Geometry of Quantum Mechanics*

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The traditional formalism of quantum theory is linear and algebraic, and classical mechanics is non-linear and geometric in nature. Remarkably, this non-linearity arises from the purely linear interactions on the quantum level. In this report, we will see on a mathematical level, classical and quantum theories are not so dramatic as they appear initially. We will start with a critical observation that the true space of quantum states is not linear but a projective Hilbert space. Ordinary quantum theory is intrinsic to this projective space, and the Hermitian inner product of traditional quantum mechanics induces a natural symplectic structure on this projective space and transforms it into phase space.

I. INTRODUCTION

There are two main pillars of modern-day physics: classical mechanics, which includes Einstein's theory of gravity, and quantum mechanics, which discusses the other three forces of nature.

Classical mechanics is defined over a phase space - a genuine manifold. The points of this space label classical states. A geometric structure, called a *symplectic form*, is imprinted on this manifold. Observable quantities are described by functions on the phase space. Each observable preserves the symplectic structure by following a specific mechanism.

On the other hand, quantum mechanics has often been dubbed the most successful but incomplete theory ever invented. It is defined in a linear and complex vector space, Hilbert space, equipped with Hermitian inner products. States of the physical system are described by points on Hilbert space, and certain *linear* operators are used to represent observable quantities on this vector space. The inner product is preserved in Hilbert space.

In quantum mechanics, the evolution of time is determined by a linear equation, and the Hamiltonian operator describes the passage of time. While the classical time-evolution is "far from linear". The symplectic structure of the classical theory seems analogous to the inner-products in Hilbert space, but their roles are entirely different in many respects. The classical symplectic structure links observables and dynamics of the underlying system, while the Hermitian inner-product is a piece of machinery to compute transition amplitudes that have no classical analogs.

Conclusively, quantum mechanics is intrinsically linear and algebraic, while the formalism of classical theory is intrinsically non-linear and geometric. Moreover, classical theory is an approximation of quantum mechanics, which is a more fundamental theory of nature. Here comes the mysterious thing. How could an intrinsically geometric and non-linear theory be an approximation of an essentially algebraic and linear theory? One can expect the reverse situation where linear equations are approximate forms of non-linear ones but not the other way round. How is the geometric description of nature encoded in Hilbert space? In this project, we will try to answer this question to some extent.

Ordinary quantum theory is understood to be linear, but it is not quite so linear upon deeper reflection. An element of Hilbert space determine the state of the system, but the converse is not true. The physical state of any system does not correspond to a unique element in Hilbert space. One may get the same physical state by choosing a vector from Hilbert space and multiplying it by a complex number. It is a sort of "gauge ambiguity" or "arbitrariness" inherent to the standard formalism of quantum mechanics. Thus, a physical state of a system, then, corresponds to a *ray* in the Hilbert space and the collection of these rays makes a true space of quantum states, called the *projective* Hilbert space. This true space serves the purpose of a manifold. However, at this point, it is fairly natural to look for a quantum formulation that is intrinsic to this projective space. If it exists, then such a "gauge-invariant" formulation would rely on the geometrical description. For instance, the Hilbert space of a spin$-\dfrac{n}{2}$ system is isomorphic to $\mathbb{C}^{n+1}$ and the corresponding projective space is $\mathbb{CP}^n$ – the Kähler manifold. It is important to note that Kähler manifolds are symplectic so that one can construct physical observables immediately. Classical mechanics, studied by Hamilton's equation, gives a flow associated with energy function (given by Hamiltonian vector field) and quantum evolution is studied via Schrodinger equation and provides a flow on the projective space. In the realm of current approaches, *coherent states* provide the strongest hint of geometric structure, from quantum to classical limit [1].

The aim of this report is to formulate the postulates of quantum theory in a way which is intrinsic to the true space of the states. This formulation can be further ex-

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tended to study non-linear modifications of quantum theory.

II. CLASSICAL MECHANICS

There is a famous metaphor attributed to Sir Issac Newton: "If I have seen further it is by standing on the shoulders of Giants." If I have to restate this metaphor, I would like to say: "If I have seen further it is by standing on the shoulders of *classical physicists*." Classical mechanics is described in the language of Lagrangian and Hamiltonian. In this report, we will briefly review the Hamiltonian formalism.

