuitively appealing. The formalism developed in section V is essentially algebraic; however, we do not restrict ourselves to $C^*$-algebras.

The plan of the remaining sections is as follows. Section II is devoted to some preliminaries relating to the general probabilistic description of dynamics of systems [26, 27] and the probabilistic version of Hamilton-Jacobi theory (called Hamilton-Jacobi fluid in ref [25, 28]). In section III, we consider unification of dynamics and probability in particle dynamics in configuration space and show that the appropriate single mathematical object unifying the Hamilton-Jacobi function $S(x,t)$ and the probability density function $\rho(x,t)$ must be a Schrödinger type wave function $\psi(x,t)$ which is ‘essentially’ $\sqrt{\rho}\exp[iS/\hbar]$; the probability interpretation of $\psi$ is then automatic. The physically realizable wave functions belong to a dense subset $\Omega$ of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$ consisting of an appropriate class of smooth functions. A $\ast$-algebra $\mathcal{A}_Q$ of (not necessarily bounded) operators mapping $\Omega$ into itself appears as the natural arena for quantum kinematics. After presenting the detailed treatment of GASSes as mentioned above (with $\mathcal{A}_Q$ as the underlying algebra) in section IV, we develop quantum kinematics and dynamics of a particle in the framework of a GASS based in $\mathcal{A}_Q$ in section V. Quantum-classical correspondence is treated in section VI. The last section contains some concluding remarks.

The paper has been written in an easy style with the hope that students just being introduced to QM will enjoy reading a substantial part of it. We shall generally maintain a pretension that we are at the pre-1925 stage when the papers of Heisenberg and Schrödinger had not appeared and evolve an autonomous formalism for QM from scratch.

A preliminary version of the essential ingredients in section IV and VI appeared in the article [10] which was given a limited circulation back in 1993. A brief account of the same (along with some background material on classical symplectic geometry) also appeared in ref [29].

II. PRELIMINARIES

In this section we shall collect some useful results relating to probabilistic description of systems and the probabilistic version of Hamilton-Jacobi theory.
A. General Probabilistic Description of Systems

A substantial part of this subsection is an adaptation from ref [26, 27].

In every physical theory, there are three primitive elements [30,31] which are always present (explicitly or implicitly):
(i) observations/measurements;
(ii) description of evolution of systems (typically in terms of a discrete or continuous parameter called time);
(iii) conditional predictions about systems: given some information about a system (typically in terms of values of appropriate measurable quantities), to make predictions/retrodictions about its behaviour.

A physical theory generally involves additional ingredients in the form of hypotheses concerning the relevant aspects of nature; the structure of the theory is then developed into a consistent mathematical formalism based on those hypotheses and incorporating the above mentioned three elements.

A useful concept which serves to integrate the three items above is that of a state. A state of a system encodes, in a conveniently usable mathematical form, the information available about the system at a particular time. A standard way to describe the evolution of a system is to describe the change of state with time. At the initial stages in its formulation, the main business of any physical theory is to provide appropriate mathematical description of observable/measurable quantities (generally called observables) and states and the relationship(s) between them.

We shall be mainly concerned with the nonrelativistic kinematics and dynamics of a particle. In Newtonian mechanics, a particle is characterized by a Galilean invariant parameter m called its mass [32, 33]. Its motion in space is described by giving its position vector $\vec{r}(t)$ as a function of time which is assumed to be smooth so that one can talk about velocity ($\vec{v} = d\vec{r}/dt$), acceleration ($\vec{a} = d^2\vec{r}/dt^2$) etc. The equation of motion (Newton's second law) gives acceleration in terms of force which is supposedly a function of position and velocity. We can, therefore, take, at each time t, the vectors $\vec{r}(t)$ and $\vec{p}(t)$ [or, equivalently, $\vec{r}(t)$ and $m\vec{v}(t)$] as independent observables. These are the fundamental observables; all other observables (angular momentum, kinetic energy etc.) are functions of these. The state of the particle at time t is given by the pair ($\vec{r}(t), \vec{p}(t)$) and its change with time is given by the equations

$$\frac{d\vec{r}(t)}{dt} = \frac{1}{m}\vec{p}(t) \quad \frac{d\vec{p}(t)}{dt} = \vec{F}(\vec{r}(t), \vec{p}(t), t).$$
Given the initial state \((\vec{r}(0), \vec{p}(0))\), at any later time \(t\), the state \((\vec{r}(t), \vec{p}(t))\) (and, therefore, the values of all other observables at time \(t\)) can be found by integrating eqs (1): we have a deterministic theory.

The mechanics underlying atomic phenomena cannot be deterministic. Given, for example, an atomic electron in a sufficiently high excited Bohr energy state, it can generally make transition to more than one possible lower energy states; a theory of atomic phenomena is expected to predict probabilities of these transitions. Moreover, if radiation is assumed to consist of photons, a description of interference and diffraction of light can be given only in a probabilistic framework [34].

A probabilistic situation can arise in a deterministic theory if the initial state is inadequately specified. This is the case in classical statistical mechanics where a state is generally represented by a probability density \(\rho(q, p, t)\) in phase space. The single particle states \((\vec{r}(t), \vec{p}(t))\) mentioned above are special cases of this corresponding to

\[
\rho(\vec{r}, \vec{p}, t) = \delta(\vec{r} - \vec{r}(t))\delta(\vec{p} - \vec{p}(t)).
\]

A formalism of this type, however, is not adequate [34] for the treatment of quantum phenomena. To the best of understanding achieved to date, the dynamics of atomic and subatomic systems is intrinsically/irreducibly probabilistic.

What is the appropriate framework for the treatment of such dynamics? We shall obtain below a standardised form for the description of states and observables in a probabilistic framework which is sufficiently general for our purpose.

Consider a typical experiment in which a system is prepared with some prescribed initial conditions and a measurement of some quantity is made. The measured values are generally expected to be measurable subsets in a measurable space \((S, \mathcal{B}(S))\) where \(S\) is a subset of some Euclidean space and \(\mathcal{B}(S)\) is its Borel \(\sigma\)-algebra. For example, measured values of a length (with error margins) are Borel subsets of the real line; measured values of a direction are Borel subsets of the unit sphere etc. In the latter case, the direction measurements can be analysed in terms of two real parameters \(\theta\) and \(\phi\). More generally, all measurements can be analysed in terms of simpler measurements giving single real numbers (with appropriate error margins) as measured values. For the treatment of fundamentals, it is generally adequate to consider only these simpler measurements. We shall, therefore assume henceforth that \(S\) is a subset of the real line.
We shall start by trying to give an operational meaning to the probability \( w_{\alpha}^{Q}(B) \) of an observable \( Q \) having values in a Borel set \( B \) when the system is in a state \( \alpha \).

Let the experiment be performed with an experimental setup or instrument \( \tilde{Q} \) with the system prepared so as to satisfy some initial conditions \( \tilde{\alpha} \). In each performance of the measurement, the measured value will lie in some Borel subset of \( S \). Let the experiment be repeated a large number \( (N) \) of times. If the measured value lies in a Borel set \( B \) in \( N_B \) runs of the experiment, we have, adopting the traditional relative frequency definition of probability, an operationally defined probability

\[
w_{\tilde{\alpha}}^{\tilde{Q}}(B) \sim \frac{N_B}{N} \quad (N \text{ large}).
\]  

We now define an equivalence relation \( \approx \) on the set \( \Sigma \) of all initial conditions: \( \tilde{\alpha}_1 \approx \tilde{\alpha}_2 \) if \( w_{\tilde{\alpha}_1}^{\tilde{Q}}(B) = w_{\tilde{\alpha}_2}^{\tilde{Q}}(B) \) for all \( \tilde{Q} \) and \( B \). We denote the equivalence class of \( \tilde{\alpha} \) as \( \alpha \) and the set of equivalence classes in \( \Sigma \) as \( \mathcal{S} \); the members \( \alpha, \beta, ... \) of \( \mathcal{S} \) will be called states. We have, at this stage, the quantities \( w_{\alpha}^{\tilde{Q}}(B) \) defined.

We next define an equivalence relation \( \equiv \) on the set \( \mathcal{I} \) of all instruments: \( \tilde{Q}_1 \equiv \tilde{Q}_2 \) if \( w_{\alpha}^{\tilde{Q}_1}(B) = w_{\alpha}^{\tilde{Q}_2}(B) \) for all \( \alpha \) and \( B \). We denote the equivalence class of \( \tilde{Q} \) as \( Q \) and the set of equivalence classes in \( \mathcal{I} \) as \( \mathcal{O} \); the members \( P, Q, ... \) of \( \mathcal{O} \) will be called observables. A quantity \( w_{\alpha}^{Q}(B) \) can now be defined; this is the desired probability.

Given \( Q \) and \( \alpha \), we have the probability measure \( w_{\alpha}^{Q} \) defined on the measurable space \( (S, \mathcal{B}(S)) \) thus obtaining a probability space \( (S, \mathcal{B}(S), w_{\alpha}^{Q}) \). The expectation value of the observable \( Q \) in the state \( \alpha \) is defined as

\[
\alpha(Q) = \int_{S} sdw_{\alpha}^{Q}(s).
\]  

Given an observable \( Q \) and a Borel - measurable function \( f \) on the real line, we can define the function \( f(Q) \) of \( Q \) as the observable which takes a value \( f(q) \) whenever \( Q \) takes a value \( q \). The expectation value of \( f(Q) \) in the state \( \alpha \) is given by

\[
\alpha(f(Q)) = \int_{S} f(s)dw_{\alpha}^{Q}(s).
\]  

Given the expectation values \( \alpha(Q) \), we can find the quantities \( w_{\alpha}^{Q}(B) \) by the rule

\[
w_{\alpha}^{Q}(B) = \alpha(\chi_{B}(Q))
\]
where $\chi_B$ is the characteristic function of the Borel subset $B$ of $S$.

We next consider the structure of a ‘mixture space’ [26] on the state space $S$. Given a finite set $\{\alpha_i\}$ and weights $\{p_i\}$ ($0 \leq p_i \leq 1$, $\sum p_i = 1$), the joint collection $(\{\alpha_i\}, \{p_i\})$ defines a state $\alpha$ by the relation

$$w^Q_\alpha(B) = \sum_i p_i w^Q_{\alpha_i}(B) \quad \text{for all } Q, B. \quad (6A)$$

The state $\alpha$ is interpreted as a mixed state in which the state $\alpha_i$ appears with a probability $p_i$. The expectation value of an observable $Q$ in this mixed state is given by

$$\alpha(Q) = \sum_i p_i \int_S s d w^Q_{\alpha_i}(s).$$

A general mixture space is defined as a set $M$ with the property that any finite collection $\{\mu_i\}$ of elements of $M$ and weights $\{p_i\}$ defines a unique element $\mu$ of $M$ subject to the condition that if $\mu_i = \mu_0$ for all $i$, then $\mu = \mu_0$. The set $S$ is clearly a mixture space. [\alpha_i = \alpha_0 \text{ for all } i \text{ in eq(6A) implies } \alpha = \alpha_0.]$

An important example of a mixture space is a convex set $K$ of a real vector space $V$. [Given points (i.e., vectors) $K_i$ lying in $K$, we have $\sum_i p_i K_i$ lying in $K$.] We shall call such a mixture space a standard mixture space.

