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Geometric Structure for Quantum Mechanics

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A geometric connection between quantum mechanics and classical mechanics is described and an operator version of the Poisson bracket is developed.

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Quantum mechanics owes much to the development and presence of the extensive existing theoretical framework which has been created for classical mechanics (Abraham and Marsden, 1978). This important influence is yet to be fully exposed. It has been of continuing interest to examine the correspondence between these two formalisms, and to develop and clarify the overlapping common elements. It can be imagined that by extending the structure of classical mechanics, many of the essential features of quantum mechanics can be accounted for. It will be shown here that this correspondence can be enlarged and deepened by slightly modifying and enlarging ideas which already exist in classical mechanics. The setting for classical mechanics is a classical phase space, and it is natural to define observables for a system as real-valued functions which are defined and are regular on that phase space. From the physical point of view, what is of interest is examining the sets of transformations of the states which do not change the basic underlying structure, or nature of the system. These obviously include, for example, time evolution or a change of inertial frame of reference. In quantum mechanics, one is analogously interested in the unitary transformations of the underlying Hilbert space. These are the basic automorphisms which are of interest in the new point of view.

The usefulness of working within the formalism of classical mechanics is that there is already a well developed underlying geometric formalism. If it could be applied more generally, it would be of use to quantum theory as well. Here we would like to illustrate that by enlarging the formalism and structure of classical mechanics, one can parallel corresponding elements of quantum mechanics. A more generalized form of classical mechanics can then accomodate many aspects

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of quantum mechanics. The main advantage of doing this is that a very unified view of both classical and quantum mechanics emerges.

In the classical theory, the dynamics and evolution of a system takes place in a phase space, and this leads to defining a particular observable as a real-valued regular function on that space. The space of states $\mathcal{S}$ of a quantum system is the projective space of a complex separable Hilbert space $\mathcal{H}$, that is, a state M in $\mathcal{S}$ can be identified with a nonzero vector $|M\rangle$ in $\mathcal{H}$, defined up to a complex factor. When the Hilbert space has finite complex dimension n, as a real space, it has then an even dimension of $2n$. The normalization condition reduces this dimension by one. Because of phase arbitrariness, the dimension is again reduced by one. Thus the complex projective space also has even dimension, a necessary condition for it to carry a Poisson bracket structure.

Begin by considering a given quantum system over some orthonormal basis, which we call $\{|\varphi_k\rangle\}$, of its Hilbert space of states. Given a state vector $|\psi\rangle$, it can be expanded in terms of the elements of this basis set

$$|\psi\rangle = \sum_k \alpha_k |\varphi_k\rangle, \tag{1}$$

and the coefficients α_k are of course complex valued. They will be written in terms of their real and imaginary parts normalized in the following way

$$\alpha_k = \frac{1}{\sqrt{2\hbar}}(x_k + i p_k). \tag{2}$$

As will be seen, the notation here is suggestive. In the case in which the Hilbert space has finite dimension, or by simply truncating the expression for the state $|\psi\rangle$, the set of components $(x_k, p_k)_{k=1}^N$ can be used to construct a local coordinate system on a manifold for the space of states. In fact, even in the infinite dimensional case, the set of components can be used for the same function, that is constructing an infinite dimensional manifold. We prefer to restrict ourselves to the finite dimensional case here. In this way, the set of (x_k, p_k) provides the space of states $\mathcal{S}$ with a smooth manifold structure in an intrinsic way.

At this point, additional structure can be defined on this manifold that one would find in a usual classical system. In terms of these coordinates (x_k, p_k), a symplectic form can be defined in terms of (x_k, p_k) as follows

$$\omega = \sum_i dx^i \wedge dp_i. \tag{3}$$

In terms of these coordinates, this form is a symplectic form on the space of states $\mathcal{S}$, thus the coordinates are canonical in the sense of the Darboux theorem (Abraham and Marsden, 1978). Moreover, any symplectic form is the negative imaginary part of some Hermitian inner product. This follows from a theorem which states that if $\mathcal{H}$ is a real Hilbert space and B a skew symmetric weakly nondegenerate bilinear form on $\mathcal{H}$, then there exists a complex structure J on $\mathcal{H}$ and a real inner product $\mathcal{S}$ such that $s(x, y) = -B(Jx, y)$. Setting $h(x, y) = s(x, y) - iB(x, y)$, h is a hermitian inner product (Abraham and Marsden, 1978). Thus any symplectic form is the negative imaginary part of some Hermitian inner product. We can then identify