Hamilton's mechanics is essentially done in phase space, Γ, which is equipped with a closed and non-degenerate two-from, Ω_{ab}. This differential form is regarded as *symplectic form* and (Γ, Ω) is the symplectic manifold. Since, Ω is a two-from, Γ is essentially even-dimensional. On any given point, p, on the manifold, Γ, the one-to-one and onto maps for tangent and cotangent spaces are defined as:

$$v^a \mapsto (i_v\Omega)_a = v^b\Omega_{ba}, \tag{1}$$

$$v_a \mapsto (i_v\Omega)^a = \Omega^{ba}v_b, \tag{2}$$

respectively. Here, Ω^{ba} is the skew-symmetric tensor field. It satisfies,

$$\Omega_{ac}\Omega^{bc} = \delta_a{}^b. \tag{3}$$

Moreover, will assumed this diffeomorphic mapping preserves the structure and is called *canonical transformation.* Assume a vector field X that generates a motion in phase space and preserves the symplectic structure, that is,

$$\mathcal{L}_X\Omega = 0, \tag{4}$$

$$(i_X\,\mathrm{d} + \mathrm{d}i_X)\,\Omega = 0, \tag{5}$$

$$\mathrm{d}i_X\,\Omega = 0. \tag{6}$$

Eq. (6) implies that one-form corresponding to vector field, X, is closed. Such vector fields are called "locally Hamiltonian" vector fields (or *infinitesimal canonical transformation* more familiarly.) Also, if $i_X\Omega$ is exact (for a simply-connected Γ), there exists a function $f : \Gamma \longrightarrow \mathbb{R}$, for which

$$i_X\Omega = \mathrm{d}f\,. \tag{7}$$

It implies,

$$X^a = \Omega^{ab}\partial_b f. \tag{8}$$

Eq. (8) is used to construct a vector field, X, from any smooth function f, if and only if $f : \Gamma \longrightarrow \mathbb{R}$. This corresponding vector field is regarded as Hamiltonian vector field, X_f. Intuitively, Ω gives the area of the parallelogram, spanned by two tangent vectors and points on Γ describe the states of the system. It is also important to note, in conventional metric manifolds, the space of Killing vector fields (infinitesimal symmetries) is finite-dimensional while in the case of infinite canonical transformations, the space is itself infinite-dimensional.

A. The Algebra of Classical Observables

Assume a space $\mathcal{O}_{\mathrm{cl}}$ of classical observables. It consists of all smooth functions on Γ. If a physical state is labeled as $p \in \Gamma$, then an ideal measurement of $f : \Gamma \longrightarrow \mathbb{R}$ will simply give the value of f at p, that is, $f(p)$ and Hamiltonian evolution will remain uninfluenced. Poisson bracket for two arbitrary functions, f and g, is defined as:

$$\{f, g\} \coloneqq (\partial_a f)\,\Omega^{ab}\,(\partial_b g) = X_g(f), \tag{9}$$

$$\{f, g\} = \Omega\,(X_f, X_g)\,. \tag{10}$$

Eq. (9) shows that Poisson bracket is actually a Lie bracket on $\mathcal{O}_{\mathrm{cl}}$. If $f, g, h \in \mathcal{O}_{\mathrm{cl}}$, then:

$$\{f, gh\} = g\,\{f, h\} + \{f, g\}\,h. \tag{11}$$

It is also important to show that $f \mapsto X_f$ is an anti-homomorphic mapping from Poisson algebra of observables to the Lie algebra of smooth vector fields in phase space Γ. That is,

$$\mathrm{d}\,\{f, g\} = \mathrm{d}\,[\Omega\,(X_f, X_g)] = \mathrm{d}i_{X_g}i_{X_f}\,\Omega, \tag{12}$$

$$= \left(\mathcal{L}_{X_g} - i_{X_g}\,\mathrm{d}\right) i_{X_f}\Omega, \tag{13}$$

$$= \mathcal{L}_{X_g}i_{X_f}\Omega - i_{X_g}\mathcal{L}i_{X_f}\Omega, \tag{14}$$

$$\mathrm{d}\,\{f, g\} = i_{[X_g, X_f]}\Omega. \tag{15}$$

Here, the Poisson bracket is defined as:

$$\{f, g\} = \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i}. \tag{16}$$