We shall now show [26] that the space $S$ can be taken, without loss of generality, to be a standard mixture space. We shall do this by showing a one-to-one correspondence between $S$ and a standard mixture space which preserves mixtures.

An affine functional on $S$ is a mapping $\phi$ from $S$ to the real line $R$ such that, for a mixture $\alpha = (\{\alpha_i\}, \{p_i\})$ we have

$$\phi(\alpha) = \sum_i p_i \phi(\alpha_i). \quad (7)$$

The set $F$ of affine functionals on $S$ is easily seen to be a real vector space. Let $F^*$ be the algebraic dual of $F$, i.e., the space of linear functionals on $F$; this space is also a real vector space. A one-to-one correspondence of $S$ onto a convex subset of $F^*$ is obtained by associating with a state $\alpha$, the element $\hat{\alpha}$ of $F^*$ given by

$$\hat{\alpha}(\phi) = \phi(\alpha) \quad \text{for all } \phi \text{ in } F. \quad (8)$$
The correspondence $\alpha \leftrightarrow \hat{\alpha}$ preserves mixtures: if $\alpha = (\{\alpha_i\}, \{p_i\})$, we have

$$\hat{\alpha}(\phi) = \phi(\alpha) = \sum_i p_i \phi(\alpha_i) = \sum_i p_i \hat{\alpha}_i(\phi)$$

implying $\hat{\alpha} = \sum p_i \hat{\alpha}_i$.

Remarks: (i) We have implicitly used, in the argument above, the fact that $S$ is a ‘separated’ mixture space which means that, given two states $\alpha_1 \neq \alpha_2$ in $S$, there is at least one affine functional $\phi$ on $S$ such that $\phi(\alpha_1) \neq \phi(\alpha_2)$. This is clear from the definition of states given above. [For given $Q$ and $B$, the object $w^Q(B)$ given by $w^Q(B)(\alpha) = w^Q_\alpha(B)$ is an affine functional on $S$, etc.]

(ii) Note that the treatment of states and observables presented above is quite general; nowhere in our proceedings did we commit ourselves to any specific type of origin of the probabilistic aspect of the phenomena.

(iii) The states in classical statistical mechanics (probability densities in phase space) already constitute a standard mixture space.

(iv) Deterministic theories are a subclass of the theories covered by the present formalism – those in which all probabilities are either zero or one. [Recall eq (2).]

(v) Note, from eqs (4) and (6A), that an observable $Q$ defines an affine functional $\phi_Q$ on $S$ (the expectation value functional) given by $\phi_Q(\alpha) = \alpha(Q)$.

B. Probabilistic Hamilton-Jacobi Theory (the Hamilton-Jacobi Fluid [25,28])

Given a system with a finite number of degrees of freedom with a Lagrangian $L(q, \dot{q}, t)$, its state at any time $t$ is given by the collection $(q(t), \dot{q}(t))$ and its dynamics is given by the Euler-Lagrange equations obtained by applying Hamilton’s principle to the action $\int L dt$. An equivalent description is given in phase space in terms of $q^\alpha$ and $p_\alpha = \partial L/\partial \dot{q}^\alpha$; now the state at any time is $(q(t), p(t))$ and dynamics is given by the Hamilton’s equations

$$\dot{q}^\alpha = \frac{\partial H}{\partial p_\alpha}, \quad \dot{p}_\alpha = -\frac{\partial H}{\partial q^\alpha}. \quad (9)$$

A third equivalent description is obtained in terms of the Hamilton-Jacobi function $S(q,t)$ which, for a fixed time $t_0$ and configuration $q_0$, is given by

$$S(q,t) = \int_{q_0,t_0}^{q,t} dt' L(q(t'), \dot{q}(t'), t') \quad (10)$$
where the integration is along the physical trajectory between \((t_0, q_0)\) and 
\((t, q(t))\) (assumed, for simplicity, unique). It satisfies the Hamilton-Jacobi

\[
\frac{\partial S(q, t)}{\partial t} + H(q, \frac{\partial S(q, t)}{\partial q}, t) = 0.
\] (11)

A solution \(S(q, t)\) of eq(11) with the initial condition \(S(q, t_0) = S_0(q)\), when

supplemented with the initial condition

\[q(t_0) = q_0,\] (12)

can be used to obtain the (unique) dynamical trajectory given by the Hamilton’s equations (9) with initial condition \((q(t_0), p(t_0)) = (q_0, p_0)\) where

\[p_0 = \frac{\partial S_0(q)}{\partial q} \bigg|_{q=q_0}.\]

To see this, define the momentum field \(p(q,t)\) and the velocity

field \(v(q,t)\) by

\[
p_\alpha(q, t) = \frac{\partial S(q, t)}{\partial q_\alpha},
\]

\[
v_\alpha(q, t) = \frac{\partial H(q, p, t)}{\partial p_\alpha} \bigg|_{p=p(q,t)}.
\]

The differential equation

\[
\dot{q}_\alpha(t) = v_\alpha(q(t), t)
\]

with the initial condition (12) gives the unique solution \(q_\alpha(t)\). Finally

\[
p_\alpha(t) = p_\alpha(q(t), t).
\]

Note that, in this picture, the state at time \(t\) is given by the quantities

\(q_\alpha(t)\) and \(S(q, t)\). The corresponding phase space density function is

\[
\tilde{\rho}(q, p, t) = \delta(q - q(t))\delta(p - \frac{\partial S(q, t)}{\partial q}).
\]

Given a Hamiltonian \(H(q, p, t)\), the change of state with time is given by

the differential equations (15) and (11). The particle picture (in situations

distinct from which the system consists of one or more particles) can be recovered from

the field \(S(q, t)\) through the equations (15) and (16). It is instructive to note
that, even in classical mechanics, the description of state of a particle system can involve a field like $S(q,t)$ in configuration space.

If, instead of the condition (12), we are initially given a probability distribution $\rho(q,t_0) = \rho_0(q)$, we shall obtain, instead of the functions $q^\alpha(t)$, the probability density function $\rho(q,t)$ which is obtained as a solution of the continuity equation

$$\frac{\partial \rho(q,t)}{\partial t} + \frac{\partial}{\partial q^\alpha} [v^\alpha(q,t)\rho(q,t)] = 0$$

with the given initial condition. The corresponding phase space density function is

$$\tilde{\rho}(q,p,t) = \rho(q,t)\delta(p - \frac{\partial S(q,t)}{\partial q}).$$

We now have the state at time $t$ described by the pair of fields $\rho(q,t)$ and $S(q,t)$ whose change with time is described by eqs (18) and (11). We have (mathematically) a hydrodynamics-like situation. ( Hence the name Hamilton-Jacobi fluid for this system. ) The results at any stage in the formalism can be analysed in terms of a particle picture through the equations (15) and (16).

### III. UNIFICATION OF DYNAMICS AND PROBABILITY IN CONFIGURATION SPACE; RATIONALE FOR A COMPLEX HILBERT SPACE

As stated in the introduction, in the author’s opinion, the main unifying concept in quantum mechanics is the unification of dynamics and probability. In this section it will be shown that when this unification is considered in the context of particle dynamics at the configuration space level, the wave mechanical formalism of Schrödinger naturally emerges.

#### A. States

We are looking for a unification of the kind one has, for example, in classical relativistic electrodynamics: the electric field $\vec{E}$ and the magnetic field $\vec{B}$ are unified into the electromagnetic field tensor $F_{\mu\nu}$. Here both the objects being unified are fields; the unified object is also a field having a ‘higher’ mathematical structure. Our search for unification of probability and dynamics should begin with a formulation of the probabilistic version of
classical dynamics in which aspects of probability and dynamics are both represented by similar mathematical objects. In phase space such a unification is already achieved by the phase space probability density function \( \tilde{\rho}(q,p,t) \). We would like to achieve it at the level of configuration space (which is a more fundamental level). Here the choice is obvious: the probabilistic version of Hamilton-Jacobi theory discussed in section II B; here probability and dynamics are represented by the fields \( \rho(q,t) \) and \( S(q,t) \) respectively. Restricting, for simplicity, to single particle systems, we attempt to replace \( \rho(x,t) \) and \( S(x,t) \) by a single function \( F(x,t) \) which presumably represents, in the quantum theory to be evolved, the state of the particle at time \( t \) (incorporating the statistical features of its kinematics at time \( t \)). One should keep in mind the possibility that the function \( F \) may belong to a ‘higher’ category of mathematical objects than that of \( \rho \) and \( S \) (which are real-valued functions of their arguments). Having arrived at the class of mathematical objects to which \( F \) must belong, we shall attempt a straightforward treatment of states and observables in the framework of section IIA.

In the emerging quantum kinematics and dynamics, the Planck constant \( \hbar \) is expected to appear in various quantities. We expect the function \( F(x,t) \) to involve, as parts of its structure, two functions \( \tilde{\rho}(x,t) \) (this has nothing to do with the phase space density function \( \tilde{\rho} \) used earlier) and \( \tilde{S}(x,t) \) such that, in the limit \( \hbar \to 0 \)

\[
\tilde{\rho}(x,t) \to \rho(x,t) \quad \tilde{S}(x,t) \to S(x,t).
\]  

(20)

Let \( F = f(\tilde{\rho}, \tilde{S}) \). To determine the function \( f \), we note that, for two non-interacting particles 1 and 2, the functions \( \rho_{12}(x^{(1)}, x^{(2)}, t) \) and \( S_{12}(x^{(1)}, x^{(2)}, t) \) for the two-particle system are related to the functions \( \rho_i \) and \( S_i \) \((i = 1, 2)\) for the two one-particle systems by

\[
\rho_{12}(x^{(1)}, x^{(2)}, t) = \rho_1(x^{(1)}, t) \rho_2(x^{(2)}, t) \quad (21)
\]

\[
S_{12}(x^{(1)}, x^{(2)}, t) = S_1(x^{(1)}, t) + S_2(x^{(2)}, t). \quad (22)
\]

It appears reasonable to assume that the functions \( \tilde{\rho} \) and \( \tilde{S} \) will also satisfy the conditions (21) and (22 respectively. Now the function \( f_{12}(\tilde{\rho}_{12}, \tilde{S}_{12}) \) must be related to \( f_1(\tilde{\rho}_1, \tilde{S}_1) \) and \( f_2(\tilde{\rho}_2, \tilde{S}_2) \) in a definite way. The simplest possibilities are

\[
f_{12}(\tilde{\rho}_{12}, \tilde{S}_{12}) = f_1(\tilde{\rho}_1, \tilde{S}_1) f_2(\tilde{\rho}_2, \tilde{S}_2) \quad (23)
\]
and
\[ f_{12}(\tilde{\rho}_{12}, \tilde{S}_{12}) = f_{1}(\tilde{\rho}_{1}, \tilde{S}_{1}) + f_{2}(\tilde{\rho}_{2}, \tilde{S}_{2}). \] (24)

In fact, these two possibilities are mutually related: given (23), \( g = \ln f \) satisfies (24) and given (24), \( h = \exp(f) \) satisfies (23). We assume that (23) holds. Eqs(21–23) give
\[ f(\tilde{\rho}, \tilde{S}) = (\tilde{\rho})^a \exp[b\tilde{S}] \] (25)
where \( a \) and \( b \) are constants.