$$\omega(V, W) = -Im\langle V, W\rangle. \tag{4}$$

This is of course invariant under the multiplication of $|V\rangle$ and $|W\rangle$ by a common phase factor. Hence ω is for every $U \in \mathcal{S}$ a well-defined intrinsic map $T_U\mathcal{S} \times T_U\mathcal{S} \to \mathbb{R}$, and the condition $d\omega = 0$ is exactly what is required to make Poisson brackets into a Lie algebra (Marsden and Ratiu, 1994; von Westenholz, 1981). The Hilbert space structure of $\mathcal{H}$ induces on the projective space $\mathcal{S}$ the structure of a symplectic manifold with $\mathcal{S}$ connected. The observables are those real-valued smooth functions on $\mathcal{S}$ whose canonical transformations they generate are automorphisms of $\mathcal{S}$, when considered as the projective space of $\mathcal{H}$.

In this way a direct correspondence between a quantum description and a classical description has been produced (Heslot, 1983, 1985). The space of states $\mathcal{S}$, of a physical system in classical mechanics is the system's phase space. This space is an even-dimensional smooth manifold provided with a nondegenerate and closed two form, or in other words, a symplectic structure. This symplectic structure has a physical meaning. Transformations which do not modify the nature of the system are precisely the automorphisms, or ω preserving diffeomorphisms, which are usually referred to as canonical.

The Poisson bracket for f and g in the vector space of real valued smooth functions on the space of states $\mathcal{S}$ can be defined by $\{f, g\} = \omega^{-1}(df, dg)$. Also this space is a Lie algebra under the Poisson bracket such that $[X_f, X_g] = -X_{\{f,g\}}$. In the classical sense, the elements of this space are considered to be the observables of the system. Thus we have

$$\frac{d}{dt}(f \circ \gamma_t) = \{f \circ \gamma_t, H\} = \{f, H\} \circ \gamma_t,$$

where γ_t is the flow of X_H and $f \in \mathcal{F}(P)$. This equation is often written more compactly as $\dot{f} = \{f, H\}$ and is called the equation of motion in Poisson bracket form. Transformations which do not change the structure of the system preserve the Poisson bracket and are referred to as automorphisms of that basic structure (Bracken, 1996). Thus, given a transformation P on the space of states, this induces a transformation on the observables. The transformation P is an automorphism on the state space with its associated Poisson bracket structure, if and only if, for the observables f and h, $\mathcal{P}(\{f, h\}) = \{\mathcal{P}f, \mathcal{P}h\}$, and $\mathcal{P}$ is called a canonical transformation. In this framework, observables are defined as real-valued regular functions of the state whose canonical transformations they generate and are automorphisms of the whole structure of the space of states. The automorphisms of quantum mechanics are unitary transformations.

For any state $|\psi\rangle$, in terms of the basis $|\varphi_k\rangle$, we can expand $|\psi\rangle$ as in (1). Let us show that the real and imaginary parts of the coefficients α_k in (1) satisfy Hamilton's equations. The motion of the quantum system is determined by Schrödinger's equation (Messiah, 1958)

$$i\hbar \frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle. \tag{5}$$

Schrödinger's equation will become a set of equations for the α_k, and from this, Schrödinger's equation may be written as a set of equations for the real and imaginary parts of the a_k, namely, the x_k and p_k. Suppose $\langle\psi|\psi\rangle = 1$ then we immediately have the following constraint on the x_k and p_k as follows

$$\sum_k x_k^2 + p_k^2 = 2\hbar.$$

Now define the function $H(x_k, p_k) = 2\langle\psi|\hat{H}|\psi\rangle$. The Schrödinger equation takes the form

$$i\hbar \frac{d}{dt} \sum_k \frac{1}{\sqrt{2\hbar}}(x_k + ip_k)|\varphi_k\rangle = \hat{H}|\psi\rangle. \tag{6}$$

Contracting on the left with the vector $\langle\psi|$, we obtain

$$\hbar \sum_m \langle\varphi_m|\alpha_m^* \frac{d}{dt} \sum_k \frac{1}{\sqrt{2\hbar}}(x_k + ip_k)|\varphi_k\rangle = \langle\psi|\hat{H}|\psi\rangle.$$

This reduces to a quantity which depends on the x_k and p_k,

$$i \sum_k (x_k - ip_k)\left(\frac{dx_k}{dt} + i\frac{dp_k}{dt}\right) = H(x_k, p_k).$$

Expanding this out, we obtain

$$\sum_k \left(ix_k\frac{dx_k}{dt} - x_k\frac{dp_k}{dt} + p_k\frac{dx_k}{dt} + ip_k\frac{dp_k}{dt}\right) = H(x_k, p_k). \tag{7}$$