If h is the standard classical Hamiltonian, the rate of change of observable f is described as:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = X_h(f) = \{f, h\}\,. \tag{17}$$

By combining Eqs. (16) and (17), we get:

$$\dot{q^i} = \frac{\partial H}{\partial p_i}, \tag{18}$$

$$\dot{p_i} = -\frac{\partial H}{\partial q^i}. \tag{19}$$

III. QUANTUM MECHANICS

Quantum mechanics is written in the language of Hilbert space, $\mathcal{H}$ and observables are represented by self-adjoint linear operators. Time-dependent equation of motion is the following Schrodinger equation:

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi, \tag{20}$$

where $\hat{H}$ is the Hamiltonian operator. Though the operators are self-adjoint, they do not define a structure on the Hilbert space because, in general, the commutator of two self-adjoint operators is not self-adjoint. It is one of the reasons it is useful to work with bounded (or Hermitian) operators. Interestingly, this cannot be the best choice always, since the two most important and fundamental operators, position ($\hat{Q}$) and momentum ($\hat{P}$) are not Hermitian (or unbounded). By eliminating unbounded operators from Hilbert space, it will not be possible to perfectly approximate quantum observables to their classical counterparts.

The space of quantum observables, $\mathcal{O}_{\mathrm{qu}}$, consists of self-adjoint, bounded, and linear operators defined over $\mathcal{H}$. With this definition, one can show that Hamiltonian does not remain the observable of the theory for most natural systems. It is because the time-evolution operator is unbounded. Importantly, this feature is not intrinsic to quantum theory, but it comes from the infinite dimensionality of the Hilbert space.

A. The Postulates of Quantum Theory

At this point, it is important to state the postulates of quantum mechanics explicitly and more rigorously. However, in doing so, many technical issues arise due to the infinite-dimensional Hilbert space. A rigorous and detailed mathematical treatment can be found in [2, 3].

We can straightforwardly specify the domains of bounded operators since they are defined over entire state space, but they may not have eigenvalues. It can be justified via a simple example of performing an measurement in a laboratory. For any $x_0\in\mathbb{R}$, where x_0 is corresponding to a location in laboratory in Euclidean space, we can write:

$$\left(\hat{Q}_{\mathrm{lab}}\delta\right)(x-x_0)=x_0\delta\left(x-x_0\right), \tag{21}$$

where $\delta\left(x-x_0\right)$ is the Dirac delta function and is not an element of the Hilbert space and hence x_0 is *almost* an eigenvalue.

In infinite-dimension, the *spectrum* of an operator is defined as a set of complex numbers, , from which $\left(\hat{A}-\lambda\hat{\mathbb{I}}\right)$ is not invertible. However, any eigenvalue of $\hat{A}$ would necessarily be an element of the spectrum of $\hat{A}$. If the state space is finite-dimensional, the operator can be decomposed as:

$$\hat{A}=\sum_i\lambda_i\mathbb{P}_{\hat{A},\lambda_i}, \tag{22}$$

where α_i are the eigenvalues of $\hat{A}$ and $\mathbb{P}_{\hat{A},\lambda_i}$ is the projection of $\hat{A}$ onto the eigenspace corresponding to α_i. When a measurement is made, this projection operator vanishes the part of the wavefunction which lies outside of the spectrum.

We are now in a position to state the postulates of quantum theory. One can find these in different notations and in slightly different language in any standard textbook on quantum mechanics, for instance, [4, 5]. Following postulates are copied from [6].

- **Hilbert Space** ($\mathcal{H}$)**:** "Physical states of the quantum system are in one-to-one correspondence with rays in a Hilbert space, $\mathcal{H}$."