Assuming that \( \tilde{\rho} \) is also a probability density, it is reasonable to demand that, given \( F(x,t) \), the quantity \( \tilde{\rho}(x,t) \) is uniquely determined. (This amounts to requiring that, in a given state, there is a unique probability density for the particle position.) The simplest way to achieve this is to have the parameter \( a \) real and \( b \) imaginary (say, \( b = i\lambda \) with \( \lambda \) real). Assuming this, we have
\[ F(x,t) = [\tilde{\rho}(x,t)]^a \exp[i\lambda \tilde{S}(x,t)]. \] (26)

Now, the function \( S(x,t) \) is arbitrary up to an additive (real) constant; the same is also expected of \( \tilde{S} \). It follows that a multiplicative constant phase factor in \( F(x,t) \) must be inconsequential for the representation of state. The objects which uniquely determine the state at time \( t \) are the bilocal functions
\[ w(x, x', t) = F(x,t)F^*(x', t) = [\tilde{\rho}(x,t)\tilde{\rho}(x', t)]^a \exp[i\lambda\{\tilde{S}(x,t) - \tilde{S}(x', t)\}]. \] (27)

Note that
\[ w(x, x, t) = [\tilde{\rho}(x,t)]^{2a}. \] (28)

Recalling the discussion in section IIA, we now impose the requirement that convex combinations of quantities of the form (27) must be admissible states. Let \( 0 < p < 1 \) and
\[ w_{12}(x, x', t) = pw_{1}(x, x', t) + (1 - p)w_{2}(x, x', t) \] (29)
where \( w_{1} \) and \( w_{2} \) are of the form (27). Putting \( x = x' \) in eq(29), we get
\[ w_{12}(x, x, t) = p[\tilde{\rho}_{1}(x,t)]^{2a} + (1 - p)[\tilde{\rho}_{2}(x,t)]^{2a}. \] (30)

Now a convex combination of probability densities is a probability density. Eq(30), therefore, appears to make sense only if \( 2a = 1 \). Assuming this, we
have, finally, (replacing the symbol $F$ by the conventional $\psi$) the Schrödinger type wave function

$$\psi(x,t) = [\tilde{\rho}(x,t)]^{1/2} \exp[i \lambda \tilde{S}(x,t)].$$

(31)

With $|\psi(x,t)|^2 = \tilde{\rho}(x,t)$ the probability interpretation of $\psi$ is automatic and

$$\int |\psi(x,t)|^2 dx = \int \tilde{\rho}(x,t) dx = 1$$

(32)

so that, for each fixed $t$, the functions $\psi(.,t)$ belong to the Hilbert space $\mathcal{H}$ of complex square integrable functions on $\mathbb{R}^3$.

The quantities $w(x,x',t)$ (for general states including mixed states) satisfy the conditions

$$w(x,x',t)^* = w(x',x,t)$$

$$\int w(x,x,t) dx = 1$$

(33)

so that they are kernel functions of density operators on $\mathcal{H}$:

$$w(x, x', t) = <x'|w(t)|x> .$$

(34)

Note. The functions $\psi(.,.)$ are, indeed, mathematical objects belonging to a ‘higher’ category than that of $\rho$ and $S$; they are complex valued functions. In the present setting, the appearance of complex valued functions should not be surprising: fluctuations are going to be an important part of the physics to emerge and these are most conveniently analysed in a complex variable setting.

An important consideration about states is the differentiability requirements on the wave functions $\psi$. In classical mechanics, the functions $\rho(x,t)$ and $S(x,t)$ are smooth. These functions, however, are (supposedly) limits of the functions $\tilde{\rho}$ and $\tilde{S}$ in the limit of vanishing Planck constant. The smoothness of $\tilde{\rho}$ and $\tilde{S}$ or of $\psi$ must be decided directly on the basis of appropriate physical and mathematical considerations in the quantum mechanical theory we are trying to construct, without any reference to the classical theory. Physically, the wave functions are supposed to encode the data about preparation of the system in question. Since any laboratory preparation involves some error margins, the objects employed in the encoding should be, broadly speaking, reasonably smooth so that small changes in the input data imply small change in the wave function (hence in the statistical information provided by it). We shall, therefore, assume that the physically realizable pure
states are represented by sufficiently smooth wave functions; we shall denote this subclass of functions in \( \mathcal{H} \) by \( S_1 \). (More precise specification of \( S_1 \) will appear later.) Since linear combinations of smooth square integrable functions are smooth square integrable functions, \( S_1 \) must be a vector subspace of \( \mathcal{H} \). For analytical work one must include the limits of sequences of functions in \( S_1 \) and consider its completion. This completion must be \( \mathcal{H} \) (there being no grounds for taking it to be a proper subset of \( \mathcal{H} \)); \( S_1 \) must, therefore, be a dense subspace of \( \mathcal{H} \). The space of all physical states (including mixed states constructed from pure physical states in \( S_1 \)) will be called \( \mathcal{S} \).

Remarks. (i) Smoothness of \( \psi \) has nothing to do with any possible smoothness of allowed particle trajectories. Even in classical mechanics, the smoothness of \( S(x,t) \) has nothing to do with smoothness of particle trajectories. It has, rather, to do with the fact that the Hamilton-Jacobi function is given by the integral in eq (10). In fact, there is a formalism [35] in which the wave function \( \psi \) is defined as an integral over (continuous) particle trajectories; its smoothness is then almost automatic.

(ii) The vector space nature of \( S_1 \) implies the principle of superposition of quantum mechanical (pure) states: given two elements \( \psi_1 \) and \( \psi_2 \) of \( S_1 \) (each of which represents a quantum mechanical pure state up to a constant phase factor) the superposition \( \psi = a\psi_1 + b\psi_2 \) (with \( |a|^2 + |b|^2 = 1 \)) also represent a quantum mechanical pure state up to a constant phase factor.

(iii) The space \( S_1 \) is the quantum mechanical analogue of the classical phase space of a system.

B. Observables

Recalling eq (4) and the remark (v) in section IIA, we expect observables to be objects defining affine functionals on the space \( \mathcal{S} \) of physical states. Suppressing time argument, a general physical state is of the form \( \rho(x,y) = \sum p_i \rho_{\psi_i}(x,y) \) where \( \rho_{\psi}(x,y) = \psi(x)\psi^*(y) \) and the \( \psi \)'s are in \( S_1 \). An affine functional on these objects is given by a complex bilocal function \( A(y,x) \) giving the expectation value functional

\[
<A> = \rho(A) = \int A(y,x)\rho(x,y)dxdy = \sum_i p_i \int \psi_i^*(y)A(y,x)\psi_i(x)dxdy.
\]

(35)

It is adequate to consider the pure state expectation values

\[
<A> = \int \psi^*(y)A(y,x)\psi(x)dxdy.
\]

(36)
Keeping in mind the denseness of $S_1$, reality of $<A>_{\psi}$ for all $\psi$ in $S_1$ implies $A(y, x)^* = A(x, y)$ so that $A(x, y)$ is the kernel of a self-adjoint operator:

$$A(y, x) = <y | A | x> \quad A = A^\dagger \quad (A\psi)(y) = \int A(y, x)\psi(x)dx.$$

Note. We did not show in section IIA that every affine functional on the set of states defines an observable. In the case at hand, however, we can show directly that the self-adjoint operator $A$ above defines an observable in the sense of section IIA. For this, it is enough to show that, given any pure state $\psi$, a self-adjoint operator defines a probability measure $w^A_\psi$ on the real line $R$. Given a self-adjoint operator $A$ and a Borel measurable function $f$ on $R$, the operator $f(A)$ can be defined through the spectral theorem. Now we can define $w^A_\psi$ by

$$w^A_\psi(B) = \langle \psi, \chi_B(A\psi) \rangle \text{ for every Borel set } B.$$ 

The self-adjoint operators corresponding to the expectation value functionals, therefore, qualify to be called observables.

Since the operation of the operator $A$ above needs to be defined only on the wave functions in $S_1$, it is allowed to be an unbounded operator; had we defined observables in terms of states on all of $\mathcal{H}$, we would end up with bounded self-adjoint operators as observables.

Note. Existence of the integral in eq(36) for $\psi$ in $S_1$ does not demand that the vector $A\psi$ also lie in $S_1$. Since, however, $S_1$ is dense, nothing of significance is lost in assuming that the self-adjoint operators representing observables map $S_1$ into itself. We shall henceforth assume this; this is to ensure that the observables belong to the algebra $A_Q$ defined below.

The collection $A_Q$ of linear operators which, along with their adjoints, map $S_1$ into itself, is an associative $*$-algebra (the $*$-operation being hermitian conjugation). This object is the analogue of the algebra $A_{cl}$ of (smooth) complex valued functions on phase space in classical dynamics and will play an important role in our treatment of quantum kinematics. Note that, whereas $A_{cl}$ is a commutative algebra [with product of functions defined as $fg(q, p) = f(q, p)g(q, p)$], the algebra $A_Q$ is noncommutative. This is a concrete formulation of Heisenberg’s insight [5] that kinematics underlying quantum dynamics must be based on a noncommutative algebra of observables.

Remarks.(i) There is, as we shall see, some flexibility in the choice of the spaces $S_1$ and $A_Q$. We shall eventually find it convenient to define $S_1$ as the
largest common dense domain which is mapped into itself by the so-called ‘fundamental observables’ (these are defined in section V) and $A_Q$ as the *-algebra generated by these observables. This has the advantage that $A_Q$ so defined has a trivial center (i.e. all operators commuting with every operator in $A_Q$ are multiples of the identity operator).