Taking the complex conjugate of (7) and using the fact that the right-hand side is real, then upon adding this to (7), we obtain

$$H = \sum_k \left(-x_k\frac{dp_k}{dt} + p_k\frac{dx_k}{dt}\right). \tag{8}$$

Differentiating both sides of (8) with respect to x_k and then p_k, respectively, the following pair of equations in terms of x_k and p_k are found

$$\frac{\partial H}{\partial x_k} = -\frac{dp_k}{dt}, \qquad \frac{\partial H}{\partial p_k} = \frac{dx_k}{dt}. \tag{9}$$

This analysis has produced a set of equations which has the same form as the classical Hamilton's equations of motion, if the x_k play the role of spacial variables and the p_k play the role of the momentum variables.

Expressions for the derivatives of the expectation values of the operator of an observable with respect to the state $|\psi\rangle$ can also be derived. Since the function obtained from the expectation value will depend on x_k and p_k, so too will the derivatives. Consider an operator $\hat{R}$ which is the operator of some observable, such as the Hamiltonian operator $\hat{H}$, for example, introduced in the Schrödinger equation (5). Then, defining the quantities $\tau_{kl} = \langle\varphi_k|\hat{R}|\varphi_l\rangle$ and $R(x_k, p_k) = \langle\psi|\hat{R}|\psi\rangle$, we have

$$\langle\psi|\hat{R}|\psi\rangle = \sum_{k,l} \tau_{kl}\alpha_k^*\alpha_l = \sum_{k,l} \tau_{kl} \left(\frac{x_k x_l - i x_l p_k + i x_k p_l + p_k p_l}{2\hbar} \right)$$
$$= \sum_{k,l} \left(\frac{x_k x_l + p_k p_l + i(-x_l p_k + x_k p_l)}{2\hbar} \right) \tau_{kl}. \tag{10}$$

Differentiate now the expression in (10) with respect to the variable p$_k$,

$$\frac{\partial}{\partial p_k}\langle\psi|\hat{R}|\psi\rangle = \frac{1}{2\hbar}\sum_{m,l}(\delta_{mk} p_l + p_m \delta_{lk} + i(x_m\delta_{kl} - x_l\delta_{mk}))\tau_{ml}$$
$$= \frac{1}{2\hbar}\sum_{l}(p_l\tau_{kl} + p_l\tau_{lk} + i(x_l\tau_{lk} - x_l\tau_{kl}))$$
$$= \sum_l \left(\frac{\tau_{kl} + \tau_{lk}}{2\hbar} p_l + i\frac{\tau_{lk} - \tau_{kl}}{2\hbar} x_l \right). \tag{11}$$

Differentiating (9) with respect to x_k, we obtain

$$\frac{\partial}{\partial x_k}\langle\psi|\hat{R}|\psi\rangle = \frac{1}{2\hbar}\sum_{m,l}(\delta_{mk} x_l + x_m \delta_{lk} - i p_m\delta_{lk} + i p_l\delta_{mk})\tau_{ml}$$
$$= \frac{1}{2\hbar}\sum_{l}(x_l\tau_{kl} + x_l\tau_{lk} + i(p_l\tau_{kl} - p_l\tau_{lk}))$$
$$= \sum_l \left(\frac{\tau_{kl} + \tau_{lk}}{2\hbar} x_l + i\frac{\tau_{kl} - \tau_{lk}}{2\hbar} p_l \right). \tag{12}$$

The fact that an operator $\hat{R}$ is a self-adjoint operator implies that, in terms of the matrix elements, $\tau_{kl}^* = \tau_{lk}$. This fact can be used to write any τ_{kl} as the sum of its real part and its imaginary part,

$$\tau_{kl} = \frac{\tau_{kl} + \tau_{lk}}{2} + i\frac{\tau_{kl} - \tau_{lk}}{2}. \tag{13}$$

The derivatives in (11) and (12) can then be written in the form

$$\frac{\partial R}{\partial x_k} = \left(\frac{2}{\hbar}\right)^{1/2} Re\left(\sum_l \tau_{kl}\alpha_l\right), \qquad \frac{\partial R}{\partial p_k} = \left(\frac{2}{\hbar}\right)^{1/2} Im\left(\sum_l \tau_{kl}\alpha_l\right). \quad (14)$$