- **Unitary Evolution** ($\mathcal{U}$)**:** "The system, when not subject to external influence, evolves according to the Schrodinger equation, Eq. (20), where $\hat{H}$, is a preferred self-adjoint operator on $\mathcal{H}$."

- **Observables** ($\mathcal{O}$)**:** "Every measurable physical quantity is represented by a bounded self-adjoint operator on $\mathcal{H}$."

- **Probabilistic Interpretation** ($\mathcal{P}$)**:** "Let $\Lambda\subset\mathbb{R}$ be a measurable subset of the spectrum of $\hat{F}$, and suppose the system is in the state determined by the vector $\Psi\in\mathcal{H}$. The probability that measurement of $\hat{F}$ will yield an element of Λ is given by:

$$P_\Psi(\Lambda)=\frac{\left\langle\Psi,\mathbb{P}_{\hat{F},\Lambda}(\Psi)\right\rangle}{\langle\Psi,\Psi\rangle}." \tag{23}$$

Apart from these standard postulates, it is reasonable to state the *reduction* postulates for discrete and continuous spectra (also taken from [6]) in a more concise way, as follows:

- **Reduction, discrete spectrum** ($\mathcal{R}_D$)**:** "Suppose the spectrum of an observable $\hat{F}\in\mathcal{O}_{\mathrm{qu}}$ is discrete. This spectrum provides the set of possible outcomes of the ideal measurement of $\hat{F}$. If measurement of $\hat{F}$ yields the eigenvalue λ, the state of the system immediately after the measurement is given by the associated projection, $\mathbb{P}_{\hat{F},\Lambda}(\Psi)$, of the initial state Ψ."

- **Reduction, continuous spectrum** ($\mathcal{R}_C$)**:** "A measurable subset Λ of the spectrum of $\hat{F}$ determines an ideal measurement that may be performed on the system. This measurement corresponds to inquiring whether the values of $\hat{F}$ lies in Λ. Immediately after this measurement, the state of the system is given by $\mathbb{P}_{\hat{F},\Lambda}(\Psi)$ or $\mathbb{P}_{\hat{F},\Lambda^c}(\Psi)$, depending on whether the result of the measurement is positive or negative, respectively."

B. The Algebra of Quantum Observables

We can define the commutator of two linear operators as:

$$\left[\hat{F},\hat{G}\right] \coloneqq \mathrm{i}\hbar\left\{\hat{F},\hat{G}\right\}_{\mathrm{qu}}. \tag{24}$$

On the space of observables, a Jordan product, is defined as:

$$\left\{\hat{F},\hat{G}\right\}_{+} \coloneqq \frac{1}{2}\left[\hat{F},\hat{G}\right]_{+}, \tag{25}$$

where $\left[\hat{F},\hat{G}\right]_{+} = \hat{F}\hat{G}+\hat{G}\hat{F}$ is the anti-commutator. Similarly, the quantum Lie bracket can also be defined as follows:

$$\left\{\hat{F},\left\{\hat{G},\hat{H}\right\}_{+}\right\}_{\mathrm{qu}} = \left\{\hat{G},\left\{\hat{F},\hat{H}\right\}_{\mathrm{qu}}\right\}_{+} + \left\{\left\{\hat{F},\hat{G}\right\}_{\mathrm{qu}},\hat{H}\right\}_{+}. \tag{26}$$

IV. THE INNER PRODUCT AS A KÄHLER STRUCTURE

In standard quantum theory, Hilbert space is a complex vector space. We can also view this Hilbert space as a real vector space on which a complex structure, J, is embedded. Here, J is a linear operator and $J^2 = -1$. Since $\mathcal{H}$ is now real space, we can decompose inner product into real and imaginary parts as follows:

$$\langle \Phi,\Psi\rangle \coloneqq \frac{1}{2\hbar}G\left(\Phi,\Psi\right) + \frac{\mathrm{i}}{2\hbar}\Omega\left(\Phi,\Psi\right). \tag{27}$$