(ii) One can introduce, at this stage, a topology $\tau$ on the space $S_1$ such that the pair $(S_1, \tau)$ becomes a topological vector space and the operators in $A_Q$ are continuous operators on this topological vector space. Let $S_1^*$ be the topological dual of $(S_1, \tau)$ i.e. the space of continuous linear functionals on $S_1$. We then have (with a little bit more of mathematical finesse) the rigged Hilbert space or Gelfand triple [36–38]

$$S_1 \subset H \subset S_1^*$$

($S_1^*$ is the space to which the generalized eigenvectors of the operators in $A_Q$ belong—for example, the generalized eigenfunctions $e^{ikx}$ of the momentum operator $-i\hbar \frac{d}{dx}$; these functions obviously don’t belong to $H$.) One can then have a mathematically rigorous development [39, 40, 38] of the Dirac bra-ket formalism [41]. We shall skip the details.

C. Transition Probabilities; Fundamental Invariances

In any scheme of dynamics, geometrical properties of the basic spaces play an important role. In classical mechanics, for example, the symplectic structure on a phase space and related canonical transformations play very important role. Among the two basic spaces, $S_1$ and $A_Q$ introduced above, we consider here the geometry of $S_1$; that of $A_Q$ (which will involve noncommutative geometry) will be taken up in section V.

Apart from the vector space structure (which, as we have seen, implies the principle of superposition), the space $S_1$ has a scalar product defined on it. The first question we must consider is the physical significance of the quantity $(\phi, \psi)$ for $\phi$ and $\psi$ in $S_1$. Note, in this connection, that the state represented by $\phi$ can also be equivalently represented by the projection operator $P_\phi$ for $\phi$. Since $P_\phi$ is a self-adjoint operator belonging to $A_Q$, it is an observable; it tests whether or not the given state is $\phi$. The expectation value of $P_\phi$ in the state $\psi$ is easily seen to be $|\langle \phi, \psi \rangle|^2$; the natural interpretation of this quantity is the probability that, given the system in the state $\psi$, on measurement it is found to be in the state $\phi$ (transition probability from the state $\psi$ to $\phi$ which happens to be equal to that from $\phi$ to $\psi$). The quantity
(\phi, \psi) (the orthogonal component of \psi along \phi) is, therefore, given the name 'transition amplitude from the state \psi to the state \phi'.

Note that, whereas in classical stochastic theory (for example, in the context of Markov processes [42–44]) one only talks about transition probabilities, in QM we have transition amplitudes as well. This feature is, of course, closely related to the principle of superposition.

Transformations on states which leave transition probabilities invariant are traditionally considered as fundamental invariances of the quantum mechanical formalism. According to Wigner's theorem [45–47], an invertible transformation on \( S_1 \) (which, by continuity, can be extended to \( \mathcal{H} \)) mapping a state \( \psi \) to \( \psi' \) such that

\[ |(\phi', \psi')|^2 = |(\phi, \psi)|^2 \]

(37)
can, by appropriate choice of phases in the representation of states (by vectors in \( \mathcal{H} \)) be represented by a unitary or an antiunitary transformation (\( \psi' = U\psi \) where \( U \) is unitary or antiunitary).

Note. If we stick to the convention that only the transformations leaving the fundamental geometrical structure (scalar product or, equivalently, transition amplitudes, in the present case) invariant are to be called fundamental invariances, then only the unitary transformations in the conclusion of the above theorem qualify to be fundamental invariances. These are the analogues of canonical transformations in classical mechanics. The antiunitary ones (which leave the transition probabilities but not the transition amplitudes invariant) also happen to be of considerable importance because, in practice, transition probabilities are more important objects than the phases of transition amplitudes. We shall see in section V that it is the unitary transformations only that qualify as the quantum mechanical canonical transformations defined as invariances of the noncommutative symplectic structure on \( \mathcal{A}_Q \).

IV. GENERALIZED ALGEBRAIC SYMPLECTIC STRUCTURES

In this section we shall construct, employing noncommutative differential geometric techniques, a class of mathematical objects which can accommodate, as a special case, the classical Hamiltonian systems and also provide the proper setting for a satisfactory treatment of quantum symplectics.

First, a few algebraic preliminaries.

A. Algebras and Derivations
By an algebra we shall mean a complex associative algebra with unit element (usually denoted as I) and a *-operation (involution). We shall denote algebras by script letters $\mathcal{A}$, $\mathcal{B}$, ... and elements of an algebra by capital letters $A, B, ...$ The star operation, by definition satisfies the relations

$$(AB)^* = B^*A^* \quad (A^*)^* = A \quad I^* = I$$

(38)

A (\*-\) homomorphism of an algebra $\mathcal{A}$ into $\mathcal{B}$ is a linear mapping $\Phi : \mathcal{A} \rightarrow \mathcal{B}$ which preserves products (and involutions):

$$\Phi(AB) = \Phi(A)\Phi(B) \quad \Phi(A^*) = \Phi(A)^*;$$

(39)

if it is, moreover, bijective, is called a (\*-\) isomorphism.

A derivation of an algebra $\mathcal{A}$ is a linear mapping $X : \mathcal{A} \rightarrow \mathcal{A}$ obeying the Leibnitz rule

$$X(AB) = X(A)B + AX(B).$$

(40)

The set $\text{Der} \mathcal{A}$ of all derivations is a Lie algebra (with commutator as the Lie bracket). The inner derivations $D_A$ of $\mathcal{A}$ defined by

$$D_A B = [A, B]$$

(41)

satisfy the relation

$$[D_A, D_B] = D_{[A,B]}$$

(42)

so that the set $\text{IDer} \mathcal{A}$ of inner derivations of $\mathcal{A}$ is a Lie subalgebra of $\text{Der} \mathcal{A}$.

An algebra isomorphism $\Phi : \mathcal{A} \rightarrow \mathcal{B}$ induces a mapping $\Phi_* : \text{Der} \mathcal{A} \rightarrow \text{Der} \mathcal{B}$ given by

$$(\Phi_* X)(B) = \Phi(X(\Phi^{-1}(B)))$$

(43)

for all $X \in \text{Der} \mathcal{A}$ and $B \in \mathcal{B}$. We have the relations

$$\Phi_* [X, Y] = [\Phi_* X, \Phi_* Y].$$

(45)

B. Generalized Algebraic Differential Forms

The noncommutative generalization of differential geometry is based on the observation that most of the developments relating to differential forms
can proceed in purely algebraic terms [ starting with the commutative algebra $\mathcal{C}^\infty(M)$ ]:

(i) Vector fields can be obtained as derivations of $\mathcal{C}^\infty(M)$.

(ii) Definition of differential forms of various degrees can be given in algebraic terms (by defining their contractions with vector fields).

(iii) Among the two basic operations on differential forms, the exterior product and the exterior derivative, the former is already algebraic; the latter can also be defined algebraically [48]:

\[(d\omega)(X_1, X_2, ..., X_{k+1}) = \sum_{i=1}^{k+1} (-1)^{i+1} X_i \omega(X_1, X_2, ..., X_{i-1}, X_{i+1}, ..., X_{k+1}) + \sum_{i<j} (-1)^{i+j} \omega([X_i, X_j], X_1, X_2, ..., X_{i-1}, X_{i+1}, ..., X_{j-1}, X_{j+1}, ..., X_{k+1})\] (46)

where $\omega$ is a differential $k$-form and the $X$s are vector fields.

In noncommutative geometry (NCG), one replaces the commutative algebra $\mathcal{C}^\infty(M)$ by a general complex associative algebra (not necessarily commutative). The formalism of NCG closest to our needs is the one developed by Dubois-Violette and others [2–4]. In their work, derivations of the basic algebra play a role analogous to that of vector fields in traditional differential geometry. Several developments proceed parallel to the commutative case. In particular, $d\omega$ (for $\omega$ a noncommutative differential $k$-form) is defined by eq (46) where $X$s are now derivations. The formalism developed in the present section is a generalization of that of these authors. The generalization is based on the observation that, in eq (46), the $X$s appear either singly or as commutators. It follows that one can restrict the allowed derivations to a Lie subalgebra $\mathcal{X}$ of $\text{Der}\mathcal{A}$ and develop NCG based on the pair $(\mathcal{A}, \mathcal{X})$; we shall call such a pair an algebraic differential system (ADS). Those ADSs in which $\mathcal{A}$ is noncommutative with a trivial centre and $\mathcal{X} = \text{IDer}\mathcal{A}$ will be called special. They will play a special role in quantum symplectics.

In the construction of tensorial objects on an ADS $(\mathcal{A}, \mathcal{X})$, the algebra $\mathcal{A}$ plays the role of the algebra $\mathcal{C}^\infty(M)$ of smooth functions on a manifold $M$ and $\mathcal{X}$ that of $\mathcal{X}(M)$, the Lie algebra of smooth vector fields on $M$. There is one point of contrast between the two situations: whereas the product $fX$ of a smooth function and a vector field is a vector field, the product $AY$ of an element $A$ of $\mathcal{A}$ and $Y$ of $\text{Der}\mathcal{A}$ is not a derivation of $\mathcal{A}$ (except when $A$ is in the centre of $\mathcal{A}$).

A covariant tensor $T$ of rank $k (=1, 2, ...,)$ on $(\mathcal{A}, \mathcal{X})$ is a $k$-linear mapping of $(\mathcal{X})^k$ into $\mathcal{A}$. The space of such tensors will be denoted as $\mathcal{T}_k(\mathcal{A}, \mathcal{X})$. We
define $T_0(A, X) \equiv A$. The interior product $i_X$ is defined as usual:

$$(i_X T)(X_1, X_2, ..., X_{k-1}) = T(X, X_1, ..., X_{k-1})$$  \hspace{1cm} (47)

for $k \geq 1$ and $i_X T = 0$ for $T \in T_0(A, X)$. We have, of course, $i_X^2 = 0$.

The space $\Omega^k(A, X)$ of differential $k$-forms on $(A, X)$ is, for $k \geq 2$, the subspace of $T_k(A, X)$ consisting of elements $\omega$ satisfying the antisymmetry condition

$$\omega(X_{\sigma(1)}, ..., X_{\sigma(k)}) = \epsilon_\sigma \omega(X_1, ..., X_k)$$  \hspace{1cm} (48)

where $\epsilon_\sigma$ is the parity/signature of the permutation $\sigma$. We have $\Omega^0(A, X) = T_0(A, X)$ and $\Omega^1(A, X) = T_1(A, X)$. In the notation of ref[3], our $\Omega^k(A, X)$ is the same as $C^k(X', A)$.