It has been shown that an observable in the classical sense can be produced from an operator, which can be written explicitly as $R(x_k, p_k) = \langle\psi|\hat{R}|\psi\rangle$. There is a natural correspondence between operators and observables which is linear as is addition and product by a scalar of observables. This correspondence can also be extended to the Poisson bracket. The Poisson bracket can also be represented formally in terms of operators using (14). The Poisson bracket of the real functions f, g is given by

$$\{f, g\} = \sum_k \left(\frac{\partial f}{\partial x_k}\frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k}\frac{\partial g}{\partial x_k}\right).$$

Substituting the derivatives in (14) and the identity $z^* w - z w^* = 2i(Re\, z\, Im\, w - Re\, w\, Im\, z)$, which holds for any complex z, w, the Poisson bracket of the two observables f, g can be written in the following way

$$\begin{aligned}
\{f, g\} &= \frac{2}{\hbar}\sum_k \left(Re\sum_l f_{kl}\alpha_l\, Im\sum_j g_{kj}\alpha_j - Re\sum_j g_{kj}\alpha_j\, Im\sum_l f_{kl}\alpha_l\right)\\
&= \frac{1}{i\hbar}\sum_k \left(\left(\sum_l f_{kl}\alpha_l\right)^*\left(\sum_j g_{kj}\alpha_j\right) - \left(\sum_l f_{kl}\alpha_l\right)\left(\sum_j g_{kj}\alpha_j\right)^*\right)\\
&= \frac{1}{i\hbar}\sum_{k,l,j}(f_{lk}g_{kj}\alpha_l^*\alpha_j - f_{kl}g_{jk}\alpha_l\alpha_j^*)\\
&= \frac{1}{i\hbar}\sum_{l,j}((\hat{f}\hat{g})_{lj}\alpha_l^*\alpha_j - (\hat{g}\hat{f})_{jl}\alpha_l\alpha_j^*)\\
&= \frac{1}{i\hbar}\sum_{l,j}[\hat{f}, \hat{g}]_{lj}\alpha_l^*\alpha_j = \frac{1}{i\hbar}\langle\psi|[\hat{f}, \hat{g}]|\psi\rangle,
\end{aligned}$$

where $[\hat{f}, \hat{g}] = \hat{f}\hat{g} - \hat{g}\hat{f}$ is the commutator. An operator version of the Poisson bracket has been produced which can be summarized in the form

$$\{f, g\} = \frac{1}{i\hbar}[\hat{f}, \hat{g}]. \quad (15)$$

Thus, we have seen that as the imaginary part of the scalar product is antisymmetric, it may be considered as an antisymmetric covariant tensor which if written in general coordinates takes the form $\omega = \sum_{\sigma,\tau}\omega_{\sigma\tau}dx^\sigma \bigotimes dx^\tau$, where the x^σ are generic coordinates on the complex projective space. There is an association with a Poisson bracket structure through

$$\{f, g\} = \sum_{\sigma,\tau} \omega^{\sigma\tau} \frac{\partial f}{\partial x^\sigma} \frac{\partial g}{\partial x^\tau},$$

where $\omega^{\sigma\tau}$ is the inverse of $\omega_{\sigma\tau}$. The real part of the scalar product induces a metric in the usual sense, that is, a symmetric covariant tensor $g = \sum_{\sigma\tau} g_{\sigma\tau} dx^\sigma \bigotimes dx^\tau$. Thus there exists a way of placing an intrinsic curvature on the space of states in this formalism.

Suppose we subject the α_k to a unitary transformation $\hat{U}$ such that $U_{kl} = \langle \varphi_k \mid \hat{U} \mid \varphi_l \rangle$, then if $U_{kl} = Q_{kl} + iP_{kl}$ the transformed coordinates satisfy the bracket

$$\{x'_k, p'_k\} = \left\{ \sum_j Q_{kj} x_j - P_{kj} p_j, \sum_m Q_{kj} p_j - P_{kj} x_j, \right\} = \sum_j (Q_{kj} Q_{lj} + P_{kj} P_{lj})$$

However, $\langle \varphi_k \mid \hat{U}\hat{U}^\dagger \mid \varphi_l \rangle = \delta_{kl} = \sum_j U_{kj} U^*_{lj} = \sum_j (Q_{kj} + iP_{kj})(Q_{lj} - iP_{lj}) = \sum_j (Q_{kj} Q_{lj} + P_{kj} P_{lj}) + i(P_{kj} Q_{lj} - Q_{kj} P_{lj}) = \sum_j (Q_{kj} Q_{lj} + P_{kj} P_{lj})$. Thus, $\hat{U}$ preserves Poisson brackets and is canonical. To conclude, it has been shown that the (x_k, p_k) constitute a system of canonical coordinates and that Schrôdinger's equation is a special case of Hamilton's equations.

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