Since,

$$\langle \Phi,\Psi\rangle = \overline{\langle \Psi,\Phi\rangle}, \tag{28}$$

we can write

$$G\left(\Phi,\Psi\right) = G\left(\Psi,\Phi\right), \tag{29}$$

$$\Omega\left(\Phi,\Psi\right) = -\Omega\left(\Psi,\Phi\right). \tag{30}$$

We can also see that G describes a positive-definite inner product because the inner product is itself positive-definite. That is,

$$G\left(\Psi,\Psi\right) \geq 0, \tag{31}$$

where

$$G\left(\Psi,\Psi\right) = 0, \tag{32}$$

if and only if

$$\Psi = 0. \tag{33}$$

From the basics of complex algebra, we know that Hermitian inner-product respects multiplication by complex factor i, such that,

$$\langle J\Phi,J\Psi\rangle = \langle \Phi,\Psi\rangle. \tag{34}$$

Using Eq. (34), we can write similar relation for G and Ω as follows:

$$G\left(J\Phi,J\Psi\right) = G\left(\Phi,\Psi\right), \tag{35}$$

$$\Omega\left(J\Phi,J\Psi\right) = \Omega\left(\Phi,\Psi\right). \tag{36}$$

Eqs. (35) and (36) show that J is preserved by G and Ω. Using

$$\langle \Phi,J\Psi\rangle = \mathrm{i}\langle \Phi,\Psi\rangle, \tag{37}$$

we can also write a relation between G,Ω and J as follows:

$$\Omega\left(\Phi,\Psi\right) = -G\left(\Phi,J\Psi\right) = G\left(J\Phi,\Psi\right), \tag{38}$$

or,

$$G\left(\Phi,\Psi\right) = \Omega\left(\Phi,J\Psi\right) = -\Omega\left(J\Phi,\Psi\right), \tag{39}$$

Eq. (38) is called Kähler form and these relations define *Kähler structure.*

A. Schrodinger's Equation in Hamilton's Principle

Employing Kähler structure, the time-dependent Schrodinger wave equation can be written as:

$$\frac{\mathrm{d}\Psi}{\mathrm{d}t} = -\frac{1}{\hbar}J\hat{H}\Psi. \tag{40}$$

Eq. (40) motivates us to associate a vector field to each observable $\hat{F}\in\mathcal{O}_{\mathrm{qu}}$, that is,

$$Y_{\hat{F}}(\Psi) \coloneqq -\frac{1}{\hbar}J\hat{F}\Psi, \tag{41}$$

where $Y_{\hat{F}}$ is the Schrodinger vector field determined by $\hat{F}$. This vector field preserves the Hermitian inner-product, and thus, the metric, G, and symplectic structure, Ω are also preserved. In Eq. (41), $Y_{\hat{F}}$ is a *locally* Hamiltonian vector field. We can explicitly show this beautiful result. Assume, we are given an observable $\hat{F}$, whose expectation value is denoted by $F : \mathcal{H} \longrightarrow \mathbb{R}$. Now, the expectation value function can be written as:

$$F(\Psi) := \left\langle \hat{F} \right\rangle (\Psi) = \left\langle \Psi, \hat{F}\Psi \right\rangle = \frac{1}{2\hbar} G\left(\Psi, \hat{F}\Psi\right). \tag{42}$$

If η is a tangent vector at Ψ, then:

$$(\mathrm{d}F)(\eta) = \frac{\mathrm{d}}{\mathrm{d}t} \left\langle \Psi + t\eta, \hat{F}(\Psi + t\eta) \right\rangle \Big|_{t=0}, \tag{43}$$

$$(\mathrm{d}F)(\eta) = \left\langle \Psi, \hat{F}\eta \right\rangle + \left\langle \eta, \hat{F}\Psi \right\rangle. \tag{44}$$

Using the symmetry of $\hat{F}$, and Eqs. (38) and (41), we get

$$(\mathrm{d}F)(\eta) = 2\mathrm{Re} \left\langle \eta, \hat{F}\Psi \right\rangle, \tag{45}$$

$$= \frac{1}{\hbar} G\left(\hat{F}\Psi, \eta\right), \tag{46}$$

$$= G\left(JY_{\hat{F}}(\Psi), \eta\right), \tag{47}$$

$$(\mathrm{d}F)(\eta) = \Omega\left(Y_{\hat{F}}, \eta\right). \tag{48}$$

Therefore, we have

$$\mathrm{d}F = i_{Y_{\hat{F}}}\Omega. \tag{49}$$

We can then state [6]: "The Schrodinger vector field $Y_{\hat{F}}$ determined by the observable $\hat{F} \in \mathcal{O}_{\mathrm{qu}}$ is exactly the Hamiltonian vector field X_F generated by the expectation value of ."