Exterior product of a $p$-form $\alpha$ and a $q$-form $\beta$ is defined as usual [48] (with vector fields replaced by derivations in $X'$):

$$(\alpha \wedge \beta)(X_1, ..., X_{p+q}) = \frac{1}{p!q!} \sum_{\sigma \in S_{p+q}} \epsilon_\sigma \alpha(X_{\sigma(1)}, ..., X_{\sigma(p)})\beta(X_{\sigma(p+1)}, ..., X_{\sigma(p+q)}).$$  \hspace{1cm} (49)

We have the associativity property

$$(\alpha \wedge \beta) \wedge \gamma = \alpha \wedge (\beta \wedge \gamma)$$  \hspace{1cm} (50)

and the antiderivation property of $i_X$:

$$i_X(\alpha \wedge \beta) = (i_X \alpha) \wedge \beta + (-1)^p \alpha \wedge (i_X \beta)$$  \hspace{1cm} (51)

but, in general, not $\alpha \wedge \beta = (-1)^{pq} \beta \wedge \alpha$. (Recall that the differential forms have now values in $A$ which need not be commutative.)

The exterior derivative $d : \Omega^p(A, X) \to \Omega^{p+1}(A, X)$ is defined, for $p = 0$ by $(dA)(X) = X(A)$ and, for $p \geq 1$, by eq (46) which, for $p = 1$ gives

$$(d\omega)(X, Y) = X(\omega(Y)) - Y(\omega(X)) - \omega([X, Y]).$$  \hspace{1cm} (52)

We have $d^2 = 0$ and the usual antiderivation property for $d$. As usual, we call a differential form $\alpha$ closed closed if $d\alpha = 0$ and exact if $\alpha = d\beta$ for some form $\beta$.

C. Induced Mappings and Lie Derivatives
An isomorphism between two ADSs \((\mathcal{A}, \mathcal{X})\) and \((\mathcal{B}, \mathcal{Y})\) is a \(\ast\)-isomorphism \(\Phi : \mathcal{A} \to \mathcal{B}\) such that the induced mapping \(\Phi_* : \mathcal{X} \to \mathcal{Y}\) is a Lie algebra isomorphism. Such a mapping induces a mapping \(\Phi^* : \mathcal{T}_k(\mathcal{B}, \mathcal{Y}) \to \mathcal{T}_k(\mathcal{A}, \mathcal{X})\):

\[
(\Phi^*T)(X_1, \ldots, X_k) = \Phi^{-1}[T(\Phi_*X_1, \ldots, \Phi_*X_k)].
\]

We have

\[
(\Psi \circ \Phi)^* = \Phi^* \circ \Psi^* \quad (54)
\]

\[
\Phi^*(\alpha \wedge \beta) = (\Phi^*\alpha) \wedge (\Phi^*\beta) \quad (55)
\]

\[
\Phi^*(d\alpha) = d(\Phi^*\alpha). \quad (56)
\]

Now, given an ADS \((\mathcal{A}, \mathcal{X})\), let \(\Phi_t : \mathcal{A} \to \mathcal{A}\) be a one parameter set of transformations (i.e. ADS isomorphisms) given, for small \(t\), by

\[
\Phi_t(A) = A + tg(A) + o(t) \quad (57)
\]

where \(g\) is some mapping of \(\mathcal{A}\) into itself. The condition \(\Phi_t(AB) = \Phi_t(A)\Phi_t(B)\) gives \(g(AB) = g(A)B + Ag(B)\) implying that \(g(A) = Y(A)\) for some derivation \(Y\) of \(\mathcal{A}\); we call \(Y\) the infinitesimal generator of \(\Phi_t\). We restrict ourselves to transformations whose infinitesimal generators are in \(\mathcal{X}\). The induced mappings can now be used to define Lie derivatives of various objects. For \(X \in \mathcal{X}\) and \(T \in \mathcal{T}_k(\mathcal{A}, \mathcal{X})\) we define the Lie derivatives \(L_YX\) and \(L_YT\) by

\[
(\Phi_t)_*X = X + tL_YX + o(t) \quad (58)
\]

\[
(\Phi_t)^*T = T - L_YT + o(t) \quad (59)
\]

( A minus sign appears in the second equation because \((\Phi_t)^*\) is essentially \((\Phi_t^{-1})_*\). Straightforward calculations give

\[
L_YX = [Y, X] \quad (60)
\]

\[
(L_YT)(X_1, \ldots, X_k) = Y[T(X_1, \ldots X_k)] - \sum_{i=1}^{k} T(X_1, \ldots, X_{i-1}, [Y, X_i], X_{i+1}, \ldots, X_k). \quad (61)
\]

The Lie derivative has the usual properties

\[
[L_X, L_Y] = L_{[X,Y]} \quad (62)
\]

\[
[L_X, i_Y] = i_{[X,Y]} \quad (63)
\]

\[
L_Y = i_Y \circ d + d \circ i_Y \quad (64)
\]

\[
L_Y \circ d = d \circ L_Y \quad (65)
\]

\[
L_Y(\alpha \wedge \beta) = (L_Y\alpha) \wedge \beta + \alpha \wedge (L_Y\beta). \quad (66)
\]
An object (whose Lie derivatives are defined) is said to be invariant if its Lie derivatives with respect to all derivations in $\mathcal{X}$ vanish.

D. Generalized Algebraic Symplectic Structures

We shall now consider noncommutative generalization of classical symplectic geometry (a quick summary of which appears in the appendix; the reader is advised to have a quick look at it before proceeding further). As we shall see, the main developments will be parallel to those in the classical case.

A 2-form $\omega$ on an ADS $(\mathcal{A}, \mathcal{X})$ is a symplectic form if it is (i) closed and (ii) nondegenerate in the sense [3] that, for every $A \in \mathcal{A}$, there exists a unique derivation $Y_A$ in $\mathcal{X}$ such that
\[ i_{Y_A} \omega = -dA. \tag{67} \]

Such a form will be taken to define a symplectic structure on $(\mathcal{A}, \mathcal{X})$ and the triple $(\mathcal{A}, \mathcal{X}, \omega)$ will be called a generalized algebraic symplectic system (GASS).

A symplectic mapping from a GASS $(\mathcal{A}, \mathcal{X}, \alpha)$ to $(\mathcal{B}, \mathcal{Y}, \beta)$ is a mapping $\Phi : \mathcal{A} \to \mathcal{B}$ such that (i) it is an ADS isomorphism between $(\mathcal{A}, \mathcal{X})$ and $(\mathcal{B}, \mathcal{Y})$ and (ii) $\Phi^* \beta = \alpha$. A symplectic mapping from a GASS onto itself will be called a canonical/symplectic transformation. The symplectic form and all its exterior powers are invariant under canonical transformations.

If $\Phi_t$ is a one-parameter family of canonical transformations generated by $X \in \mathcal{X}$, then the condition $\Phi_t^* \omega = \omega$ implies $L_X \omega = 0$ which, along with equations (64) and $d\omega = 0$ gives
\[ d(i_X \omega) = 0. \tag{68} \]

A derivation $X$ satisfying eq(68) will be called locally Hamiltonian. The subclass of such derivations for which $i_X \omega$ is exact will be called (globally) Hamiltonian. The Hamiltonian derivation $Y_A$ corresponding to $A \in \mathcal{A}$ is given by eq (67) [see eq (A.3)].

Give two locally Hamiltonian derivations $X$ and $Y$, we have
\[
\begin{align*}
  i_{[X,Y]} \omega &= (L_X \circ i_Y - i_Y \circ L_X) \omega = (i_X \circ d + d \circ i_X)(i_Y \omega) \\
  &= d(i_X i_Y \omega) = d[\omega(Y, X)] \tag{69}
\end{align*}
\]

which shows that the commutator of two locally hamiltonian derivations is a Hamiltonian derivation.
The Poisson bracket (PB) of \( A, B \in \mathcal{A} \) denoted as \( \{ A, B \} \) is defined as
\[
\{ A, B \} = \omega(Y_A, Y_B) = Y_A(B) = -Y_B(A). \tag{70}
\]
It has the usual properties of a PB: antisymmetry, bilinearity (obvious), Leibnitz rule:
\[
\{ A, BC \} = Y_A(BC) = [Y_A(B)]C + B[Y_A(C)] = \{ A, B \}C + B\{ A, C \} \tag{71}
\]
and Jacobi identity:
\[
0 = \frac{1}{2}d\omega(Y_A, Y_B, Y_C) = \{ A, \{ B, C \} \} + \text{cyclic terms} \tag{72}
\]
where eqs (46) and (70) have been used. We also have [recalling eq (69)]
\[
i_{[Y_A, Y_B]}\omega = d[\omega(Y_B, Y_A)] = -d(\{ A, B \}) \tag{73}
\]
which gives [recalling eq (67)]
\[
[Y_A, Y_B] = Y_{\{ A, B \}} \tag{74}
\]
showing that the mapping \( A \mapsto Y_A \) is a Lie algebra homomorphism.

An element \( A \in \mathcal{A} \) can act, via \( Y_A \), as the infinitesimal generator of a one-parameter family of canonical transformations. The change in \( B \in \mathcal{A} \) due to such an infinitesimal transformation is [see eq (57)]
\[
\delta B = tY_A(B) = t\{ A, B \}. \tag{75}
\]
In particular, if \( \delta B = tI \) (infinitesimal ‘translation’ in \( B \)), we have
\[
\{ A, B \} = I \tag{76}
\]
which is the analogue of the classical PB relation \( \{ p, q \}_c = 1 \).

E. Canonical Symplectic Structure on a Special ADS [10]

On a special ADS \((\mathcal{A}, IDer\mathcal{A})\) we can define a differential 2-form \( \omega_c \) (to be called the canonical 2-form) by
\[
\omega_c(D_A, D_B) = [A, B]. \tag{77}
\]
It is easily verified that \( \omega_c \) is closed. Moreover, for any \( A \in \mathcal{A} \), the equation
\[
\omega_c(Y_A, D_B) = -(dA)(D_B) = -D_B(A) = [A, B] \tag{78}
\]
has the unique solution $Y_A = D_A$. The form $\omega_c$ is easily seen to be invariant (i.e. $L_X\omega_c = 0$ for all $X \in IDerA$). The symplectic structure defined above will be called the canonical symplectic structure on the special ADS $(A, IDerA)$. The PB is now a commutator:

$$\{A, B\} = Y_A(B) = D_A(B) = [A, B].$$

(79)

The invariant symplectic structure on the algebra $M_n(C)$ of complex $n \times n$ matrices obtained in ref [2] is a special case of the canonical symplectic structure on special ADSs described above.

If, in this special ADS, instead of $\omega_c$, we take $\omega = \beta \omega_c$ as the symplectic form (where $\beta$ is a nonzero complex number), we have

$$Y_A = \beta^{-1}D_A \quad \quad \quad \{A, B\} = \beta^{-1}[A, B].$$

(80)

We shall make use of such a symplectic structure in the treatment of quantum symplectics in the next section.

F. Dynamical Systems in Algebraic Setting; Generalized Algebraic Hamiltonian Systems

In the algebraic treatment of dynamical systems [49–51], the basic object for any system S is taken to be an algebra $A$. It is often taken to be a $C^*$ algebra; we shall, however, not put that restriction. Observables of S are self adjoint elements of $A$ and states are an appropriate class of linear functionals on $A$ (details of this are not relevant at this stage). Dynamics is generally defined by a one-parameter family of $^*$- automorphisms $\Phi_t : A \rightarrow A$. Let $X$ be the infinitesimal generator of this family and $A(t) = \Phi_t(A)$. The resulting time evolution is governed by the equation

$$\frac{dA(t)}{dt} =XA(t).$$

(81)

This description of dynamics is quite general and covers almost all known forms of dynamics (with continuous time parameter). For example, the dynamics of a general deterministic system (whose state space is assumed to be a differentiable n-manifold M) is given by the equation defining the integral curves of a vector field $X$ in $M$:

$$\frac{dx^i(t)}{dt} = X_i(x(t)) \quad i = 1, 2, ..., n$$

(82)
with some initial conditions $x^i(0) = x_0^i$. [Eq (1), for example, is a special case of eq (82) with $n = 6$.] Now, for any smooth function $f$ on $M$, we have

$$\frac{d}{dt} [f(x(t))] = \frac{dx^i}{dt} \frac{\partial f}{\partial x^i} = (X^i \partial_i f)(x(t)) = (Xf)(x(t)).$$

Let $x(0) = x$ and $f(x(t)) = F(x,t) = F(t)(x)$. Note that $F(t)$, for each value of $t$, is an element of the algebra $C^\infty(M)$. The preceding equation can now be written as

$$\frac{dF(t)}{dt}(x) = [XF(t)](x) \Leftrightarrow \frac{dF(t)}{dt} = XF(t) \tag{83}$$

which is of the same form as eq (81) with $A = C^\infty(M)$.

The most important subclass of deterministic systems is that of Hamiltonian systems in which the underlying state space is a symplectic manifold $(M, \omega)$ and the vector field $X$ of eqs (82, 83) is the Hamiltonian vector field (see appendix) $X_H$ corresponding to the Hamiltonian $H$ of the system. Formally, the triple $(M, \omega, H)$ is called a Hamiltonian system. The equation of motion in such a system takes the form

$$\frac{dF(t)}{dt} = X_H F(t) = \{H, F(t)\}_c \tag{84}$$

where $\{,\}_c$ is the classical Poisson bracket (see appendix).

For our purposes it is useful to introduce the concept of a generalized algebraic Hamiltonian system (GAHS). We define it to be a quadruple $(\mathcal{A}, \mathcal{X}, \omega, H)$ whee $(\mathcal{A}, \mathcal{X}, \omega)$ is a GASS and $H$ a self-adjoint element of $\mathcal{A}$ ($H^* = H$; the Hamiltonian). The dynamics of such a system is given by eq (81) with $X = Y_H$:

$$\frac{dA(t)}{dt} = Y_H A(t) = \{H, A(t)\}. \tag{85}$$

A classical Hamiltonian system $(M, \omega, H)$ is easily seen to be the GAHS $(\mathcal{A}, \mathcal{X}, \omega, H)$ with $\mathcal{A} = C^\infty(M)$, and $\mathcal{X}$ the family of Hamiltonian vector fields on $M$. We shall describe, in the next section, quantum dynamics in the framework of a GAHS.

In section VI we shall need the concept of an isomorphism of GAHSs. Two GAHSs $(\mathcal{A}, \mathcal{X}, \omega, H)$ and $(\mathcal{B}, \mathcal{Y}, \zeta, K)$ are isomorphic if there exists a symplectic mapping $\Phi : (\mathcal{A}, \mathcal{X}, \omega) \rightarrow (\mathcal{B}, \mathcal{Y}, \zeta)$ which preserves the Hamiltonians (i.e. $\Phi^* K = H$).
V. QUANTUM MECHANICS OF A PARTICLE

Having assembled the necessary apparatus, we shall now do quantum symplectics by applying some results obtained in the previous section to the algebra \( \mathcal{A}_Q \) constructed in section III. The task of the essential geometrical study of the two spaces \( S_1 \) and \( \mathcal{A}_Q \) thus completed, we shall proceed to present the promised development of the quantum kinematics and dynamics of a particle. Galilean invariance plays an important role in this enterprise. We shall briefly review the essential developments relating to the projective representations of the Galilean group. Its kinematical subgroup, the Euclidean group, plays an essential role in the identification of the fundamental observables. The two pictures of quantum dynamics – the Schrödinger picture and the Heisenberg picture – naturally emerge, the latter being a special case of a GAHS.

A. The Quantum Symplectic Form

As mentioned earlier, we shall eventually take \( \mathcal{A}_Q \) to be the \(*\)-algebra generated by the fundamental observables (to be defined later in this section) ensuring thereby that it has a trivial center. Assuming this property, we can now make use of the (modified) canonical symplectic structure on a special ADS. We take our GASS to be \((\mathcal{A}_Q, \mathcal{X}_Q, \omega_Q)\) where \( \mathcal{X}_Q = IDer.\mathcal{A}_Q \) and \( \omega_Q = \beta \omega_c \) [where \( \omega_c \) is the canonical symplectic form on the special ADS \((\mathcal{A}_Q, \mathcal{X}_Q)\) and \( \beta \) is a nonzero complex number.] We shall call \( \omega_Q \) the quantum symplectic form. Note that, the form \( \omega_c \) being dimensionless, \( \omega_Q \) has the dimension of the constant \( \beta \). The quantum Poisson brackets are [see eq (80)]

\[
\{A, B\}_Q = \beta^{-1}[A, B].
\] (86)

We shall take \( \beta = -ih \). (This is the only place where we shall put the Planck constant ‘by hand’; its conventional appearance at various places will be automatic.) This choice gives \( \omega_Q \) the dimension of action (the same as that of the classical symplectic form \( dp \wedge dq \)) and makes the quantum PBs the famous Dirac PBs [7, 41].

A canonical transformation for this GASS (to be referred to later as a quantum canonical transformation) is a mapping \( \Phi : \mathcal{A}_Q \rightarrow \mathcal{A}_Q \) which is an isomorphism of the ADS \((\mathcal{A}_Q, \mathcal{X}_Q)\) satisfying the condition \( \Phi^* \omega_Q = \omega_Q \). Now

\[
(\Phi^* \omega_Q)(X_1, X_2) = \Phi^{-1}[\omega_Q(\Phi X_1, \Phi X_2)].
\] (87)
We need to consider only inner derivations. For $X = D_A$ eq (43) gives
\[ \Phi_* D_A = D_{\Phi(A)}. \] (88)

With $X_1 = D_A$ and $X_2 = D_B$ eq (87) now gives
\[ \Phi(\beta[A, B]) = \beta[\Phi(A), \Phi(B)] \text{ for all } A, B \text{ in } \mathcal{A}_Q. \] (89)

From the invariance property of the canonical symplectic form discussed in section IV E we can conclude that all 1-paramter *-automorphisms of $\mathcal{A}_Q$ generated by the inner derivations of $\mathcal{A}_Q$ are canonical transformations. [This is consistent with eq (89).]

We shall next examine as to what extent the Wigner symmetries correspond to quantum canonical transformations. A Wigner transformation on states given by $\psi \rightarrow \psi' = U\psi$ (with $U$ unitary or antiunitary ) induces a transformation on $\mathcal{A}_Q$ given by
\[ (\psi', A\psi') = (\psi, A'\psi) \Rightarrow A' = U^{-1}AU. \] (90)

With $\Phi(A) = A'$ of eq (90), eq (89) gives
\[ U[\beta[U^{-1}AU, U^{-1}BU]]U^{-1} = \beta[A, B] \] (91)
which is satisfied for general $\beta$ for unitary $U$ but for only real $\beta$ for antiunitary $U$. Since $\beta$ is, in fact, imaginary, it follows that only unitary Wigner symmetries correspond to genuine quantum canonical transformations. (This is a familiar situation in quantum mechanics; the antiunitary transformations do not preserve the canonical commutation relations. See, for example, [52], p.641. )

Under an infinitesimal unitary transformation $U = I + i\epsilon G$ where $G$ is a self-adjoint operator (belonging to $\mathcal{A}_Q$) we have, for the infinitesimal change in an element $A$ of $\mathcal{A}_Q$
\[ \delta A = -i\epsilon[G, A] = \epsilon\{T, A\} \] (92)
where $T = -i\beta G = -\hbar G$. In physical applications where $G$ and $T$ generally correspond to observables, it is generally preferable to work with the operator $T$ which has the 'right' dimension. Accordingly, we shall generally write, for an infinitesimal transformation
\[ U = I - \frac{i}{\hbar}\epsilon T. \] (93)
B. The Galilean Group

(No new result is obtained in this subsection. The contribution of the author is in collecting the right material and putting it in proper context; it serves to make the presentation reasonably self-contained.)

An important demand on the formalism being evolved is that it must obey the principle of Galilean relativity; this means that the group of (proper) Galilean transformations must be implemented unitarily. This, as we shall see, has important implications for both the kinematics and dynamics of quantum systems.

The Galilean transformations map the space-time point \((x,t)\) to \((x',t')\) given by (in matrix notation)

\[
x' = Rx + vt + a \quad t' = t + b
\]

where \(R\) is an SO(3) matrix, \(v\) and \(a\) are vectors and \(b\) a real number. These transformations constitute a connected 10-parameter Lie group \(G\). Since quantum mechanical wave functions are arbitrary up to constant phases, the unitary representatives \(U(g)\) [where \(g = (R,v,a,b)\)] are expected to constitute array/projective representation of \(G\):

\[
U(g_1)U(g_2) = \omega(g_1, g_2)U(g_1g_2)
\]

where \(\omega\) is a phase factor of modulus one. In this subsection, we briefly consider these projective representations [49, 50] in a general separable Hilbert space.

For an infinitesimal transformation with parameters \(\epsilon^\alpha (\alpha = 1, ..., 10)\), we have \(U(\epsilon) = I + i\epsilon^\alpha T_\alpha\). In a genuine group representation (i.e. when \(\omega = 1\) in eq (95)) we have

\[
[T_\alpha, T_\beta] = if_{\alpha\beta}^\gamma T_\gamma
\]

where \(f_{\alpha\beta}^\gamma\) are the structure constants of \(G\). In a projective representation, the preceding equation must be generalized to

\[
[T_\alpha, T_\beta] = if_{\alpha\beta}^\gamma T_\gamma + c_{\alpha\beta} I
\]

where \(c_{\alpha\beta}\) are complex constants.