V. THE COMMUTATOR IS A POISSON BRACKET

Article IV A suggests to formulate quantum theory in phase space, where observables are represented by real-valued functions and not by operators. One possible candidate for such a formulation is expectation value function. But it raise an essentially important question that whether the function $\left\langle \frac{1}{\mathrm{i}\hbar}\left[\hat{F}, \hat{K}\right] \right\rangle$ can be naturally expressed in terms of $\hat{F}$ and $\hat{K}$ or not? Answer is *yes* and calculation is remarkably simple. By employing the Hermiticity of operators and using the Eqs. (27), (35), (36) and (41), we can write,

$$\left\langle \frac{1}{\mathrm{i}\hbar}\left[\hat{F}, \hat{K}\right] \right\rangle (\Psi) = \frac{1}{\mathrm{i}\hbar} \left\langle \Psi, \left(\hat{F}\hat{K} - \hat{K}\hat{F}\right)\Psi \right\rangle, \tag{50}$$

$$= \frac{1}{\mathrm{i}\hbar}\left(\left\langle \hat{F}\Psi, \hat{K}\Psi \right\rangle - \left\langle \hat{K}\Psi, \hat{F}\Psi \right\rangle\right), \tag{51}$$

$$= \frac{2}{\hbar}\mathrm{Im}\left\langle \hat{F}\Psi, \hat{K}\Psi \right\rangle, \tag{52}$$

$$= \frac{1}{\hbar}\Omega\left(\hat{F}\Psi, \hat{K}\Psi\right), \tag{53}$$

$$= \Omega\left(Y_{\hat{F}}, Y_{\hat{K}}\right), \tag{54}$$

$$\left\langle \frac{1}{\mathrm{i}\hbar}\left[\hat{F}, \hat{K}\right] \right\rangle (\Psi) = \Omega\left(X_F, X_K\right). \tag{55}$$

Eq. 55 shows that algebraic expression on the expectation value function is *exactly* a Poisson bracket. However, this Poisson bracket is neither the classical Poisson bracket nor this relation is Dirac's correspondence. But it is important to notice that inherent Lie structure to the algebra of quantum observables may be *precisely* written in the language of a classical physicist.

We can then state the following lemma [6]: "Let F and K be the expectation value functions of the observables $\hat{F}$ and $\hat{K}$, respectively. Denote by H the expectation value of the Lie bracket of $\hat{F}$ and $\hat{K}$, as defined by Eq. (24). Then H is the Poisson bracket of F and K, with respect to the quantum symplectic structure; $H = \Omega\left(X_F, X_K\right)$." That is,

$$\{F, K\}_{\mathrm{qu}} = \Omega\left(X_F, X_K\right). \tag{56}$$

VI. CONCLUSION

In this report, we have seen that standard quantum theory can be written in a geometric language intrinsic to the projective Hilbert space. The Hermitian operator is constructed on Hilbert space and defines a symplectic structure. The conventional complex-valued vector space (the Hilbert space) is a real-value Kähler space. We also found that, for a bounded and self-adjoint operator, expectation value as a function on $\mathcal{H}$ contains all information about the operator under consideration. This feature can nicely lead us to a complete geometric formulation of quantum theory in terms of projective Hilbert space. Moreover, the time-dependent Schrodinger equation assumes the form of Hamilton's canonical equation of motion. We also found that the Poisson bracket of the two expectation value functions is precisely equal to the ($-\mathrm{i}/\hbar$ times) commutator of the corresponding operators. It provides us a way to view quantum mechanics as an infinite-dimensional Hamiltonian system.

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