The operators \(U(g)\) are defined modulo multiplicative phase factors which means that one has the freedom to redefine the generators:

\[
T_\alpha \rightarrow T'_\alpha = T_\alpha + b_\alpha I
\]
where $b_{\alpha}$ are real parameters. Using this freedom, the generators $J_k$ (rotations), $P_k$ (space translations), $H$ (time translations) and $G_k$ (Galilean boosts) can be shown to satisfy the commutation relations [51][recall eq (93)]

\[
\begin{align*}
[J_j, J_k] &= i\hbar \epsilon_{jkl} J_l \\
[P_j, P_k] &= 0 \\
[J_j, P_k] &= i\hbar \epsilon_{jkl} P_l \\
[G_j, G_k] &= 0 \\
[J_j, G_k] &= i\hbar \epsilon_{jkl} G_l \\
[P_j, G_k] &= i\hbar m \delta_{jk} I \\
[H, P_k] &= 0 \\
[H, J_k] &= 0 \\
[H, G_k] &= i\hbar P_k
\end{align*}
\]

where $m$ is a real parameter. For $m = 0$, we have a usual vector representation of $G$. The equations above show that the ray representations of the Galilean group are characterized by a real parameter $m$. In physical applications, this parameter is expected to correspond to a Galilean invariant intrinsic property of the system. For a particle, as we shall see below, $m$ is the traditional (Newtonian) mass.

C. The Fundamental Observables

We next consider the fundamental observables (FOs) in the quantum theoretic description of a particle. The most fundamental observables are those related to measurement of position. Recall that $|\psi(x)|^2$ has the interpretation of probability density for position (we have suppressed the time variable). The mean value $\int x_j |\psi(x)|^2 dx$ of the $j$th component of position must be interpreted as the expectation value, in the state $\psi$, of an observable represented by a self adjoint operator $X_j$:

\[
(\psi, X_j \psi) = \int x_j |\psi(x)|^2 dx
\]

which suggests the following definition of the operator $X_j$:

\[
(X_j \psi)(x) = x_j \psi(x) \quad j = 1, 2, 3.
\]

To determine the other FOs we note from eq (93) that observables are in bijective correspondence with (generators of) infinitesimal one-parameter
transformations on the states. The FOs must be determined in such a manner that, together, they serve to define the most general 'kinematically permissible' change of state at a fixed time. What does 'kinematically permissible' mean? For this we must take guidance from the operative principle of relativity which, in the present situation, is Galilean relativity. As we have seen, a wave function belongs to a projective representation of the Galilean group G. For the quantum mechanical description of a particle, this representation must be irreducible. (This is because, in a reducible representation, the states can be divided into more than one Galilean invariant subsets which is not acceptable for an 'elementary system' like a particle [52].) Now, among the various Galilean transformations, time translations relate to dynamics (change of state with time) and the boosts also relate to transformations involving time. The true 'kinematical subgroup' of G is the Euclidean group whose commutation relations appear in eqs (99–107). The remaining FOs must be (provisionally; see below) the infinitesimal generators $P_k$ and $J_k$; we shall call them the momentum and the angular momentum operators.

To determine the operators $P_j$, we consider the transformation law of the wave functions under infinitesimal space translations $x \rightarrow x' = x + \epsilon$. The standard choice for the transformation law

$$\psi'(x') = \psi(x) \Leftrightarrow \psi'(x) = \psi(x - \epsilon)$$

(110)

gives

$$\delta \psi = -\epsilon_j \frac{\partial \psi}{\partial x_j} = -\frac{i}{\hbar} \epsilon_j P_j \psi(x)$$

(111)

implying

$$P_j = -i\hbar \frac{\partial}{\partial x_j}.$$  

(112)

Eqs (109) and (112) give the canonical commutation relations

$$[X_j, P_k] = i\hbar \delta_{jk} I.$$  

(113)

It is worth emphasizing that eq (113) (in fact, all equations in this section) must be understood as operator equations in the subspace $\mathcal{S}_1$ of the quantum mechanical Hilbert space $\mathcal{H} = L^2(R^3)$. 

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Now, the orbital angular momentum operators

\[ L_j = \epsilon_{jkl} X_k P_l \]  \hspace{1cm} (114)

satisfy the commutation relations (99) and (101). Defining \( S_k = J_k - L_k \) (operators representing intrinsic angular momentum or spin), we have

\[
[S_j, L_k] = 0 \hspace{1cm} (115)
\]

\[
[S_j, S_k] = i\hbar \epsilon_{jkl} S_l. \hspace{1cm} (116)
\]

We, therefore, conclude that the fundamental observables in the quantum mechanical description of a particle are \( X_j, P_j \) and \( S_j \) (\( j = 1, 2, 3 \)). For a spinless particle we have \( S_j = 0 \) and the fundamental observables are \( X_j \) and \( P_j \) only.

We now assume that the algebra \( \mathcal{A}_Q \) is the \( * \)-algebra generated by the fundamental observables identified above subject to the commutation relations (100), (113), (116) and the relations

\[
[X_j, S_k] = 0 = [P_j, S_k]. \hspace{1cm} (117)
\]

Any operator in \( \mathcal{A}_Q \) commuting with the generators must be a multiple of the identity; the algebra \( \mathcal{A}_Q \), therefore, has a trivial center.

D. Quantum Dynamics

Dynamics involves the change of states/observables with time. The developments in the subsection B involving the time translation generator \( H \) (the Hamiltonian operator) are relevant for dynamics. A close look at eq (90) shows that one can apply a transformation to states leaving operators unchanged or apply it to operators leaving states unchanged; the two options are equivalent in a certain sense which the equation makes clear. (A unitary transformation applied to both states and operators is essentially a change of basis and can have no physical implications.) There are, accordingly, two standard descriptions of dynamics in QM: one (the Schrödinger picture) includes time dependence in states and the fundamental operators \( X_j, P_j, S_j \) (and, therefore, any function of these not involving any explicit time dependence) remain time independent; the second (the Heisenberg picture) puts time dependence in operators and the state vectors remain time independent. The two descriptions are related through eq (90) where \( U \) is now the time evolution operator obtained below [see eq (119)].
In the Schrödinger picture, we have, under an infinitesimal time translation \( t \to t' = t + \delta t \) [recall eq (93)]

\[
\delta \psi(x,t) = \frac{\partial \psi}{\partial t} \delta t = -\frac{i}{\hbar} H \psi(x,t)
\]

which gives the Schrödinger equation (in the general form)

\[
i\hbar \frac{\partial \psi}{\partial t} = H \psi.
\] (118)

When \( H \) is independent of time, we can write [notation: \( \psi(x,t) = \langle x | \Psi(t) \rangle \)]

\[
\Psi(t) = U(t,t_0) \Psi(t_0) \quad U(t,t_0) = e^{-iH(t-t_0)/\hbar}
\] (119)

In the Heisenberg picture, we have under an infinitesimal time translation

\[
\delta A(t) = -i\frac{\delta t}{\hbar} [H, A(t)]
\] (120)

which gives the Heisenberg equation of motion

\[
\frac{dA(t)}{dt} = (-i\hbar)^{-1} [H, A(t)] = \{H, A(t)\}_Q.
\] (121)

Note that eq (121) is of the form of eq (85); we have here the GAHS \((A_Q, X_Q, \omega_Q, H)\).

E. The Hamiltonian Operator

The Schrödinger equation (118) or the Heisenberg equation (121) give a concrete description of dynamics only when the expression for the Hamiltonian operator \( H \) in terms of the fundamental operators is given. We first consider the case of a free spinless particle. A free particle must be seen as a free particle by all Galilean observers; its dynamics, therefore, has full-fledged Galilean invariance and all the commutation relations (99–107) must be operative. According to eq (104) a particle is characterized by a Galilean invariant parameter \( m \) which, as we shall see presently, is the traditional mass parameter. The fundamental observables are \( X_j \) and \( P_j \). To determine \( H \), we shall use the commutators involving \( H \) [eqs (105–107)]. Eq (107) is useful only if \( G_k \)'s are explicitly known; we shall, therefore determine \( G_k \) first.
Under an infinitesimal Galilean transformation, we have
\[ \delta X_j = \delta v_k \{ G_k, X_j \} = \frac{i}{\hbar} \delta v_k [G_k, X_j]. \]
This, with \( \delta X_j = (\delta v_j)tI \) [hint: \( \delta(\psi, X_j \psi) = (\psi, \delta X_j \psi) = \delta v_j t, \) etc.] gives
\[ [G_k, X_j] = -i\hbar \delta_{jk} tI. \tag{122} \]
This gives
\[ G_k = P_k t + G'_k \text{ with } [G'_k, X_j] = 0. \tag{123} \]
Eqs (123) and (104) give
\[ G_k = P_k t - mX_k + G''_k \tag{124} \]
where the last term commutes with both \( X_j \) and \( P_k \) and, therefore, must be a multiple of the identity operator. Eq (107) now gives
\[ [H, X_k] = -\frac{i\hbar}{m} P_k \tag{125} \]
which implies
\[ H = \frac{|\vec{P}|^2}{2m} + H' \text{ with } [H', X_k] = 0. \tag{126} \]
Eqs (126) and (105) imply \([H', P_k] = 0; H', \) therefore, must be a multiple of the identity operator. This term, being inconsequential for dynamics, can be dropped giving the free particle Hamiltonian
\[ H_0 = \frac{|\vec{P}|^2}{2m} \tag{127} \]
which has the same form as the free particle Hamiltonian in classical mechanics. Notice that \( m \) is, indeed, the mass parameter.

To describe the dynamics of a particle under some given forces, we generally employ, for convenience, a definite reference frame. For example, the expression for a central force takes a simple form in a frame in which the center of force is at the origin. With the choice of frames so restricted, one cannot invoke full Galilean invariance. In particular, eq (105) is no longer
operative and we are back to eq (126). With $[H', X_k] = 0$, we can write $H' = V(X)$ giving finally

$$H = \frac{\hat{P}^2}{2m} + V(X). \quad (128)$$

From this point on, the development of QM along the traditional lines can proceed.

VI. QUANTUM-CLASSICAL CORRESPONDENCE

Quantum-classical correspondence has several aspects some of which continue to be investigated. A comprehensive work which reports on some detailed features of quantum-classical correspondence employing some techniques of noncommutative geometry is ref [53] which contains detailed references. As stated in the introduction, we shall be concerned with showing how, in the $\hbar \to 0$ limit, one recovers classical mechanics in some of its aspects (especially its Hamiltonian structure) from QM.

First we recall a slightly refined version of the well-known argument [25, 28] leading from the real and imaginary parts of the Schrödinger equation (118) with $H$ of eq (128) (after the substitution $\psi = \sqrt{\rho} \exp [iS/\hbar]$), in the limit $\hbar \to 0$, the equations (18) and (11) of the probabilistic version of Hamilton-Jacobi theory. The refinement consists in noting that, in the above-mentioned substitution, the quantities $\rho$ and $S$ will have, in general some $\hbar$ dependence. Accordingly, we make the substitution (31) (with $\lambda = 1/\hbar$) in the Schrödinger equation and take its real and imaginary parts; we get the two equations:

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot (\hat{\rho} \hat{v}) = 0 \quad \text{where} \quad \hat{v} = m^{-1} \nabla \hat{S} \quad (129)$$

$$\frac{\partial \hat{S}}{\partial t} + \frac{(\nabla \hat{S})^2}{2m} + V - \frac{\hbar^2}{2m} \frac{\Delta (\sqrt{\rho})}{\sqrt{\rho}} = 0 \quad (130)$$

where $\Delta$ is the Laplace operator. When, in the limit $\hbar \to 0$, the functions $\hat{\rho}$ and $\hat{S}$ have well defined limits (say, the functions $\rho$ and $S$), eqs (129) and (130) give, in this limit, eqs (18) and (11) of the Hamilton-Jacobi theory.

Our main concern, however, will be to recover classical symplectics from quantum symplectics in the limit of vanishing Planck constant. Our strategy will be to start with the quantum GAHS treated in the previous section,
transform it to an isomorphic GAHS involving phase space functions and
\(\ast\)-products (Weyl-Wigner-Moyal formalism [54–56]) and show that the sub-
system of this latter GAHS which go to smooth functions in the \(\hbar \to 0\) limit
produce the classical GAHS in the limit. For simplicity (and continuity with
the previous section ), we restrict ourselves to the case of a particle although
the results obtained admit trivial generalization to systems with phase space
\(\mathbb{R}^{2n}\).

Recall that, in the case at hand, we have \(\mathcal{H} = L^2(\mathbb{R}^3)\), the fundamental
observables are \(X_j, P_j\), which generate the \(\ast\)-algebra \(A_Q\). The space \(\mathcal{S}_1\) of
physically admissible wave functions consists of the largest common dense
domain which is mapped into itself by the fundamental observables ( and,
therefore, by the elements of \(A_Q\)); it contains, as a dense subspace, the space
\(\Omega = C_0^\infty(\mathbb{R}^3)\) of infinitely differentiable functions with compact support. We
have the quantum GAHS \((A_Q, X_Q, \omega_Q, H)\) with \(H\) of eq (128).

Any \(\psi \in \mathcal{S}_1\) can be approximated as closely as we wish by an element of
\(\Omega\). For \(A \in A_Q\) and \(\psi \in \Omega\) we have
\[
(A\psi)(x) = \int K_A(x, y)\psi(y)dy. \tag{131}
\]

To the operator \(A\) corresponds the Wigner function \(A_W\) on the phase space
\(\mathbb{R}^6\) given by
\[
A_W(x, p) = \int K_A(x + \frac{b}{2}, x - \frac{b}{2})e^{-ip.b/\hbar}db. \tag{132}
\]

In terms of the Fourier transform \(\tilde{A}_W\) of \(A_W\) defined by
\[
A_W(x, p) = \int \tilde{A}_W(r, s)e^{i(r.p+s.x)}drds \tag{133}
\]
the operator \(A\) can be written as
\[
A(X, P) = \int \tilde{A}_W(r, s)e^{i(r.P+s.X)}drds. \tag{134}
\]

There is a bijective correspondence \(A \leftrightarrow A_W\).

Introducing, in \(\mathbb{R}^6\), the notations \(\xi = (x, p)\) and \(\sigma(\xi, \xi') = p.x' - x.p'\) (symplectic form in \(\mathbb{R}^6\)), we have, for \(A, B \in A_Q\)
\[
(AB)_W(\xi) = (2\pi)^{-6} \int \exp[-i\sigma(\xi-\eta, \tau)]A_W(\eta+\frac{\hbar\tau}{4})B_W(\eta-\frac{\hbar\tau}{4}) \equiv (A_W \ast B_W)(\xi). \tag{135}
\]
The product $\star$ of eq (135) is the $\star$-product of Bayen et al [57] and the twisted product of Liu [58].

Simple reasoning based on eqs (131),(133) and (134) shows [58] that the functions $A_W(\xi)$ belong to the space $O_M(R^6)$ (the space of infinitely differentiable functions which, along with their derivatives, when multiplied by any Schwartz function, give functions bounded all over $R^6$). These functions are known [58] to form a complex noncommutative algebra with the star product as product. Calling this algebra (i.e. the algebra of Wigner functions of operators in $A_Q$ with the star product as product) $A_W$, we have a GAHS $(A_W, X_W, \omega_W, H_W)$ where the first two entries represent the special ADS based on $A_W$ and $\omega_W = -i\hbar \omega_c$. This GAHS is isomorphic to the initial quantum GAHS. (This is because the correspondence $A \leftrightarrow A_W$ is a $\star$-algebra isomorphism; the rest is automatic.) Under this isomorphism of GAHSs the quantum mechanical PB (86) is mapped to the Moyal bracket [56]

$$\{A_W, B_W\}_M \equiv (-i\hbar)^{-1}(A_W \star B_W - B_W \star A_W). \quad (136)$$

For functions $f,g$ in $A_W$ having no $\hbar$-dependence, we have, from eq (135)

$$f \star g = fg - (i\hbar/2)\{f, g\}_{cl} + O(\hbar^2). \quad (137)$$

The functions $A_W(\xi)$ will have, in general, some $\hbar$ dependence and the $\hbar \to 0$ limit may be singular for some of them [59]. We denote by $(A_W)_{reg}$ the subclass of functions in $A_W$ whose $\hbar \to 0$ limits exist and are smooth (i.e. $C^\infty$) functions; it is easily seen to be a subalgebra of $A_W$. Now, if $A_W \to A_{cl}$ and $B_W \to B_{cl}$ as $\hbar \to 0$ then $A_W \star B_W \to A_{cl}B_{cl}$; the subalgebra $(A_W)$, therefore, goes over, in the $\hbar \to 0$ limit, to the commutative algebra $C^\infty(R^6)$ with pointwise product as multiplication. The Moyal bracket of eq (136) goes over to the classical PB $\{A_{cl}, B_{cl}\}_{cl}$. Assuming that $H_W \in (A_W)_{reg}$, the subsystem $(A_W, X_W, \omega_W, H_W)_{reg}$ goes over to the classical GAHS $(A_{cl}, X_{cl}, \omega_{cl}, H_{cl})$ where $A_{cl} = C^\infty(R^6)$.

VII. CONCLUDING REMARKS

1. The somewhat trivial looking generalization of admitting Lie subalgebras of Der$A$ in the development NCG along the lines of ref [2–4] was quite crucial in evolving a formalism in which both classical and quantum symplectics could be described as special cases of a single mathematical object :GAHS and the quantum to classical transition could be seen transparently.
2. After having arrived at the conclusion in section III that Schrödinger wave functions are the appropriate objects for a unified description of probability and dynamics, one could have taken a different route than the one followed here and go to, for example path integrals [35]. However, evolving an autonomous formalism for QM in the path integral framework is a bird of different feather than obtaining a path integral representation of the general solution of the Schrödinger equation (which is already quite challenging). The challenge of the former bird is, in the author’s opinion, worth accepting and it promises to be quite rewarding.

APPENDIX: SYMPLECTIC MANIFOLDS

We shall follow the notational conventions of Woodhouse [60]. Other useful references are [61–63].

A symplectic manifold is a pair \((M, \omega)\) where \(M\) is a smooth manifold (we shall be concerned with finite dimensional manifolds only) and \(\omega\) is a differential 2-form (defined everywhere on \(M\)) which is (i) closed (i.e. \(d\omega = 0\)) and (ii) nondegenerate in the sense that, at each point \(u \in M\), the mapping \(T_u(M) \to T_u^*(M)\) given by \(X(u) \mapsto (i_X \omega)(u)\) (or \(X^a \mapsto X^b \omega_{ba}\)) where \(X\) is a smooth vector field, is an isomorphism (of vector spaces). The second requirement implies that the matrix \((\omega_{ij})\) must be nonsingular. The dimension of \(M\) must clearly be even, say, \(2n\).

Locally, the symplectic form \(\omega\) can be expressed in terms of canonical coordinates \((q^i, p_i)\) in the form

\[
\omega = \sum_{i=1}^{n} dp_i \wedge dq^i. \tag{A1}
\]

Given two symplectic manifolds \((M, \omega)\) and \((M', \omega')\), a mapping \(\Phi : M \to M'\) is called symplectic if it is a diffeomorphism and preserves the symplectic form (i.e. \(\Phi^* \omega' = \omega\)); if the two symplectic manifolds are the same, then \(\Phi\) is called a canonical transformation.

If \(\Phi_t\) is a one-parameter family of canonical transformations generated by a smooth vector field \(X\), then the condition \(\Phi_t^* \omega = \omega\) implies \(L_X \omega = 0\) which, with \(L_X = i_X \circ d + d \circ i_X\) and \(d \omega = 0\) implies

\[
d(i_X \omega) = 0. \tag{A2}
\]
A vector field satisfying the condition (A2) is called locally Hamiltonian. The subclass of such vector fields for which $i_{X}\omega$ is exact are called (globally) Hamiltonian. Writing this exact form as $-df$, we have a bijective correspondence between smooth functions (arbitrary up to additive constants) and Hamiltonian vector fields given by (denoting the Hamiltonian vector field corresponding to the smooth function $f$ by $X_f$)

$$i_{X_f}\omega = -df. \quad (A3)$$

The Poisson bracket (PB) of two smooth functions $f$ and $g$ on $M$ is defined as

$$\{f, g\}_cl = \omega(X_f, X_g) = X_f(g) = -X_g(f). \quad (A4)$$

In local coordinates it is given by

$$\{f, g\}_cl = \sum_{i=1}^{n} \left( \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} - f \leftrightarrow g \right) \quad (A5)$$

It differs by an overall sign from the definition generally given in classical mechanics textbooks. The adopted convention has the virtue that, with it, the mapping $f \mapsto X_f$ from smooth functions into the Hamiltonian vector fields is a Lie algebra homomorphism:

$$[X_f, X_g] = X_{\{f, g\}_cl}. \quad (A6)$$

ACKNOWLEDGEMENTS

The author would like to thank Michel Dubois-Violette for his constructive comments on the article in ref [10].

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